Chemistry Congress . 26-28 july 2022 . Tabriz

Azarbaijan
Shahid Madani University

21st ICS International Chemistry Congress

July 26-28, 2022

Azarbaijan Shahid Madani University

By:

Azarbaijan Shahid Madani University, Tabriz, Iran

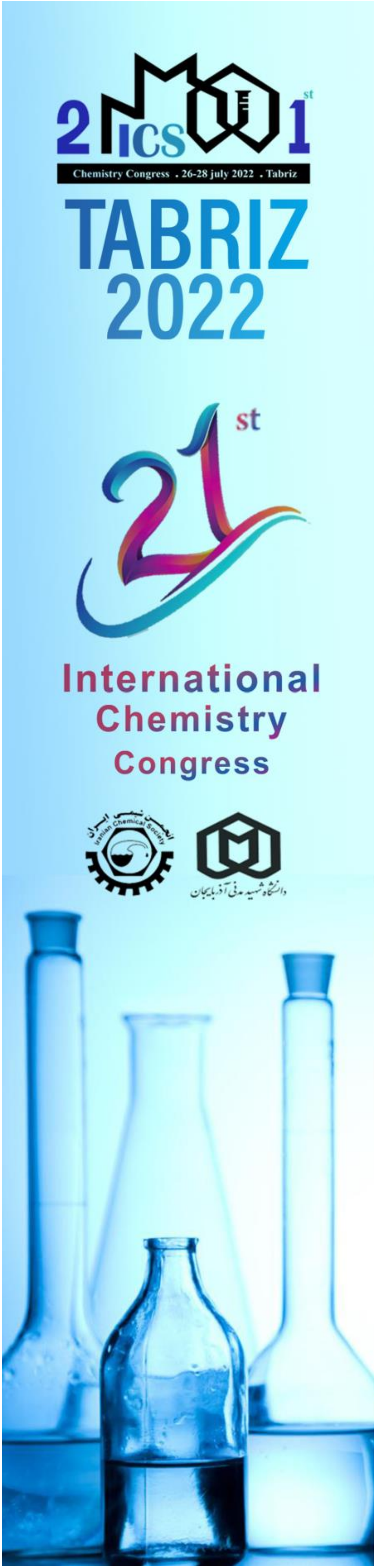
In collaboration with:

Iranian Chemical Society

In The Name of Allah, The Most

Gracious, The Most Merciful

Table of Content



Editorial Note:

Dear Friends and Colleagues,

It is a great pleasure and honor to welcome you; honorable guests, lecturers, researchers and participants, to the 21st ICS International Chemistry Congress (ICC2022) to be held 26-28 July 2022 at Azarbaijan Shahid Madani University in Tabriz. After two years of delay due to the covid-19 pandemic, we are so glad to meet you, here in Tabriz and this could not be possible without the selfless sacrifice of the health services staff, which I would like to express my deep gratitude to them. The ICC2022 is a forum for presentation and discussion of the most recent advancements in all fields of chemistry which are held biannually in one of the Iranian universities in collaboration with the Iranian Chemical Society (ICS).

Keynote and invited speakers, oral presentations, poster sessions, workshops and specialized exhibitions are arranged in the program of the present congress. We are looking forward that these specific topics could manifest the current central points and the trends of development in chemistry research thus directing us to work co-ordinately for the advancement of chemistry.

I have to thank the scientific committee members for peer-reviewing abstracts, the organizing committee members, executive committee members, Professor Hassan Valizadeh as chancellor of Azarbaijan Shahid Madani University, and Professor Ali Ajami as research vice-chancellor.

We are honoured to have Professor Mohammad Ali Zolifigol as Minister of Science, Research and Technology, Professor Peyman Salehi as vice-minister of research, Professor Mojtaba Shamsipur as ICS president and Professor Majid Moghadam as secretary-general of ICS during the congress. In addition, I would like to express our sincere thanks to all sponsors, both from industry and commercial companies, for their generous financial support.

Wishing you a pleasant time in Tabriz, we hope you rejoice in meeting old friends and colleagues, and making new connections. And let's also hope this current congress and the future ones provide means for our academic and research community to reach new spheres of scientific knowledge.

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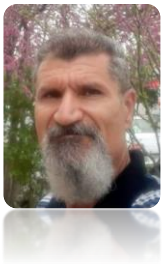

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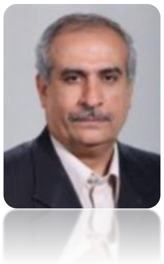

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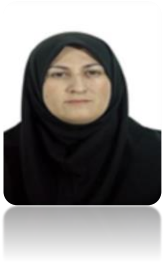

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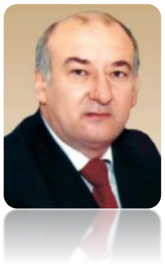

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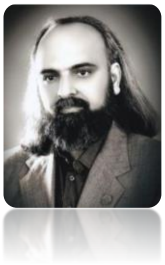

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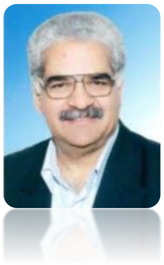

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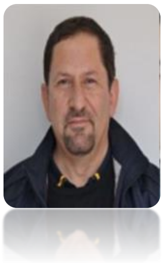

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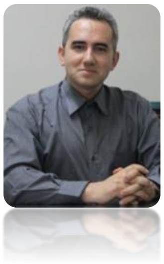

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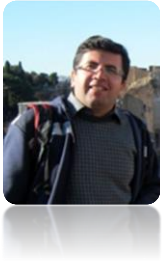

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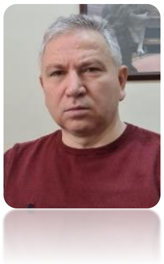

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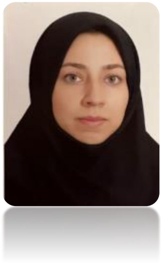

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Oral Presentations

Green Chemistry, Nobel Prizes and Sustainable Development

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To find a clue in a hot topic scientific interests and a particular cutting edge field of activity, it can be arisen from diverse sources. Nobel Prize is one of the most important ones. Due to the importance of eco-friendly processes and energy management as well as development of green aspects of chemical processes, Nobel prize laureates and their following researchers have focused on design and development of safe and clean materials and methods to aim sustainable development. The green reactions especially based on natural materials that deserve least reaction steps, high yields, high atom economy, saving energy and environment and bond forming efficiency in the aimed protocols on chemical reactions are of prime importance in sustainable development. Thus, research centers and groups try to design and develop clean and sustainable protocols and green materials in diverse chemical transformations.

Keywords: Green Chemistry, sustainable development

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Quantum Computational Chemistry of Large-Size Systems: An Introduction to QM/MM and ONIOM Methods

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In the field of quantum chemistry, although computational power has increased dramatically over the last few decades, but there is still a high computational cost associated with the description of complex molecular systems in material and life sciences. There are many efforts in the literature to reduce this cost, and the first and simplest involves extrapolation techniques. That is, calculation of the system of interest using a lower level of theory (ca. DFT/MP2) and scaling to a higher level (CCSDT). However, with very high accuracy methods comes high computational cost. To date, high-level theory is only applicable for very small molecules, involving just a few atoms, as anything more is intractable. Such an approach cannot be used for materials or life sciences. Alternative approaches are needed to tackle large polyatomic systems at the forefront of active chemical research. Instead of scaling or extrapolating, another approach is to subdivide the system of interest, compute the smaller subsystems, then combine the pieces. This has been shown to be highly effective, and such techniques are commonly called quantum embedding the act of embedding a smaller system of interest in a larger one (surrounding environment). In this perspective, the Quantum Mechanical/Molecular Mechanical (QM/MM) approach and its more general version “Own-N-Layered Integrated Molecular Orbital and Molecular Mechanics (ONIOM)” as two quantum embedding methods are briefly introduced and some examples are explained [1-2].

Keywords: Quantum Computational Chemistry, Quantum Mechanical/Molecular Mechanical (QM/MM)

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[2]. Bahrami H, Tabrizchi M, Farrokhpour H. *Chemical Physics*. **2013**, 415, 222

Layered Double Hydroxides (LDHs) as Multifunctional Nanomaterials for Different Applications: From Water Splitting to Drug Delivery

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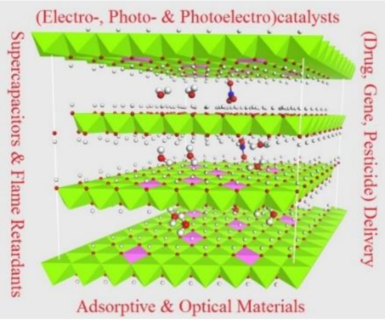
The present work involves the study of layered double hydroxides (LDHs). LDHs have been known for over 150 years since the discovery of the mineral hydrotalcite, and a large class of minerals with closely related structures are usually known to mineralogists as the sjögrenite-hydrotalcite group. The basic features of their structure, involving positively charged brucite-like layers together with charge-balancing anions and water in interlayer galleries are well understood, but some detailed aspects of their structure have been the subject of controversy in the literature. [1] With the emergence and growth of nanotechnology, more attentions were drawn to LDHs, because the possibility of synthesizing LDHs nanostructures provides a variety of applications such as (electro-, photo-, photoelectro-) catalysis, adsorption, (drug , gene , pesticide) delivery, optical materials , flame retardants and supercapacitors for these materials.



Schematic representation of the various applications of LDHs

The structural features of LDHs play an essential role in this diverse applicability. In the first part, their structural characteristics are described. Then, different methods of synthesis and especially the synthesis of LDHs nanocomposites are explained. In the last part, the potential applications of LDHs in the electrocatalysis of water splitting via oxygen evolution reaction (OER), adsorptive removal of dyes, drug delivery and supercapacitors will be discussed. The research works carried out in the last 10 years in our research laboratory at Azarbaijan Shahid Madani University have been described concerning to the topics.

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Assembly of Angular Triquinane Cores

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Polyquinanes constitute an important class of fused polycyclopentanes (three or more fused five-membered ring systems) that aroused interest due to their biological activities and synthetic challenges.[1] Among the polyquinanes, the triquinane natural products which are abundant in nature, are classified into linear, angular, and propellane-type[4] (Fig. 1). Angular triquinanes, in contrast to linear triquinanes, are a synthetic challenge, since their basic structure includes a quaternary stereocenter.

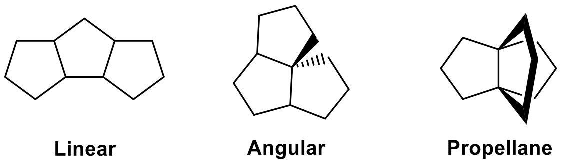

Fig. 1. Carbocyclic triquinanes.

We have developed one-pot strategies for synthesis of angular triqinane cores. The reactions provide direct access to structurally diverse angular triqinanes **1-6** shown in Figure 2.[2] Evidence for the stereochemistry of these products obtained from single-crystal X-ray analyses, and NMR spectroscopic data. Mild reaction conditions, moderate to good yields and diverse functional group tolerance are advantages of these metal-free protocols. The transformations proceeded without much sensitivity to electronic or steric hindrance factors. Various features of these transformations will be presented and discussed.

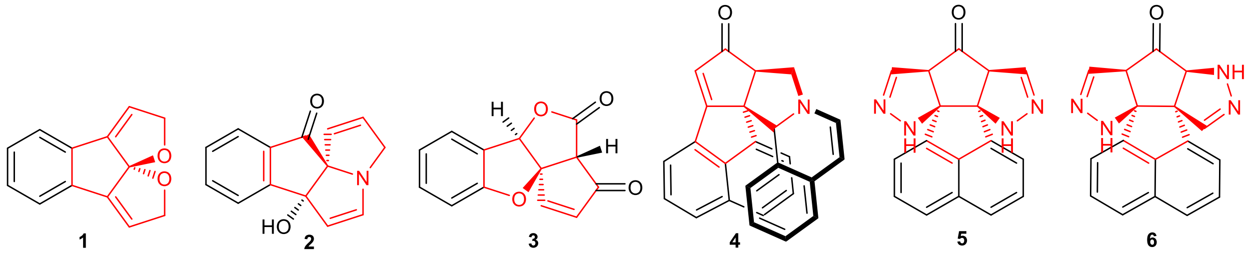

Fig. 2. Structurally diverse angular triqinanes **1-6**.

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Single atom catalysts for environmental protection: New insights from density functional theory calculations

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Single atom catalysts (SACs) have lately sparked the interest of many researchers due to their outstanding physicochemical properties and diverse catalytic applications. They are defined as catalysts in which all active metal species reside as isolated single atoms stabilized by support or alloying with another metal. The catalytic performance of SACs and their product selectivity, and stability are all influenced by the nature of the metal/support material, the interaction between metal atoms and the support, charge separation behavior, adsorption ability, active sites, and defects. This study used density functional theory (DFT) calculations to examine current progress in the design of SACs for tackling air pollution and other environmental problems. Meanwhile, the advantages of SACs in energy storage are highlighted, as are the opportunities and challenges that SACs have encountered in this research field, as well as the future development direction.

Keywords: Catalysts; Air pollution; DFT; adsorption; energy storage.

Exhaled breath condensate as a promising biological sample

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Blood, serum, plasma and urine are the most common biological samples used for quantification of different biomarkers or drugs in biomedical investigations [1]. In addition to these samples, saliva, sweat, tear, cerebrospinal fluid, sputum, bronchoalveloar lavage, nail, hair, and tissue are the common samples. The exhaled breath (EB) and exhaled breath condensate (EBC) are less commonly used potential biological samples possessing a number of advantages to follow up the analytes' concentrations. EB contains mainly volatile compounds and EBC contains both volatile and non-volatile analytes. EBC is a newly presented sample and could be collected using different collection setups. The range of analytes in EBC varies from small Na or K ions to large macromoecules such as DNA [2,3]. In this presentation, a brief history of EBC, its collection setups, recent analytical works on EBC, advantages, disadvantages and also its potential applications in furture pharmaceutical and biomedical investigations will be discussed.

Keywords: Biomarker, Pharmaceutical, Analysis, Biological sample, Exhaled breath condensate

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Large scale MOF production for Industrial applications

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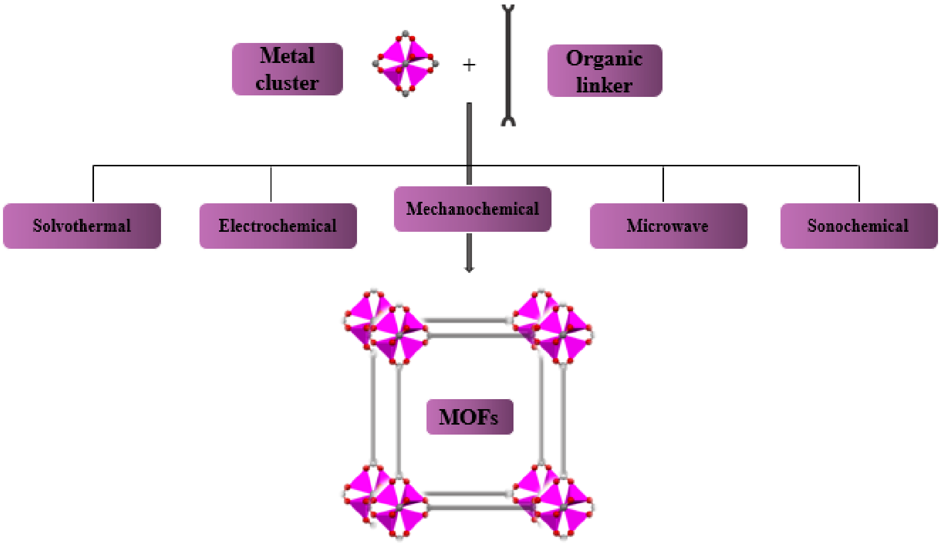
Due to the fascinating molecular structure of metal-organic frameworks (MOFs) and their widespread practical use in various industrial applications, great attention has focused on the development of various commercialization techniques for up-scaled production of these advanced porous materials via more efficient, sustainable, and cost-effective manners. Despite the impressive progress in MOFs synthesis via conventional solvothermal methods, the large-scale production of these materials has been limited due to the non-green, non-economic, and complex synthesis routes in solvothermal processes. This presentation provides an overview of recent advances on MOFs synthesis via mechanochemical methods highlighting the synthetic challenges as well as the advantages of scaling up of MOF synthesis.



Keywords: Metal-organic frameworks, mechanosynthesis, scalable

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Structural Skeletons with Unique Architectures from Iranian Native Plants; Masterpieces of nature

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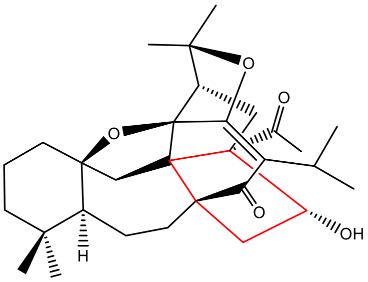
A huge diversity of molecular skeletons found in natural products enables finding better lead compounds to develop clinically useful entities. Plants are able to produce chemical metabolites with unique structures and specific properties, and therefore have always been considered as an important source for discovering new drugs or even finding suitable lead compounds [1]. Due to the increasing discovery of new drugs from plants and unique structures of biologically active natural compounds, progress in the field of separation and structure elucidation of these compounds is very important [2].

Our recent studies, aimed at identifying structurally interesting and bioactive metabolites from the Iranian endemic species, resulted in the isolation of several new compounds; some of them possess unusual and unique structures (**1-3**). The structures were elucidated by a combination of 1D and 2D NMR, HRESIMS, and X-ray crystallographic analyses. Plausible biosynthetic pathways toward these new skeletons were proposed. Biological properties of the new compounds were also investigated. Some of these compounds showed good *in vitro* antiplasmodial and anticancer activities at submicromolar concentrations and were subjected to semisynthetic modifications in order to improve their activity.



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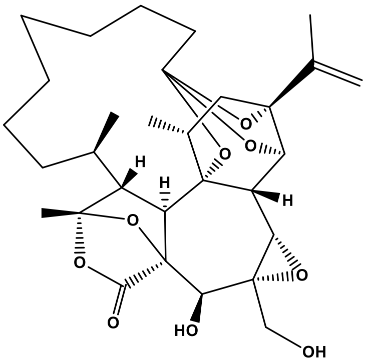

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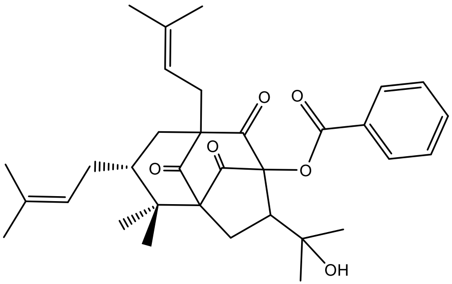

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Keywords: Drug discovery, Lead compound, Structure elucidation, Biological activity

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Non-Asymmetric Organocatalysis: A green chemistry approach

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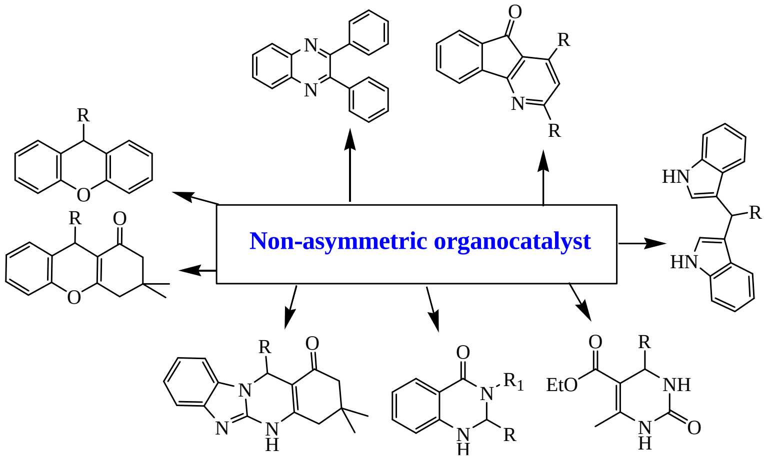
Organocatalysis has emerged as a powerful approach in organic chemistry for making/forming carbon-carbon and carbon-heteroatom bonds over the last 20 years.[1] Organocatalytic processes yielding achiral compounds have recently garnered huge attention as a low-cost, non-toxic, easily available approach yielding the corresponding products with outstanding selectivity in high yields. [2]

Heterocycles are being studied extensively for their numerous biological activity and medicinal properties [3], including GABAA receptor ligands, ϒ-secretase inhibitors, kinase inhibition, GSK3-inhibiting, and proapoptotic effects, antimalarial and anti-inflammatory.

The proposed paper addresses our recent successes in synthesizing highly functionalized heterocycles utilizing non-asymmetric organocatalysts [4, 5]. [(Scheme1)



Scheme 1. Synthesis of heterocyclic compounds using non-asymmetric organocatalyst

Keywords: Organocatalyst, achiral, heterocycle, green

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Application of nano-based materials and Molecular imprinted polymers in analytical and environmental approach

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Extraction and determination of residual hazardous organic compound in various complicated matrices including environmental and biological samples attain great importance. In complicated samples, especially at concentration below detection limit make an emphasis to researchers for designing novel approaches which benefit from remarks like high selectivity and unique ability for separation of analyte which possible clean-up of real sample before their instrumental analysis. In this regard, application of nano-based material and unique sorbents like molecular imprinted polymer [1-2] based strategy owing to high reactive center and surface area according to cooperation of sizes and functional group supply unique selectivity and enhance figures of merits. Combination of such features along high selectivity detection tolls led to more progress in method performance. Hence, molecularly/ion imprinted polymers (MIPs or IIPs) as well as nanostructure materials are most prominent and available protocol to enhance figures of merit corresponding separation methods to supply distinguished model for such purposes. MIP owing to incorporation of most complexation and trapping factors like functional group, surface imprinting, enhance in lipophilicity, dummy feature and restricted access nature and ability for supplying initial materials by low cost raw material suggested as best candidate that enable high capacity, low cost of preparation and high selectivity with target molecules/ions.

Keywords: molecularly/ion imprinted polymers (MIPs or IIPs), nano-based material, Extraction

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Electrochemical Energy Storage for Sustaining a Healthy Planet

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The electricity that is currently generated from photovoltaic panels or wind turbines exhibits potential benefits toward a sustainable energy future. However, the highly intermittent nature of renewable sources of energy is a big challenge that limits their extended applicability in modern societies. Thus, the development of advanced batteries and supercapacitors represents a feasible solution to overcome the existing constraints. In one approach, we electrosynthesized a polyaniline-lignosulfonate interpenetrating network as well as polydopamine (PDA) on carbon cloths/fibers to fabricate high-performance supercapacitors.[1] We also synthesized mesoporous carbon nitrides *via* a nano hard-templating method and then composited it with the graphene aerogel to fabricate a supercapacitor.[2] We also conjugated aromatic redox active dyes to the reduced graphene oxide surface via non-covalent π-π stacking interaction to fabricate supercapacitors.[3] Besides, we developed superbatteries as hybrid energy storage devices based on layered-double hydroxides (LDH) and metal-graphene aerogel nanocomposites.[4] We also reviewed the standard performance metrics of batteries and supercapacitors that would help the researchers of the energy storage community to evaluate the recently-developed systems based on the well-established criteria.[5]

Keywords: energy storage, supercapacitors, advanced materials, batteries, standard metrics

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Merging Chemistry with Technology: Nanomaterial, 3D printers and mobile phones in micro total analytical systems (uTAS)

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The significant progress in technology in last few decades reflected strongly on the progress in analytical chemistry. The concept of merging optics, fluidics, electronics and biosensors in very small scaled channels is a state-of-art. It is undisputed that many virtues can be effectuated by using extremely small fluid volumes (micro to pico litres) of solvents and chemicals with high throughput, high degree of control, reduced waste generation and relatively less energy. This ultimately can be dedicated in many chemical analyses and rather replace a couple numbers of traditional bench-top analytical procedures. In addition, the utility of greening approach in analytical analysis will be fulfilled by micro total analytical systems (uTAS). However, new challenges appeared and novel approach were required to overcome these challenges. The approach is based on utilizing new materials that can be easily utilized in these uTAS.

Metal-organic frameworks (MOFs) are special type of inorganic crystalline porous nanomaterials. These nanomaterials consist of certain multidentate organic bridges connected to cationic central parts. The main advantages of MOFs are high ordered porosity, tunable pore sizes, great surface areas, high stability and tailor-made functionality [1]. These properties give the MOFs a superior room in various fields, especially in catalysis and sensor developments and made them valuable adsorbents for extraction and separation goals.

Carbon based nanomaterials due to the benefits of marvellous electronic and physicochemical features in addition to the abundant external morphology, carbonaceous nanostructures, like graphene sheets, fullerenes, carbon nanotubes and carbon quantum dots (CQDs), have inspired broad studies on them. C-based QDs is especially interesting because it exhibits the highest effectiveness of luminescent and light emission, which can be tuned to any wavelength in the visible spectrum by varying the size and shape. Compared with macroscopic carbons and traditional semiconductor quantum dots (QDs), C-based QDs exhibit exemplary merits, encompasses low toxicity, dispersing well in water, good photobleaching resistance, ease of synthesis and surface modification [2].

In our labs, we integrate the use of these novel materials along with mobile phones in a 3D printed platform, to create a state of art micro total analytical systems [3-4].

This presentation, will highlight some of the latest developments in this exciting field.

Keywords: Metal-organic frameworks, nanomaterials, 3D printer, micro total analytical systems, Mobile Phone.

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Where Are We in Antioxidant Capacity Measurement Eighteen Years After the Discovery of the CUPRAC Method?

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The cupric ion reducing antioxidant capacity (CUPRAC) assay as an electron-transfer (ET) method measuring total antioxidant capacity (TAC), and its modifications can indirectly measure the scavenging capacity of antioxidants toward reactive oxygen species (ROS). This method is widely used in food chemistry and biochemistry laboratories and research centres, and the two leading CUPRAC publications [1,2] have retrieved a total number of ≈ 3500 citations (Google Academic). CUPRAC has definite advantages over other similar ET-based methods: (i) The CUPRAC reagent is low-cost, accessible and stable. (ii) The method works at physiological pH, simulating biologically relevant redox reactions of antioxidant defense against reactive species. (iii) The CUPRAC reagent is selective toward true antioxidants, because its redox-active components, cupric/cuprous-neocuproine couple, has the most suitable redox potential of 0.6 V close to that of most biological and food antioxidants. (iv) The cupric neocuproine chelate has favorable kinetics toward slow-reacting antioxidants; it reacts with simple and protein thiols and certain phenolic acids at an appreciable rate. (v) CUPRAC yields perfectly linear curves over a wide concentration interval. (vi) It is a robust method unlike other methods extremely sensitive to light, air oxygen, temperature and pH. (vii) CUPRAC measurements do not give rise to redox-cycling of phenolics, altering analytical precision. (viii) CUPRAC can determine both hydrophilic and lipophilic antioxidants, enabling the measurement of plasma and oil antioxidants in different solvent systems. (ix) The reagent can be adsorbed on a Nafion membrane sensor and operate like a pH-paper. (x) CUPRAC can measure antioxidants individually by adaptation to online HPLC with the use of a postcolumn reactor. (xi) It has been implemented in microplate and flow modes. (xii) It can be applied to insoluble food components (such as bound phenolics). (xiii) CUPRAC can indirectly measure ROS and their scavengers by careful selection of CUPRAC-reactive probes or their oxidation products. (xiv) CUPRAC can indirectly determine a number of oxidative and antioxidative enzymes through substrates or enzymatic conversion products. As a result, the CUPRAC method has evolved into a train of antioxidant activity/capacity assays [3] useful for indicating the full antioxidant potential of food and biological systems, and other materials (such as ammunition) requiring antioxidative protection.

Keywords: Antioxidant capacity, electron transfer, CUPRAC method, ROS scavenging

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Development and evaluation of novel positron emission tomography radiotracers for targeting neurodegenerative disorders

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Major neurodegenerative diseases (NDD) are defined by the deposition of pathogenic neuroproteins, particularly amyloid-β (Aβ), tau, and α-synuclein fibrils. Alzheimer's disease (AD) is most likely caused by the aggregates of Aβ and tau. Molecular imaging using nuclear medicine modalities can help diagnose the AD by using Aβ- positron emission tomography (PET) and Tau-PET. Neuroimaging offers a long-term vision of creating a paradigm shift in the early diagnosis and understanding of Parkinson's disease (PD) too by enabling early detection of aggregated α-synuclein (aSYN) in brain using a novel tracer. Preclinical studies in mice and translational studies toward clinical applications will be accomplished by rational design for developing new molecular tracers for whole body PET. A highly desired, but so far unmet medical need is the in vivo demonstration and quantification of the presence, severity and regional distribution of aSYN and its clinical manifestations in individuals with α-synucleinopathies, including PD, dementia with Lewy bodies (DLB), and multiple system atrophy (MSA).

Different candidates from among different classes of substances have been identified which bind selectively and with high specificity to Aβ, tau, and α-synuclein aggregates. For the best specific, [^{18}F]FIBT[1] with its excellent binding to Aβ, the entire development process was performed up to the patient investigation. It has also been shown that some candidates from this portfolio of promising ligands open up the possibility of stratification and differentiation of NDDs. This methodology can provide valuable contributions to disease development and individual care. Recently, highly innovative molecules utilized as diagnostic probes, based on 4,4'-diaryl-2,2'-bithiazole (DABTA) were also developed in my group as sensitive, selective and specific tracers suitable for the visualization and quantification of α-synucleinopathy by PET imaging. With the help of these newly developed substances, the presence, distribution and progression pattern of α-syn can be investigated in the living rodent and human brain, reflecting the disease entity and stage. Preliminary results with leads with high binding affinity for α-syn (Ki < 3 nM) and high selectivity (>>100 fold) versus Aβ and tau) in a E46K-Tg rats, nonhuman primates, and extended single dose toxicity study followed by first-in-human application are promising with regard to safety and sensitivity. Based on all these data carried out the optimization of DABTA candidates toward improved pharmacokinetics (PK)[2].

In summary, a broad range of new and powerful radiopharmaceuticals have been developed for the diagnosis of NDDs new labeling strategies and translational PET imaging research.

Keywords: Molecular Imaging, AD, PD, LBD, MSA

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Cyclometalated luminescent complexes of the nickel triad (Ni, Pd, Pt)

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Besides the important d^6 configured cyclometalated Ir(III) complexes, d^8 configured Pt(II) complexes containing cyclometalated heterocyclic ligands have gained enormous interest as efficient triplet emitters for applications in light emitting diodes (OLED), for photocatalysis, or as luminescent probes in biomedicine.[1-3] In the last few years attempts have been made to replace these precious (rare and expensive) elements by earth abundant homologues such as Fe(II) (d^6) or Ni(II) (d^8).[4] However, these lighter homologues pose a number of problems which hamper their exploration. The lecture will highlight these problems but also the opportunities showcasing recent research on complexes of the Ni – Pd – Pt triad carrying tridentate or tetradentate heteroaromatic cyclometalated ligands (examples in Figure 1).

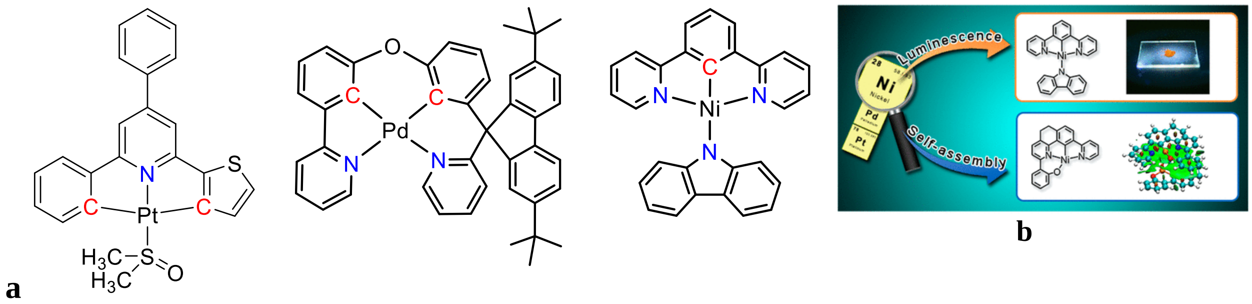

Figure 1. a) Cyclometalated Pt(II)[5], Pd(II)[2], and Ni(II)[7] complexes, b) Cyclometalated Ni(II) complexes showing luminescence and π-stacking. From ref. [7]; Courtesy by the American Chemical Society (ACS)

In the last decades the "golden rule" was that Pt(II) complexes are generally better emitters than their Pd(II) homologues.[5,6] In typical cases, Pt(II) complexes showed efficient triplet emission in solution at ambient temperature, while for the Pd(II) homologue emission was only observed at 110 K in the solid. For Ni(II) virtually no triplet emitting complexes were reported; luminescent Ni(II) complexes owed their emission exclusively to their fluorescent ligands (singlet emission). Very recently, Vivian Yam reported the first Ni(II) complex (Figure 2) that is luminescent from an metal-perturbed triplet π–π* excited state $({}^3\pi{-}\pi^*/{}^3\mathrm{MLCT})$ at 298 K in the solid and at 77 K in glassy frozen matrices, alongside with π stacking of another cyclometalated Ni(II) complex, which is a key step to form luminescent aggregates from d^8 configured metal complexes.[7]

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Diamondoids: Ranging from Nature's Bounty to Pharmaceutical Applications

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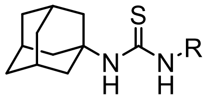
Diamondoids are cage and hydrogen-terminated hydrocarbon molecules that are superimposable on the diamond lattice.[1] Thus, diamondoids as nanometer-sized diamond-like molecules, nanodiamonds, are likely to share some of the unique properties of macroscopic diamond that are very attractive for a number of applications, ranging from material science to medicinal chemistry. Adamantane, the simplest member of the diamondoids, was primarily discovered and isolated from crude oil (natural abundance ~0.0004% petroleum content) in 1933 and became widely available through Schleyer's synthesis in 1957. Thereafter, synthesis of adamantane derivatives started fueling pharmaceutical studies thereof, and drugs incorporating the adamantane motif were quickly introduced to the market.[2] On the other hand, nowadays, adamantane scaffold is viewed as a "lipophilic bullet" for the modification of known drugs in order to enhancing lipophilicity and stability of them, thereby improving their pharmacokinetics and pharmacodynamics.[3] There are many diverse drug candidates based on adamantane-modification of known drugs.[3,5] Hence, the present study will outline the synthesis of privileged structures incorporating an adamantane scaffold, including, thioureas **1**, 1,4-dihydropyridines **2**, pyrimidines **3**, propranolol derivative **4**, and Schiff bases **5**, that are pursued in the group of the author.



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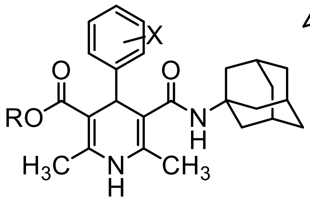

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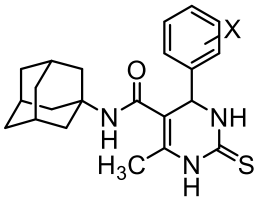

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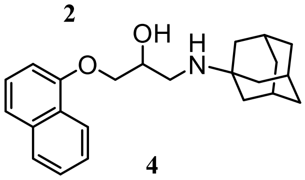

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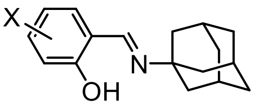

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Keywords: Diamondoid, Nanodiamond, Adamantane motif

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Porous nanostructures from MOFs, COFs and SBA-15, to PMO microporous and mesoporous nanoreactors: 14 years with ONG

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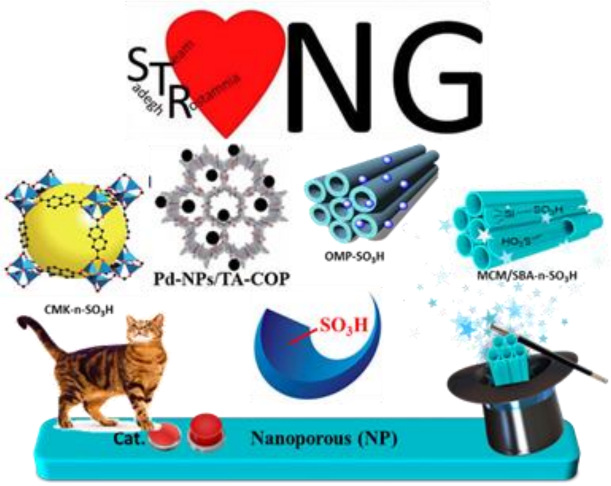
Within the feld of materials, chemistry, catalysis, energy, drug-delivery and even industry the nanostructures as a nanoreactor has possessed much attention. Normally, the synthesis of these materials are based on supramolecular and self-assembly phenomna in solvothermal condition [1]. Post-synthetic modification synthesis of these materials have main role in our group for desighned meta-organic frameworks (MOFs), covalent organic frmaeworks (COFs) for vrious application. Furthermore, these porous materials, from MOFs, COFs and SBA-15, to PMO, can be an excellent candidate for the stabilization of metal nanoparticles in their pore cages that it is our goal in Oganic and Nano Group (ONG) at IUST [2-4].

Keywords: Metal-organic frameworks, covalent organic frameworks, nanoreactors.



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Green chemistry approaches for the separation and enrichment of trace organic and inorganic species

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Separation-preconcentration for trace species is the one of the main parts of the sample pretreatment step. Solvent extraction, solid phase extraction, coprecipitation etc. are widely used separation-preconcentration techniques. In the last decade, the miniaturization of these techniques for the green chemistry purposes is very popular in analytical chemistry. Nowadays microextraction and solid phase microextraction procedures for traces organic and inorganic species from environmental samples with different strategies are the main part of separation-preconcentration techniques with new nanomaterials including graphene-based materials, MOFs, COFs and HOFs etc. [1]. and new generation solvents including ferrofluids, switchable solvents, deep eutectic solvents, supramolecular solvents etc. [2].

In this presentation, the main strategies for the microextraction of organic and inorganic species at trace levels with new generation solvents and solid phase microextraction with new nanomaterials have been discussed with some examples from our research group.

Keywords: Green chemistry, Enrichment, Microextraction

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Localized X-Ray Photoelectron Impedance Spectroscopy (Lo-XPIS) for Capturing Screening Dynamics of Electrical Double Layer in Solid/Liquid Interfaces

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Many electrochemical devices are based on the fundamental process of ion migration and accumulation on surfaces. Complex interplay of molecular properties of ions and device dimensions control the entire process and define the overall dynamics of the system. Particularly, for ionic liquid-based electrolytes it is often not clear which property and to what extent contributes to the overall performance of the device. Herein we use X-ray photoelectron spectroscopy (XPS), while the device is under electrical bias. Such a procedure reveals localized electrical potential developments, through binding energy shifts of the atomic core levels, in a chemically specific fashion. Combining it with Square-Wave AC Modulation, the information can also be extended to time domain, and investigate devices configured as a coplanar capacitor, having an ionic liquid as the electrolyte, in macro-dimensions. Our analysis reveals that nonlinear voltage profile across the device emerge from spatially nonuniform electrical double layer formation on electrode surfaces. Interestingly coplanar capacitor has extremely slow time response which is particularly controlled by IL film thickness. XPS measurements can capture the ion dynamics in tens of seconds to microseconds range, and reveal that ionic motion is all over the device, including those on metallic electrode regions. This behavior can only be attributed to motion in more than one dimension. The ion dynamics can also be faithfully simulated by using a modified PNP equation, taking into account steric effects, and device dimensions. XPS measurements on two devices with different dimensions corroborated with and validated the simulation results. The present results propose a new experimental approach and provide new insights into the dynamics of ions across electrochemical devices.

Keywords: XPS, Ionic Liquids, Electrified Interfaces, Ion Dynamics

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Easy Applicable Approaches for Sensitive Analysis for Drug Molecules

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Sample preparation has been recognized as a major step in the chemical analysis workflow. As such, substantial efforts have been made in recent years to simplify the overall sample preparation process. Sensitive analysis of drug molecules in biological samples is a challenge due to low concentration of target molecules and comlexity of sample matrix[1]. Major focusses of these efforts have included miniaturization of the extraction device; minimizing/eliminating toxic and hazardous organic solvent consumption; eliminating sample pre-treatment and post-treatment steps; reducing the sample volume requirement; reducing extraction equilibrium time, maximizing extraction efficiency etc. All these improved attributes are congruent with the Green Analytical Chemistry (GAC) principles[2]. Classical sample preparation techniques such as solid phase extraction (SPE) and liquid-liquid extraction (LLE) are being rapidly replaced with emerging miniaturized and environmentally friendly techniques such as Solid Phase Micro Extraction (SPME), Stir bar Sorptive Extraction (SBSE), Micro Extraction by Packed Sorbent (MEPS), Fabric Phase Sorptive Extraction (FPSE), and Dispersive Liquid-Liquid Micro Extraction (DLLME). These techniques manifest a rapid development of sample preparation techniques in different fields, such as biological, environmental, food sciences, natural products, forensic medicine, and toxicology. In the biological and forensic fields, where a wide variety of drugs with different chemical properties are analyzed, the sample preparation is required to make the sample suitable for the instrumental analysis, which often includes gas chromatography (GC) and liquid chromatography (LC) coupled with mass detectors or tandem mass detectors (MS/MS)[3]. Application of magneic nanoparticles as high-performance extraction sorbents has undoubtedly elevated the extraction efficiency and method sensitivity of modern chromatographic analyses to a new level. Combining magnetic nanoparticles with many microextraction sorbents has opened up new possibilities to extract target analytes from sample matrices containing high volumes of matrix interferents. By developing this type materials, highly sensitive and selective analyzes can be performed easily and effectively even in laboratories with a conventional chromatographic system.

Keywords: Pharmaceutical Analysis, Microextraction techniques, HPLC, GC, Biological samples

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Plasmonic Metal-based Photocatalysis; an Efficient Method for Modifying Semiconductors

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Metal nanoparticles have shown great potential in heterogeneous photocatalysis. Noble metal nanoparticles such as Au, Pt, and Ag have drawn great attention in this area, due to their visible-light activity and selectivity in various chemical reactions [1-3]. But the challenge is that they are easily deactivated during the catalysis and their high cost. Therefore, composition of the metal nanoparticles with other metals and preparation of bimetallic nanoparticles based on surface plasmonic resonance effect becomes one of the most promising strategies to overcome the stability issue. In this paper, we provide a summary of the recent progress in the synthesis of Bi, Cu, and Ag nanoparticles as co-catalysts to improve the photocatalytic activity of metal oxides and metal sulfides. This paper begins with an introduction to the preparation method for synthesis of metal nanoparticles, and composition with semiconductors. The advantages of the designed materials are then discussed, such as improved photocatalytic efficiency for removal of organic pollutants, enhanced stability, and improved selectivity in photo-, and electrocatalysis.

Keywords: Photocatalysis, Surface Plasmon Resonance, Metal Nanoparticles, Bimetallic Nanoparticles, Organic Pollutants.

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Structural Behaviors of Nicotinamide Complexes of Cd(II) Arylcarboxylates

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Cadmium(II) is compatible with a wide range of stereochemical settings due to its d^{10} electronic structure. Cadmium(II) has four, five, six, seven and eight coordination numbers. In a study comparing the structures of the 200 cadmium(II) complexes with crystal structure, it was found that in 19.8 % of these complexes, coordination numbers of cadmium had four and five. In addition, in 56 % of these complexes, the coordination number of cadmium was reported to be six. In the same study, seven-coordinate cadmium(II) complexes were reported to be less common in the literature [1].

Cadmium(II) complexes with carboxylic acid and carboxyate ligands play an important role in coordination chemistry. In this study, the crystal structures of nicotinamide complexes of cadmium arylcarboxylates were examined. These complexes exhibit different structural properties such as monomeric, dimeric, ionic, polymeric and supramolecular. Six of these complexes, which have eleven different examples in the literature, have a dimeric structure. The coordination number of cadmium in all dimeric complexes is seven, and these dimeric complexes contain the coordinated water molecules. The number of coordination in the monomeric complex containing 2-nitrobenzoate anion is six, while the number of coordination in the monomeric complex containing 2,4,6-trimethylbenzoate anion is seven. The 4-formylbenzoate anion in the ionic complex is located outside the coordination sphere. The main ligand of the polymeric complex is terephthalate anion, and it is the only complex that does not contain a water molecule among the nicotinamide complexes of cadmium arylcarboxylates. The asymmetric unit in the supramolecular complex, which has an interesting structural architecture, contains two different molecules. In the supramolecular structure, 2-hydroxybenzoate ligand is a monodentate coordinate in one molecule and a bidentate coordinate in another. In a study in which dimeric nicotinamide complexes of cadmium 3-fluorobenzoate were synthesized by classical and hydrothermal methods, 3-fluorobenzoate anions form a bridge in the complex synthesized by the classical method, while nicotinamide molecules form a bridge in the complex synthesized by the hydrothermal method. This complex is the only literature example in which the nicotinamide molecule is bidentate coordinated among the nicotinamide complexes of cadmium arylcarboxylates [1, 2].

Keywords: Cadmium complexes, arylcarboxylate, nicotinamide, crystal structure.

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Smartphone-Based Electrochemiluminescence for Visual Simultaneous Detection of RASSF1A and SLC5A8 Tumor Suppressor Gene Methylation in Thyroid Cancer Patient Plasma

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Visual one-step simultaneous detection of low-abundance methylation is crucial challenge in early cancer diagnosis in simple manner [1]. Through the design of closed split bipolar electrochemistry system (BE) [2], detection of promoter methylation of tumor suppressor genes in papillary thyroid cancer, RASSF1A and SLC5A8, was achieved using electrochemiluminescence. For this purpose, electrochemiluminescence of luminol loaded into the Fe_3O_4@UiO-66 and gold nanorods-functionalized graphite-like carbon nitride nanosheet (AuNRs@C_3N_4 NS), separately, on the anodic and cathodic pole bipolar electrode (BPE) in two different chambers of bipolar cell were recorded on a smartphone camera. To provide same electric potential (ΔE_{elec}) through the BPEs to conduct simultaneous light emission,as well as to achieve higher sensitivity, anodic and cathodic poles BPEs was separately connected to ruthenium nanoparticles electrodeposited on nitrogen-doped graphene-coated Cu foam (fCu/N-GN/RuNPs) to provide hydrogen evolution reaction (HER) and polycatechol-modified reduced graphene oxide/pencil graphite electrode (PC-rGO/PGE) to provide electrooxidation of hydrazine. Moreover, taking advantages of strong cathodic ECL activity due to the roles of AuNRs, as well as the high density of capture probe on the UiO-66 and Fe_3O_4 role in improving the signal-to-background ratio (S/B) in complicated plasma media, a sensitive visual ECL immunosensor was developed to detect two different genes as a model target analyte in patient plasma samples. The ability of discrimination of methylation levels as low as 0.01% and above 90% clinical sensitivity in thyroid cancer patient's plasma implies the present strategy is able to diagnose cancer early as well as monitoring responses patients to therapeutic agents.

Keywords: Electrochemiluminescence, Smartphone, DNA Methylation, Thyroid cancer, Metal organic framework

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Quantum close coupling, classical MM and molecular dynamics calculation of the transport properties of the atom-diatom molecular systems

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The classical Boltzmann kinetic theory and its Chapmann-Enskog solution is a unique method to describe the transport properties of the atomic gases governed by the van der Waals (vdW) interactions. However, in polyatomic systems some other properties arise from the spatial distribution and quantal effect. The quantum mechanical Waldman-Snider equation is the extension of the classical Boltzmann equation to the molecular systems in which the internal degrees of freedom are also considered. The exact solution of the Hamiltonian of the simple atom-diatom system was provide by close-coupling (CC) method. Coupling of the CC method with WS equation provides an exact method to calculate the transport and also relaxation properties for such molecular systems. In this paper, CC, classical Mason-Monchick (MM), and classical molecular dynamics (MD) simulations were used to calculate the viscosity and diffusion coefficient of some atom-linear molecular vdW complexes in the limit of zero density. The selected systems are He-HCl, He-HBr, He-BeH2 and He-CO2 vdW complexes. In this respect, the potential energy surface (PES) of these systems were calculated at CCSD(T)-aug-cc-pvXz (X=3,4,5) level of theory and the obtained PESs then were used to calculate the transport properties. In MD simulations the effect of 2-body and 3-body interactions were also considered. In summary, we found that, by increasing the size of the systems, i.e., increasing the molecular mass and the number of atoms, the accuracy of the MD and MM methods were decreased compared to the exact CC results. Also, the consideration of 3-body interactions has a crucial effect on the accuracy of the results especially at higher temperatures.

Keywords: He-BeH$_2$, Non-equilibrium thermodynamics, Viscosity, Diffusion coefficient

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Green Chemistry: Historical Developments and its 12 Golden Principles

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In this work, the development of green chemistry is presented in a historical background. From 1970's in which the environmental damages caused by human have been received to a critical level, some countries tried to establish environmental protecting organizations. One of pioneering them is environmental protecting organization of the United State. The most important finding of the woks done in these years is that the chemical industries have made the most severe damage to the soil, water and air.

Then the chemical scientists categorized those aspects of the chemical technologies that destroy the environment and give us the solutions. These solutions are directions about how the wastes are managed, how byproducts production is avoided, how unsafe reactions are bypassed and other directions and comments. These are named as Green Chemistry and involve 12 principles about various aspects that following them leads to reduction the amounts of wastes, toxic byproducts, using renewable row materials, energy costs of processes and other aspects helping to protect the environment.

Here we discuss these principles, their historical source and some industrial examples related to each principle.

Microextraction as a solution for real-life challenges

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Microextraction methods, as important part of separation science, have proven to gain sufficient strength to solve new challenges caused by huge consumption of chemicals resulted from the expansion of industries and agriculture. These methods, along with the well-established spectroscopy- and chromatography-based strategies, can be implemented to monitor and follow the chemistry behind the interactions of the hazardous molecules with the developed extractive phases [1,2].

Due to the high annual consumption of foods and drinks, there is a great demand for monitoring their safety while the producers prefer to use pesticides and non–steroidal anti–inflammatory drugs to prevent any possible loss which might occur. In this contribution, the applicability of some extractive phases such as monolithic polymers, cryogel–based semi–interpenetrating polymer networks (Cryo–SIPNs), nature based biochars and zein, gradient derived base layers, graphene oxide–starch–based nanocomposites, organic-inorganic nanofiber composites and MOFs which have been successfully implemented to deal with the challenge of analyzing real life samples are discussed. Water, honey, fruiting vegetables, milks, and meats, are among the vital samples which have been monitored to evaluate their health safety [3-6].

Keywords: Microextraction, Real-life analyis, Food safety

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Metabolomics-based biomarker discovery from medicinal plants quality control toward human therapeutics improvement

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Most frequently, metabolomics is employed in a comparative mode, where metabolic profiles of samples (herbal extract to biofluids) set from a normal state (authenticated herbal extract to healthy biofluids) and a perturbed state (Non-Authenticated herbal extracts to non-healthy samples) are compared to find changes related to the unusual conditions. It as a holistic approach to the quality control has the potential to become an increasingly effective tool for clinical studies, in drug development, and in food and plant biotechnology. Here, we are addressing our recently research for the usage of chromatographic techniques, particularly in combination with mass spectrometry as the most standard techniques for biomarker findings. First, we explored the role of amino acids in vitiligo using targeted metabolomics. 22 amino acids were derivatized and precisely determined in 31 patients and 34 healthy individuals. Eight amino acids, including cysteine, arginine, lysine, ornithine, proline, glutamic acid, histidine, and glycine were observed deferentially. The ratios of cysteine, glutamic acid, and proline increased significantly in vitiligo patients, whereas arginine, lysine, ornithine, glycine, and histidine decreased significantly compared to healthy individuals [1]. Second, looking for metabolites are associated with varying rates of ovarian aging, GC-MS untargeted metabolomics by which showed 29 metabolites correlated with the annual decline rate of AMH, of which 14 metabolites increased significantly across its tertiles [2]. Third, growing concern for quality control and authentication of Saffron leads to set MALDI-TOF mass spectrometry as a fast and straightforward method for a comprehensive fingerprinting. This provides conformity between the MALDI-TOF-MS method as a relatively new method and the HPLC-DAD method as a common and reliable method [3]. Fourth, chicory and chicory distillate have long enjoyed a special status among Iranians. But despite the absence of any kind of essential oil in chicory distillate, it still has its therapeutic effects on its consumers. In addition, due to the low metabolic content of this product, one of the main concerns can be standardization and quality control of it. we tried to investigate the content of this herbal distillate with the help of extraction and chromatography techniques. Chromatographic based metabolomics introduced sesquiterpene lactone compounds especially 11,13-dihydro-8-deoxylactucin and magnolialide as chicory quality biomarkers [unpublished].

Keywords: metabolomics, biomarkers, quality control, medicinal plants, disease

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Futures of Medicinal Chemistry

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Pharmaceutical chemistry was presented as the fundamental branch of pharmaceutical science as soon as pharmacy became a profession in the middle of the 19th century. Pharmaceutical chemistry is required to provide a solid scientific foundation for obtaining targeted professional objectives. The evolution of medicinal chemistry as a multidisciplinary field incorporating a variety of basic and practical sciences and skills, including chemistry, biology, and clinical practices, while interacting with physics, mathematics, and many other branches of science over the years was a result of the paradigm shift of pharmacy from basic science to clinical profession. **[1-4]**

Over the past few decades, medicinal chemistry has advanced quickly as an exact and data-driven field. Technology progress has made it easier, personalized medical methods have made it more complex, and green medication development has raised questions about it.
We need to look at the history of medicinal chemistry, assess its current situation, and envision its future by utilizing the futures study method to meet the state and demands of the future in this field. The current study provides a summary of research that has been done in addition to professional judgments about medicinal chemistry's past, present, and future. We underlined the relationship between medicinal chemistry and paradigm-shifting chemistry in the future. The primary difficulties and achievements of medicinal chemistry, as well as the primary knowledge and scientific profile of future medicinal chemists, were highlighted.

Keywords: Medicinal chemistry, Futures study, Science Map, crosstalk between sciences

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From Science to Business: Advanced Polymer Technology

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Today, an important part of human life is dependent on polymer materials. This covers different macromolecules such as proteins, sugars, enzymes as well as synthetic polymers used in various industries. Nowadays, industries such as road and construction, electronic, automobile, textile and fibre, rubber and plastic, adhesive, paint, and coating are directly dependent on polymer. In recent years, development of advanced polymers, classified as the engineering polymers (type of polymers that are better substitute for metal and materials with high mechanical properties) and smart materials, has created a revolution in human life.

The present work aims to provide a comprehensive overview on novel applications of engineered and smart polymers based on our own experience. These applications have been successfully developed and commercialized as knowledge-based products by our pioneering team.

Various application including Artificial Muscles, Sensors, Smart windows, displays light emitting polymers, Self-healing polymers, Shape memory, Cochlear Insertion, Robots and Micro-Machines, smart membranes, Electronic Nose, Electronic Fabrics, drug delivery systems, Novel adhesives, polymer flooring and waterless cleaning system will be discussed considering to their basic science.

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Chromic behavior of Aryl and Heteroaryl Azo Quinoline Dyes

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Photophysical and photochemical behavior of the new synthesized aryl and heteroaryl azo quinoline dyes (Fig. 1) were studied in various media with different nature. Tautomerism, solvatochromism, halochromism, dichromism, and Ionochromism of the compounds were studied. It was established that in the media with basic nature, only one tautomeric form and corresponding anion exist, which the latter is the main species. According to the dichroism results, the dichroic ratios of the dyes are larger than one. This means that the absorption bands for these dyes may be considered as $\pi - \pi^*$.

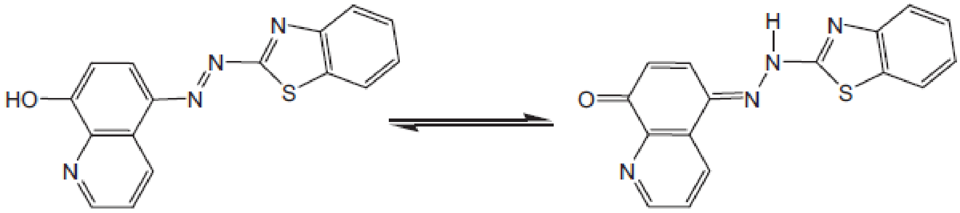

Fig. 1. Azo/hydrazone tautomerism

Application and Risk assessment of Synthesized Metal and Metal Oxide Nanoparticles as Bio Detection Devices

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Bio detectors or biosensors measure the analyte fast and accurate, directly in a sample or environment. They should continuous and reversible. In this field, nanomaterials suggestively increase the accuracy and sensitivity of the detection system. Bio detection devices have parts that are nano sensitive to materials (the part of the system used to attach to the analyte and specifically detect it is a biological element such as a nucleotides strand, antibody, enzyme, whole cell), responsive (various types of biosensors and biochips including an array of biosensors, emphasizing the nanostructures) and recorders (biological element as a diagnostic component or the electrode as a transducer). The use of nanoparticles (mainly metal and metal oxide) in these systems is commonly done to qualified the converter and the bioreceptor interaction. In this research, the synthesis, characterization and application of modified metal nanoparticles (CQD modified Au) and metal oxide (CQD modified ZnO) and the identification of proteins related to the liver system (lipase, amylase, AST and ALT) have been discussed. For this purpose, synthesized nanoparticles and their structure was determined. The synthesized nanoparticle properties were assayed using UV-Vis, dynamic light scattering, X-ray powder diffraction, circular dichroism and 1D gel electrophoresis. Also, the dangers of the synthesis and use of these materials for users were examined. Moreover, the level of interaction and their response to the mentioned enzymes was investigated. The results show that the spherical nanoparticles of gold and zinc oxide modified with carbon quantum dots, with dimensions below 20 nm, have a crystalline structure. Enzymes can be detected in amounts of at least 10 to 25 ppb by the this system directly.

Keywords: Biodetector, Liver enzyme, Au-CQD, ZnO-CQD.

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Ultrasound Synthesis of Nano Metal-Organic Frameworks and Their Potential Application in Catalysis, Gas sorption, and Controlled Drug Delivery Systems

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The relatively new class of porous material known as metal-organic framework (MOF) exhibits unique features such as high specific surface area, controlled porosity, and high chemical stability. Very recently, much attention has started to explore the synthesis and applications of nanoscale MOFs (nanoMOFs), the particles of which feature at least one dimension at the nanoscale. So far, nanoMOFs have shown particular advantages compared to their bulk materials with unique properties, such as accelerated adsorption/desorption kinetics and accessibility to the internal active sites for enhanced catalysis, suitable sizes for biomedical application, and their assembly to diverse nanostructured materials for energy and membrane separation-related applications, etc.

The pore size, shape and particle size of nano-MOFs are mostly related to the structure of organic ligands. In the process of preparing nano-MOFs such as solvothermal and hydrothermal syntheses, the formation of a regular framework material between metal ions and organic ligands requires external energy supply, like high temperature and high pressure. In addition, the way to change the energy supply form also enriches the preparation methods of nano-MOFs including sonochemical, microwave-assisted, mechanochemical, electrochemical synthesis.

As for the sonochemical method, ultrasonic waves are typically used to perform strong ultrasonic treatment on the liquid by adjusting the frequency of the sound wave so that the ions in the reaction liquid can obtain high energy, promoting the progress of the chemical reaction. In this process, by controlling the sound wave frequency, the reaction time can be greatly shortened and the uniformity of the formed product can be improved as well. In addition, this method is conducive to improving yield, operating safety, and reducing reaction costs. For example, using ultrasoundassisted methods, HKUST-1, MOF-5, and MIL-88A (Fe) were successfully synthesized with uniform crystal structures.

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Outlook of liquid fuel cells

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In recent years, the energy and environmental crises have been identified as the global challenges all over the world. To date, different kinds of energy storage and conversion technologies have been developed to deal with the problem. Among them, fuel cell technology has attracted more attention because of high power density, high reliability, flexibility in installation and operation, and reduced greenhouse gas emissions [1]. Direct liquid fuel cells (DLFCs) have recently attracted widespread attention, because liquid fuels such as methanol, ethanol, formate, and borohydride possess some advantages over hydrogen in terms of transportation, storage, and handling [2]. The main obstacle for the commercialization of DLFCs is the high cost of electrocatalysts, poor electrocatalytic activity and stability problems under the experimental environment. So, the challenge lies in the design of very effective and low-cost catalysts with high stability and reusability. A variety of metallic nanoparticles (NPs) that composed of noble and transition metals were reported for DLFCs. These NPs such as Ni@Pt, Ni@Pd, Ni@Ru, and Co-Pd showed higher electrocatalytic activity than pure noble metal electrocatalysts because of the synergistic effect between the two metals [3]. The addition of catalyst supports like multiwall carbon nanotubes (MWCNTs), graphene oxide (GO), reduced graphene oxide (rGO), nitrogen doped graphene oxides (NrGO), Ni foam, and conductive polymers that are mesoporous and conductive are frequently conducted to promote catalyst durability and charge transfer efficiency. Excellent catalyst support effectively disperses metal nanoparticles and reduces the noble metals consuming and enhancing the catalytic activity [4]. Therefore, it can be said that the research perspective is focused on the production of inexpensive electrocatalysts with high electrocatalytic performance toward the oxidation of fuel used in fuel cells using nanotechnology.

Keywords: Direct liquid fuel cell, Electrocatalyst, Catalyst support, Metallic nanoparticles.

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Miniaturized Spectrometers Powered by Chemometrics for High-throughput Food Authenticity

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Nowadays, miniaturized spectrometers have been emerged as new technologies with many different applications [1]. Owing to the important role of miniaturized near-infrared (NIR) spectrometers, this technology and its applicability is explored for food authentication [2]. Unlike a rather uniform design of a mature benchtop FT-NIR spectrometer, miniaturized instruments employ diverse technological solutions, which have an impact on their operational characteristics. Continuous progress leads to new instruments appearing on the market. The current focus in analytical NIR spectroscopy is on the evaluation of the devices and associated methods, and to systematic characterization of their performance profiles. The technologies are not specifically aimed at certain commodities or product features, and no single technology can be applied for authentication of all commodities. Nevertheless, many useful applications have been developed for many food commodities [3].

The trade-off for using these devices is that the spectral region and resolution are limited compared to benchtop technologies. Additionally, scattering effects and instrumental and ambient noise make robust chemometric and machine learning methods crucial to extract the relevant information from the spectra.

The focus of the present contribution is summarizing miniaturised technologies, commercially available devices, chemometric data analysis methods and device applications for food authentication or measurement of features that could potentially be used for authentication [3]. We focus on the handheld technologies and their generic characteristics: (1) technology types available, (2) their design and mode of operation, and (3) chemometric data handling. Subsequently, two examples of recent applications are reviewed with details [4, 5]. It is important to note that the use of these applications in practice is still in its infancy. This is largely because for each single application, new spectral databases need to be built and maintained. Therefore, apart from developing applications, a focus on sharing and re-use of data and calibration transfers is pivotal to remove this bottleneck and to increase the implementation of these technologies.

Keywords: Handheld spectrometer, Chemometrics, Food authenticity.

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Microextraction on a Screw

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In the recent three decades, researchers have focused on miniaturization and automation of the sample preparation methods [1]. These systems can decrease the extraction time, sample volume, and solvent consumption to reduce costs and achieve a green analytical procedure. Numerous miniaturized methods such as microextraction by packed sorbent (MEPS), in-tube solid-phase microextraction (IT-SPME), and needle trap microextraction (NTME) have been developed [2]. Although the MEPS has several advantages, it suffers from some shortcomings like being easily clogged by small particles existing in sample solutions, improper for viscous or highly concentrated samples, and undesirable for sample volumes larger than 500 μL. On the other hand, NTME can be used for liquid and gaseous samples, but is sufficient for gaseous samples. The difficulties in coating and characterizing the inner surface of the tube, high back pressures and possibility of tube clogging by suspended particles in the sample solutions are some shortcomings of the IT-SPME.

Efforts are made to eliminate some of these disadvantages by presenting new SPME methods. In research experiments, we attempted to solve some problems of the mentioned methods by introducing microextraction on a screw (MES), which was a miniaturized form of solid phase-based extraction techniques without any backpressure or column clog [3,4]. In this technique, the pass length of the microchannel is too high and thus its surface covered with suitable coatings provides high surface area, enhanced extraction efficiency and sensitivity, and shorter extraction time. Different chemical, electrochemical, electrospinning, electrophoretic deposition, etc., can be used for deposition of various coatings on the screw. Also, characterization of the coatings can be performed using different instruments.

In this speech, MES will be introduced. Different methods that can be applied for coating various polymers and composites on the screw will be discussed. Some examples on application of MES for extraction, identification and determination of pollutants in environmental samples and biomarkers in biological samples will be presented. Possibility of automation of MES will be investigated. Moreover, its potentials and limitations in comparison with other microextraction methods and future view will be evaluated.

Keywords: Microextraction, Screw; Pollutants, Preconcentration; Automation

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Sparse methods in chemometrics with application in metabolomics investigations

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“Sparseness” is a property of matrices in numerical analysis and scientific computing when the matrix has many zeros and is less crowded while the information is preserved. Different signals in the chemistry realm are “sparse” rather than “continuum.” Examples of sparse signals in chemistry are the mass and ion mobility spectra, NMR spectra of single molecules, 2D-NMR of complicated mixtures, gas chromatograms (GC), electropherogram of charged molecules in electrophoresis, and signals related to GC×GC and LC×LC. Along with creating sparse datasets in different fields of science, numerical methods for processing such datasets were developed and evolved in recent years. Such methods mainly use L1- norm constraint for confining the length of vectors when processing data matrices. This eventually led to less crowded vectors that would be ideal for visualization and interpretation. In the present contribution, we review the concept of “sparsity” in chemical data analysis. Different measures for the quantification of “sparseness” are reviewed. The sparse versions of different chemometric methods are presented, and the advantages and limitations of methods are discussed. We will discuss how “sparseness” helps chemists with pattern recognition, multivariate calibration, classification, and clustering. Different applications of sparse methods for processing GC-MS, excitation-emission (EEM) fluorescence, FT-IR, and UV-Vis data are discussed [1-4]. We discuss the enormous potential use of sparse methods for solving the challenges in the metabolomics realm for biomarker discovery, noise removal, and improving the accuracy of predictions. Finally, we compare the use of such methods in chemistry and other fields of science. We conclude that while not well-recognized in chemistry, “sparse methods” are currently well-known and used in different areas of science. This emphasizes introducing such methods in the chemometrics community more than before for handling large datasets and improving the interpretation of complicated models.

Keywords: chemometrics, Sparseness, sparse methods

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Sustainable catalytic and photocatalytic H_2 production

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H_2, as a fuel, could be the last resort for the production of sustainable energy sources. Nowadays, many efforts have been made to investigate catalytic and photocatalytic approaches to develop sustainable and economical processes for H_2 production. The utilization of nanomaterial architecture can be a rational solution for sustainable and efficient H_2 production in all these H_2 production approaches. Nanoarchitecture of materials can be obtained either by top-down or bottom-up synthesis approaches, such as templated materials synthesis. Chemically, nanomaterials for H_2 production can be nitrides, oxides, sulfides, carbides, and carbon-based. A fraction of these nanomaterials is naturally abundant, while others can be developed from abundant nanomaterials and precursors. In theory and sometimes in the experimental analysis, Nanostructures should possess a high surface area. However, they are usually unfavorably less active or inactive in the natural form. For example, in the case of layered materials, their interlayer nano space and surfaces are inaccessible to catalytic reactions. As a result, these layered nanomaterials require additional post-modifications (e.g., exfoliation or functionalization) to envoke their great physio-chemical potentials in the photocatalytic/electrocatalytic/catalytic H_2 production. Therefore, breakthroughs in competitive catalytic H_2 production mandates developing new layered nanomaterials and frameworks that supersede traditional layered nanomaterials' boundaries.

Colloidal lithography: From surface modifications to applications

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Engineering the surfaces and controlling their properties in nano/micro scales attracted a lot of attention due to their wide applications in various fields. Different studies have been carried out to find easy and cost-effective methods to control the surface properties. Among these, colloidal lithography is a clever, straightforward, and economic method to fabricate different structures using nano/micro sacrificial spheres which are usually made of Polymethylmethacrylate (PMMA), (Polystyrene) PS, and SiO_2 [1]. Having used the proposed method, it is possible to fabricate inverse opal photonic crystals (three-dimensional ordered porous structures) and control their pore size according to the application. Also, different metal nanoparticles arrays can be fabricated, such as nano-pyramid, nano-discs, nano-crescent arrays, etc. Having unique optical properties such as photonic bandgap (PBG) and localized surface plasmon resonance (LSPR), the fabricated photonic crystals and plasmonic structures can be used in different applications that need trapping and manipulation of the light. For example, the observed PBG in inverse opal photonic crystals and the resonance frequency of plasmonic structures are highly dependent on the refractive index of the media that fill the pore or surround the metal nanoparticles, respectively. Thus, the introduced structures can be applied as highly sensitive chemical/biosensors [2]. Furthermore, the fabricated structures can provide increased light trapping, which is essential for some other applications such as solar cells and photocatalysts [3]. Also, surface-enhanced Raman scattering is another field in which the introduced structure can be beneficial.

In this presentation, the colloidal lithography method and some of its applications are going to be discussed in detail.

Keywords: Colloidal Lithography, Photonic Crystals, Localized Surface Plasmon Resonances, Photonic Band Gap.

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Characterizing DNA Dynamics with a Smart Fluorescent Nucleobase Rotor

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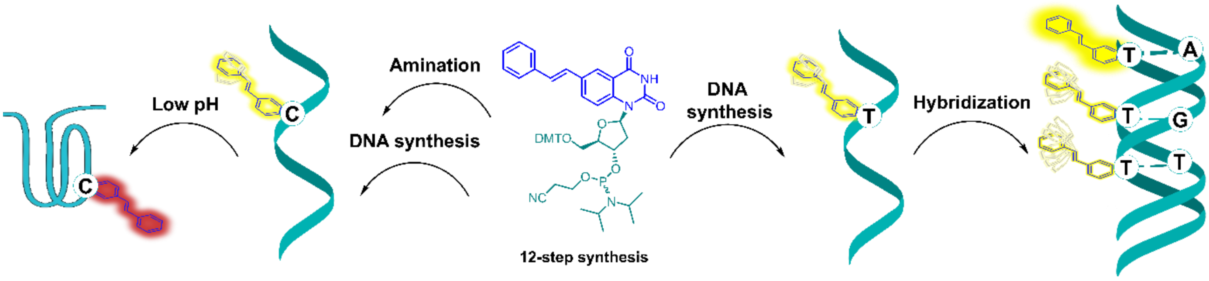
Observing the nature and understanding the function of DNA require "tools" with high sensitivity and precise positioning. These tools are synthetic fluorescent nucleobase analogs that mimic nucleobases [1]. Here, we introduce highly fluorescent base mimics equipped with a robotic arm. These microenvironment-sensitive probes have provided novel information about local dynamics of DNA bases and global dynamics of diverse DNA secondary structures.

To probe local dynamics, a molecular rotor, *trans*-stilbene, was incorporated into thymidine [2]. Followed by a 12-step synthesis, the resulting probe (^{ts}T), which is the brightest and most mismatch-sensitive fluorescent base analog reported to date, acted like a smart mechanical arm, rotating and sensing the microenvironment around it. The amount of rotation (monitored by fluorescence signal) depends on the mechanical motions in DNA. Thus ^{ts}T could discriminate between single- *vs* double-stranded DNA and sense single-nucleotide polymorphism by reporting single mismatched, well-matched, and damaged nucleobases. Moreover, by means of DNA-mediated charge and energy transfer, it acted as a molecular ruler and determined the distance between specitfic bases with Angstrom resolution.

In the context of global dynamics, inspired by the high sensitivity of ^{ts}T towards DNA dynamics, we synthesized its cytosine analog, ^{ts}C, to probe pH-dependent folding of C-rich DNA into i-motif structures. In addition, we developed the first reversible switching of different DNA secondary structures (A, B and Z) by coordination of Hg^{II} to TT mismatches [3].

Keywords: Fluorescent DNA, Modified nucleobases, Molecular rotor, DNA dynamics



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An Optimized Method to Estimate the Glutaminase Activity in Biological Samples

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Spectrophotometric methods have been used to estimate glutaminase activity, using diverse reagents to form colored complexes that absorb light within the visible spectrum. The current study describes a simple, precise, and accurate protocol for measuring the activity of glutaminase, is an important enzyme in the glutamine hydrolysis and is also responsible for the modification of glutamine metabolism.

The current protocol assesses glutaminase activity by incubating glutaminase samples at 37°C for 30 min with suitable concentrations of glutamine dissolved in a buffer (pH 8.6). The enzymatic reaction contains suitable activity of glutamate oxidase, which acts to convert glutamate to hydrogen peroxide and 2-oxoglutarate. After the incubation period, a working solution that contained vanadate (V) and pyridine-2,6-dicarboxylic acid was added to stop the enzymatic reaction.

The reaction between undissociated hydrogen peroxide and the added reagent forms a stable orange-colored chelate complex known as oxo-peroxo-pyridine-2,6-dicarboxylato-vanadate (OPDV) that demonstrates maximum absorbance at 435nm. To optimize the formation of the method (the OPDV-Glutaminase assay), we applied the Box-Behnken design (BBD) by utilizing the response surface methodology (RSM) as an index of precision of the assay. This novel method was validated against a Bland-Altman plot analysis of catalase activity using the Nessler method in matched samples. The comparison between the two methods resulted in a correlation coefficient equal to 0.99, demonstrating that the new method is just as effective as the reference method.

Keywords: Box-Behnken design; glutaminase activity; pyridine-2,6-dicarboxylic acid; response surface methodology; spectrophotometry; vanadate (V).

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Bioactive glass coatings for bone tissue engineering

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Metallic prostheses are widely used to treat joint and skeletal injuries and disease. However, metal alloy implants can sometimes fail due to complications of fibrous encapsulation and poor stress transfer between the bone and the implant. Bioactive glass (BG) coatings may promote the formation of a strong bond with living bone tissue thus decreasing the likelihood of fibrous encapsulation and have the added benefit that their dissolution ions stimulate cell activity [1,2]. Strontium (Sr) ranelate, a drug used to treat and prevent osteoporosis, works via the action of Sr ions which stimulate the formation of new bone and prevent osteoclast-mediated resorption [3]. We have previously shown that Sr-substituted BGs promote osteoblast activity *in vitro* [4] and explored the effect of altering phosphate content on the material structure of soda-lime-phosphosilicate glasses [5]. The effect of increasing phosphate content in Sr-substituted BG on cultured osteoblasts, however, remains unexplored. Here, we created Sr-substituted BG coatings with a range of phosphate contents and thermal expansion coefficients that matched that of Ti alloy, producing materials that combine the bone remodelling benefits of Sr and BG with phosphate to mediate pH changes which can affect cell viability. In the study presented here we report the characterization of these multicomponent BG coatings in terms of their bioactivity and interaction with cells.

Keywords: Metallic prostheses, Bone, Tissue engineering

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Analytical detection methods for food frauds

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Fraud in food commodities is very common around the world and today occurs at different places of the supply chain: the demand for rapid and confirmatory analytical methods has increased in recent years. Recently, consumers have increased attention on the safety, authenticity and quality of food commodities [1], and the development of reliable methods to detect fraud could better preserve the quality of production, with an advantage for the industry and the final consumer, who would have more confidence in the quality and safety of the product. Current governance of food supply chains, through certifications, inspections and audit controls, has historically been indeed developed, with a focus on food safety. However, criminal actions not only involve the adulteration of raw materials or finished products, but also the fraudulent declaration of the geographical origin of commodities. However, sometimes it seems that the new analytical methods developed and presented in the peer-reviewed journals are not applied or even not known by the industrial quality control laboratories. An effective analytical testing strategy is a key element in the fight against food fraud and one of the major components of a Food Fraud Vulnerability Mitigation Plan. Its purpose is not just to detect a potential fraud event but also to act as a deterrent and contribute to its prevention [2]. A fraudster is likely to think twice about supplying suspicious product to a company known to operate a comprehensive testing system. Indeed, the same notion could apply to a country that has stringent and regularly enforced regulations in place when compared to one with a lax regulatory system. Chromatographic techniques are widely used in food authentication as a means of separating and quantifying chemically similar constituents of a foodstuff. The components areseparated between two phases, a stationary and a mobile phase, the separation resulting from the different strengths of adsorption of the different molecules between the two phases. Techniques used in food analysis include gas chromatography (GC) and liquid chromatography (LC) depending on the state—gas or liquid—of the mobile phase. Highperformance or high-pressure LC (HPLC) is the most commonly used LC technique, in which the solvent of the mobile phase is pumped through the column. Other variants of chromatography include thin-layer chromatography that uses a solid, planar surface and a liquid mobile phase, and capillary electrophoresis involving electrokinetic separation.

Keywords: Analytical detection methods, Food frauds, Chromatographic techniqueshnique

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Low Temperature and Economic Method of Carbon Nanotubes Synthesis

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Flame fragment deposition (FFD) method was used to synthesize carbon nanotubes (CNTs) from Iraqi liquefied petroleum gas (LPG), as a carbon source. It was found that 30 minutes is sufficient to prepare the carbon nanotubes in nine sample collection sites at the top of the locally manufactured device and under the temperature in the collection site up to 150 ^{o}C. This technology does not need to use electrical energy since it depends only on burning the gas used as a carbon source after mixing it with pure nitrogen gas to control the combustion process.

Purification of synthesized CNTs was accomplished by calcination at 350 ℃ for 2 hours, oxidation with hydrogen peroxide H_2O_2, and treatment with acetone. In this method, an ultrasonic water bath was used to disperse for one hour 100 mg of synthesized CNTs in 50 mL of H_2O_2. The mixture was chilled for 24 hours at 4 ℃ before bringing it to room temperature and was gradually heated to 50 ℃ until all hydrogen peroxides were extracted. After that, the solid was rinsed with deionized water and dried for 6 hours at 80 ℃. The CNTs were then dispersed in 15 mL of acetone, but before they were treated with acetone, they have to be sonicated for 15 minutes. After 15 minutes, the obtained suspension was centrifuged. Then the obtained solid was dried overnight at 100^{0}C , characterized and finally compared with standard CNTs (MWCNTs (95%), Sigma ,Aldrich) by using X-ray diffraction (XRD), thermogravimetric analysis (TGA), Raman spectroscopy, scanning electron spectroscopy (SEM), Energy Dispersive X-ray Spectroscopy (EDS), and transmission electron microscopy (TEM). After applying the suitable experimental circumstances, the obtained characterization results confirm the synthesis of multi-wall carbon nanotubes (MWCNTs) with portion from few wall carbon nanotubes (FWCNTs). The average diameter of the synthesized Carbon nanotubes appeared to range from 31.26 to 78.00 nm with a purity of about 70%.

Keywords: Carbon nanotubes, liquefied petroleum gas, flame fragment deposition

Non-metal doped chemiresistive oxide thin film- based ethanol sensor

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Indium oxide (In_2O_3) and Zinc oxide (ZnO), which are n-type SMOs, have been widely investigated for their suitability in developing efficient ethanol sensors. Out of various strategies explored for improving gas sensing performance of semiconducting metal oxides (SMOs) incorporation of suitable dopants have drawn significant interest. Typically, various metal-based dopants have been considered for modifying the receptor function of the SMOs, whereas non-metallic dopants have drawn only limited attention. In this talk the impact of nitrogen incorporation on the ethanol sensing properties of In_2O_3 and ZnO thin films shall be discussed. Synthesis of nitrogen doped In_2O_3 and ZnO thin films via wet chemical route using urea as the nitrogen source leads to interstitial doping of In_2O_3 while substitutional doping is observed in case of ZnO thin films. While N-doped In_2O_3 offers fast response and improved resilience against humidity, N-doped ZnO offers siginificantly improved selectivity towards ethanol in comparison to various other volatile organic compounds. Microscopic mechanism of the improved ethanol sensing properties of the individual nitrogen doped oxides shall be discussed in light of chemical sensitization and microstructure modification. It shall be demonstrated that combining the benefits of fast sensing and superior selectivity offered by N-In_2O_3 and N-ZnO, nitrogen doped In_2O_3-ZnO nano-composite mesoporous thin films hold the potential of realizing highly sensitive and selective ethanol sensor [1-4].

Keywords: metal oxide thin films, nitrogen doping, chemiresistive gas sensing, VOC sensing

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Thermal decomposition of cyclopentadienyl compounds of Mn, Fe, Co immobilized on oxide surfaces

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Supported catalysts with metal particles smaller than 10 nm in size can be obtained by thermal decomposition of organometallic compounds immobilized on porous substrates. Development of the chemistry of organometallic compounds in recent years has made it possible to develop methods for the synthesis of various homo- and heterometallic clusters, which can be used to obtain catalysts containing ultrafine particles of transition metals on substrates of various organic and inorganic nature [1]. This paper presents the results of a study of the thermal decomposition of mono- and binuclear cyclopentadienyl compounds of 3d-metals (Mn, Fe, Co) deposited on oxide (aluminum oxide, silicon dioxide, aluminosilicates) substrates. The main goal of this work was to develop new approaches to the preparation of catalysts containing nanosized particles of 3d metals on oxide supports and to develop methods for controlling their catalytic properties in the hydrogenation of carbon dioxide to C_2,C_3 olefins. SEM JSM-6610LV, JEOL scanning electron microscope combined with an element analyzer (SEM/EDS) is used to control the surface morphology and distribution of active elements in the substrate structure. The phase analysis of the synthesized samples was studied using XRD 3500 TD diffractometer, China and Phaser D2, Germany, with CuK_α radiation. The textural characteristics (the specific surface area and total pore volume) of the samples was determined by low-temperature adsorption of nitrogen using Belsorp Mini II, BEL Japan Inc. instrumtnts device. The infrared spectra of the synthesized samples were recorded on an Alfa Fourier spectrometer, Bruker, Germany, and the EPR spectra - on an EMRmicro spectrometer, Bruker, Germany. Thermal analysis was carried out on a STA 449 C Jupiter setup (NETZSCH, Germany) in a nitrogen flow in the temperature range of 25–700°C at a temperature rise rate of 10°C/min, as well as in an isothermal mode at 120, 200, 400°C for 3 hours at each temperature. Test portions 10 mg, in the case of the original compound, and 25-30 mg, in the case of applied samples. The transformations occurring upon heating of the samples were judged from thermogravimetric (TG) and differential (DTG, DTA) curves.

Keywords: Thermal decomposition, cyclopentadienyl compounds of Mn, Fe, Co, oxides

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NMR characterization, conformational energy and nonlinear optical property calculations of 1,3-bis(2,4-dimethoxyphenyl) imidazolidine-2-thione molecule

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Thioureas and their cyclic derivatives are known to exhibit a broad spectrum of biological activities such as antibacterial and antifungal properties and regulating activities for plant protection in agriculture [1-3]. They also have a wide variety of uses in the mining industry. Therefore, the interest in these compounds continues to increase [4-5].Conformational analysis of the 1,3-bis(2,4-dimethoxyphenyl) imidazolidine-2-thione molecule was performed by calculating the molecule's potential energy surface (PES) as a function of the θ[C4-C3-N1-C2] and φ[C13-C12-N2-C11] dihedral angles. In potential energy surface calculation, density functional DFT/B3LYP methods and the 6-31G basis set were used and and θ[C4-C3-N1-C2] and φ[C13-C12-N2-C11] torsion angles were scanned from -180° to 180° at intervnals of 15°. By performing geometry optimization calculations of the lowest energy conformations on the PES, the ground state geometry of the molecule was determined. Using the optimized structure, the geometry of the molecule, the highest occupied molecular orbital (HOMO), the lowest unoccupied molecular orbitals (LUMO), harmonic vibration waves, linear optical properties (polarizability) and nonlinear optical properties (NLO) (hyperpolarizability) values has been examined at both *ab initio* Hartree Fock (HF) and DFT/B3LYP methods using the 6-311++G(d,p) basis set. The energy gap ($\Delta E = E_{LUMO}-E_{HOMO}$) of the molecule were determined using E_{HOMO} and E_{LUMO} energy values of the molecule. The total energy distribution (TED) of the studied molecule was calculated in VEDA4f program. Also, the ^{1}H as well as ^{13}C NMR chemical shifts values of studied compound in the ground state have determined by both methods employing different basis sets such as the 6-31G, 6-31+G, 6-31+G(d), 6-31++G(d,p), 6-311++G(d,p) and 6-31+G(2d,p) using Gauge independent atomic orbital (GIAO) technique. The structural parameters of the 1,3-bis(2,4-dimethoxyphenyl) imidazolidine-2-thione molecule calculated in both methods were compared with the previous experimental data on the molecule in literature [3]. The approximate geometry of the molecule in three dimensions was drawn in the GaussView 5.0 molecular imaging program, and all theoretical calculations were used with the Gaussian 09W package program.

Keywords:conformational energy, NMR characterization, Dipole moment, Polarizability, Hyperpolarizability.n

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Association of *ATP1A2*, rs373796693 Gene Variant with Preeclamptic Patients in Placental Tissue

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Preeclamptic is a human pregnancy-specific disorder defined by the appearance of proteinuria-related hypertension after the twenty weeks of gestation in a previously normotensive woman and entirely cured by the sixth postpartum week. It is the main cause of morbidity and mortality during pregnancy. It is a multisystem sickness, but its etiology is unknown. Preeclamptic has been associated with system anomalies, such as ion transport deficits in neonatal, maternal, and placental cell lines.

This is the first study in Iraq, the objective is to evaluate the relation of rs373796693 variant with preeclamptic and study the sequence of gene alpha 2 to obtain genotyping, by conducting a case-control association study. This study was consisting of 90 cases that were divided into two groups, 50 normal pregnancies (control), and 40 preeclamptic (patients). For genotyping, we designed and optimized a ‘polymerase chain reaction- single strand conformation polymorphism (PCR-SSCP) method with the presence of internal splicing. While the sequence employed by sending the PCR products of ATP1A2 gene to macrogen company in Korea for performed DNA sequencing. The results were analyzed using the statistical package for social sciences (SPSS®) software version 28.0. A p-value of ≤ 0.05 was considered significant.

The results of the genetic test showed that there was no significant allelic or genotypic association recorded between patient and control groups for the gene studied. While the sequence data for gene *ATP1A2* (rs373796693) showed TCCT deletion in the investigated samples.

Keywords: Preeclamptic, ATP1A2, , rs373796693, Sequence, PCR-SSCP.

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Simple and Precise Protocol to Assess Trypsin Activity in Biological Samples

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Trypsin is a digestive enzyme that assists in the digestion of food. The small intestine contains trypsin. Fungus, plants, and bacteria may all be used to produce it. However, it is mainly manufactured for commercial uses from livestock pancreas. Serum trypsin determination seems to be a specific diagnostic for acute pancreatitis. In clinical diagnostics and drug research, it's critical to develop innovative detection techniques for trypsin activity assays.

A simple spectrophotometric procedure for trypsin, a protease generated in the pancreas, was developed in this study. Trypsin could preferentially cleave cytochrome c, a fundamental component of trypsin, into heme–peptide fragment. The resulting peroxidase-like activity catalyzes the oxidation of 3,3′,5,5′-tetramethylbenzidine (TMB) in the presence of hydrogen peroxide. This produces a blue-colored product with a maximum absorption wavelength of 620-525 nm. We used the Box-Behnken design (BBD) with response surface methodology (RSM) as an index of assay precision to optimize the synthesis of a blue colored product. In matched samples, this new method was compared to a Bland-Altman plot study of trypsin activity using the standard method.

With a detection limit of 0.5 IU/L, the procedure was able to measure trypsin in the range of 2–250 IU/L. For the assessment of 100 IU/L trypsin solution, the protocol exhibited improved accuracy, with a relative standard deviation of 1.4 percent. This protocol was used to investigate the inhibitor of trypsin, and the IC50 values for benzamidine hydrochloride were determined to be 2.2 g/mL, suggesting its potential use in drug development and disease treatment. Our research showed a simple, simple, low-cost, sensitive, and selective protocol for assessing trypsin enzyme that may be utilized to investigate its clinical value and pharmacological interference.

Keywords: Box-Behnken design; trypsin activity; response surface methodology; spectrophotometry; tetramethylbenzidine.

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Approaches Towards First Total Synthesis of Onosmone and Analogues

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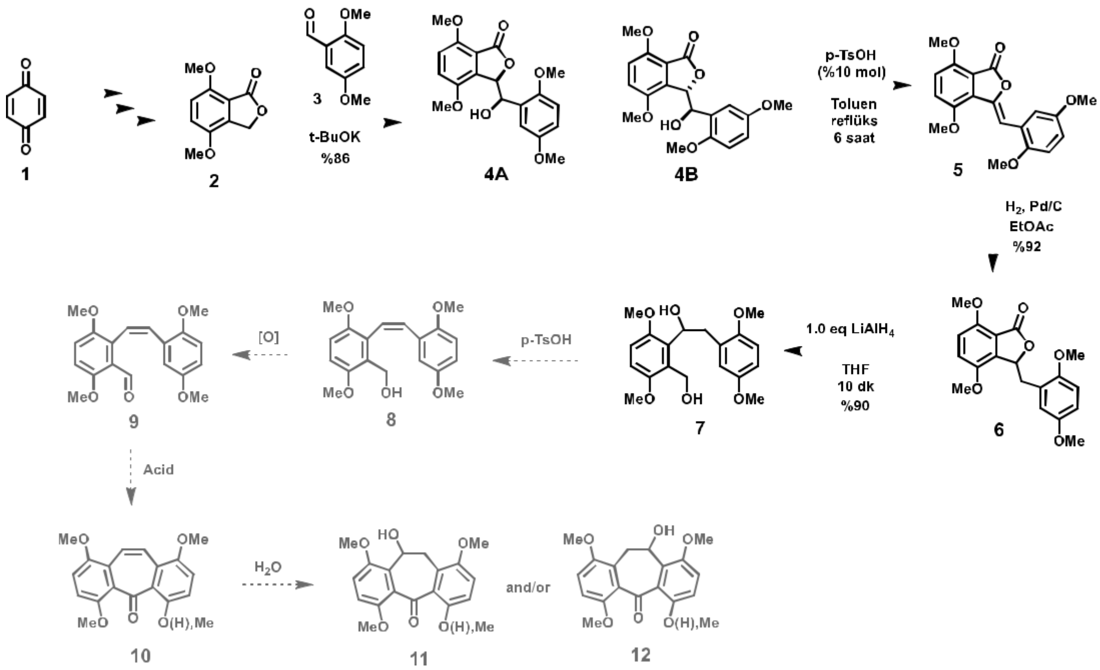
Onosma plant is used as tonic, demulcent, diuretic and refrigerant. Onosmone is isolated from *Onosma Limutaneum* plant in trace amounts and is a dibenzosuberone derived compound [1]. The total synthesis of this molecule has not been done yet. In this study, the first total synthesis of onosmon is aimed. For this purpose, lactone **2** was synthesized from *p*-benzoquinone **1** according to the methods in the literature[2-4]. So far, the synthesis steps from lactone **2** to diol **7** have been carried out successfully (Scheme1). Our work continues intensively for the synthesis of **8-12** compounds.



Scheme 1. Total Synthesis of Onosmone and Analogues

Keywords: Onosmone, *Onosma Limutaneum*, Dibenzosuberone, Natural product synthesis, Total synthesis

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Magnetic solid phase extraction of Ni(II) with Fe_3O_4@ Diaion HP-2MG particles as the adsorbents prior to flame atomic absorption spectrometry

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Heavy metal pollution increasing due to human activities and especially the problems experienced in trace level detection are increasing gradually. While heavy metals negatively affect the soil, food and water ecosystem, they also accumulate in the body through the air, skin or digestive system[1]. Nickel is an essential element for human metabolism, but high nickel intake is toxic. Therefore, the analysis of Ni(II) especially in complex matrices is important. Accelerating technological developments, even if analytical devices that can perform heavy metal analysis such as FAAS, ICP-MS and X-Ray fluorescence spectroscopy have been developed, they often do not allow analysis later because they are less sensitive than the detector can detect in the analysis of trace species. For this purpose, separation-enrichment methods are needed. Magnetic solid phase extraction method has been developed due to its high enrichment factor, low cost, low reagent consumption, ease of automation and environmental friendly features[2].

In this study, magnetic Diaion HP-2MG resin was synthesized for rapid extraction, enrichment and determination of trace amounts of Ni(II) ions. Diaion HP-2MG polymer with polymethacrylate matrix is relatively hydrophilic. Among the parameters affecting the Ni(II) extraction efficiency, pH, resin amount, matrix effect, sample volume, eluent type and volume were optimized and analyzes were performed in the FAAS device after pre-concentration[3]. After optimizing the analytical parameters such as LOD, LOQ, PF and reusability, the accuracy of the developed method was applied to natural water and food samples by adding-recovering increasing Ni(II) and validation was carried out with water and food certified reference material analyzes with known Ni(II) content.

Keywords: Nickel, Diaion HP-2MG, magnetic solid phase microextraction, separation-preconcentration, FAAS

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Deep eutectic solvent-based liquid phase microextraction Sudan IV prior to UV-Vis spectrophotometric determination

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Sudan dyes are a group of azo dyes that have significant toxic effects on human organs due to their azoic structure and aromatic rings. Sudan dyes are prohibited for use because they are classified as Group 3 carcinogens by the International Agency for Research on Cancer. Therefore, effective and reliable methods are of great importance for the rapid detection of Sudan dyes in the samples [1]. In recent years, green analytical chemistry has been one of the key steps in developing extraction and sample preparation methods. The main goals of green analytical chemistry are to reduce the use of expensive and hazardous chemicals, to minimize time and energy consumption and to increase safety in the laboratory. In this context, deep eutectic solvents (DESs) are introduced as a new generation solvents that has all the qualities as mention above. DESs can be easily prepared by simply mixing two or more compounds classified as hydrogen bond donors and acceptors to obtain a eutectic mixture using basic laboratory equipment. Deep eutectic solvents (DESs) appear to be successfully used as a new generation solvent system that is effective, safe, inexpensive, non-toxic, biodegradable and biocompatible for important analytical and other chemical applications [2,3].

In this study, a deep eutectic solvent was prepared and used as an extraction solvent for the deep eutectic solvent-based liquid phase microextraction, separation and preconcentration of Sudan IV. After the preconcentration step; accurate and precise determination of Sudan IV analyte in the extraction phase was performed using UV-Vis spectrophotometer. Important analytical factors that affect the extraction efficiency of DESs such as pH of the solution, mole ratio of DES components, DES volume and sample volume were determıned and optimized. Quantitative recovery values of Sudan IV were determined at pH 4.0. The validity of the developed method has been proven by applying addition-recovery tests to environmental water and food samples under optimum conditions.

Keywords: Sudan IV, Deep Eutectic Solvent, UV-Vis spectrophotometer

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Electrocatalytic Hydrogen Production with a Molecular Co(III) Complex

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Water splitting is one of the most effective ways to produce high-purity hydrogen and oxygen [1]. The most significant progress has been made in designing of the molecular catalysts for hydrogen production using earth-abundant transition metals as the catalyst. Cobalt complexes with polypyridyl ligands have received great interest because of their stability and electroactivity at both metal and ligand centers [2]. In this context, a Co(III) complex with the formula of $[CoL(X)(OH_2)]$, where L = N,N bis (pyridine-2-carboxamido) benzene dianion and X= N_3^-, has been synthesised and characterised by the CHN elemental analysis, IR, UV-Vis and X-ray powder diffraction techniques. The crystal structure determination of complex showed a dianionic ligand L providing N4 set is located in equatorial plane, and the two H_2O and N_3^- ligands occupy the two axial positions, leading to a distorted octahedral geometry around Co(III) center [3]. The electrocatalytic activity of this complex in water splitting reactions was investigated.. The results exhibit good electrocatalytic activity in hydrogen evolution reaction with a high TOF at neutral pH. Furthermore DFT computations provide further insights into the mechanisms, and explain the activities of the complex in H_2 production reaction. Our approach to synthesise effective and stable molecular catalyst with earth-abundant transition metal ions offers a simple way to design and fabricate molecular electrocatalysts for HER process.

Keywords: Water Splitting, Carboxamide, Co(III) Complexes.

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Solvatochoromic explains strong emission wavelengths of Carbon Dots

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Carbon Dots (C-dots) are a novel class of carbon-based nanoparticles discovered in 2004[1]. C-dots synthesis from bio-sourced has displayed excellent potential and ease of synthesis for applications in bio-imaging, printing inks, photocatalysis, biosensors, drug delivery and, light-emitting diodes (LED) owing to their remarkable properties [2]. The synthesized C-dots exhibit excellent solubility in a series of organic solvents and we have extensively investigated the C-dots + solvent interactions to understand the solvatochromic behavior of C-dots, which has hardly been studied. In this study, the photoluminescence (PL) emission spectra of C-dots indicate the blue-green color under UV light; various mechanisms have been proposed in relation to the color of C-dots releases. One of these mechanisms shows that surface heteroatoms such as nitrogen and oxygen from surface energy levels between HOMO and LUMO, leading to the propagation of long wavelengths from these surfaces [3]. In addition, we indicate exploring C-dots + solvent interactions to elucidate the nature of their tunable fluorescence. The photoluminescence quantum yield (QY) of the aqueous dispersion of C-dots was calculated to be 23.5%. Which increases as the lipophilic character of the solvent promote. The quantum yield of synthesized C-dots was studied in the range of protic and aprotic solvents. If surface states are complicated in the emission mechanism, the interactions of C-dots with the surrounding solvent should be vital in causal their optical properties. The result shows the fluorescence of C-dots is a combination of an excited state of the -COOH group and an excitation wavelength-dependent fluorescence from the polar groups such as the -OH moiety in the C-dots. Additionally, solvatochromic provided a semi-quantitative method to analyze the C-dot behaviors in connection with its surface localized electronic transitions in terms of non-specific and specific solute-solvent mutual interactions. The results of C-dots + solvents and photoluminescence influence will be useful for future application of drug delivery, cell imaging, biosensors and, another medical study.

Keywords: solvatochromic, Carbon dots, photoluminescence

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Computational chemistry as a powerful tool in investigating the optical properties of organic compounds

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Molecular Science and Engineering Research Group (MSERG)

Non-linear optics is the study of interaction of electromagnetic radiations with matter, resulting new electromagnetic radiations with change frequency, phase or other physical properties. Atomic, molecular, solid-state physics, surface interface science, material science, medicine, chemical dynamics and biophysics are diverse disciplines in which nonlinear optical materials have been used. In recent years, due to advances in laser technology non-linear optics become a field of major study. Acoustic-optic conversions, optical computing, optical signal processing, data storage, super-resolution lithography, and microscopy to higher harmonic and terahertz (THz) generation and optoelectronics are important technical areas in which nonlinear optical materials are used.

The development of non-linear optical (NLO) material with better response is very important. Some family of organic compounds was considered with a large non-linear optical property such as hetroaromatics, charge-transfer complexes and Schiff bases. Organic materials have low energy transitions in the UV–vis region which enhanced the NLO efficiency, but result in a trade off between nonlinear efficiency and optical transparency and they may have low thermal stability. Inorganic crystals have several drawbacks: high quality single crystals are difficult to grow, are expensive, and are not easy to incorporate into electronic devices.

The practical measurement of β is challenging, but this can be resolved by using theoretical methods. Theoretical understanding of factors which control the non-linear optical properties is very important to develop materials with enhanced non-linear optical properties. Time Dependent Density Functional Theory offers a good accuracy/computational cost ratio among different methods used to predict the electronic structure for molecules of practical interest. The Coupled Electronic Oscillator (CEO) formalism was recently shown to accurately predict NLO properties of organic compounds when combined with Time Dependent Density Functional Theory.

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Epoxy coating with super corrosion protection containing 2-mercaptobenzothiazole modified ZnO with core shell structure as anticorrosion pigment

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Corrosion of the metallic structures has undesirable effects on the industry and daily life in both economically and safety points of view [1]. Organic coatings were extensively used for protecting purposes in the corrosive media [2]. Epoxy (EP) coating which has low cost, good barrier properties, and good adhesion is preferred to other organic coatings [3].

In this study, 2-mercaptobenzothiazole modified ZnO with the core-shell structure (ZnO@PANI@MBT) was synthesized by layer by layer (LBL) method and characterized successfully by fourier transform infrared spectroscopy (FTIR), scanning electron microscopy (SEM), thermogravimetric analysis (TGA), Zeta potential, raman spectroscopy and dynamic light scattering (DLS) techniques.

Different weight percentages of pure ZnO nanoparticle and ZnO@PANI@MBT core shells (0.5,1,2 wt.%) were embedded into epoxy and coated on mild steel. The corrosion protective performance of coatings were studied by electrochemical impedance spectrometry (EIS) in saline electrolyte (NaCl 3.5 wt.%, 65 °C). The EIS study indicated that epoxy resin with the 1 wt.% addition of ZnO@PANI@MBT core shell nanoparticles had higher corrosion protection and lower permeability to water penetration. Also, using modified ZnO nanoparticles with the core shell structure as anti-corrosion pigment increased the hydrophobicity of epoxy coatings. The highest coating corrosion resistance (R_{coat}) after 200 h immersion time in saline electrolyte was obtained in the presence of 1 wt.% ZnO@PANI@MBT (4.8×10^{8} Ωcm^2) which is higher than that of epoxy/pure ZnO coatings ($R_{coat} = 9.2\times10^{6}$ Ωcm^2) and net epoxy ($R_{coat} = 9.1\times10^{3}$ Ωcm^2). The water uptake amount of epoxy/ZnO@PANI@MBT 1 wt.% was 1.04 time smaller than epoxy/pure ZnO and 1.90 time smaller than net epoxy after 200h immersion.

Keywords: Epoxy, Core shell, ZnO, corrosion inhibitor, layer by layer synthesis.

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Design and synthesis of a new type dibenzosuberenone-dihydropyridazine based fluorescent dyes for heavy metal ion and multi-analyte sensing applications

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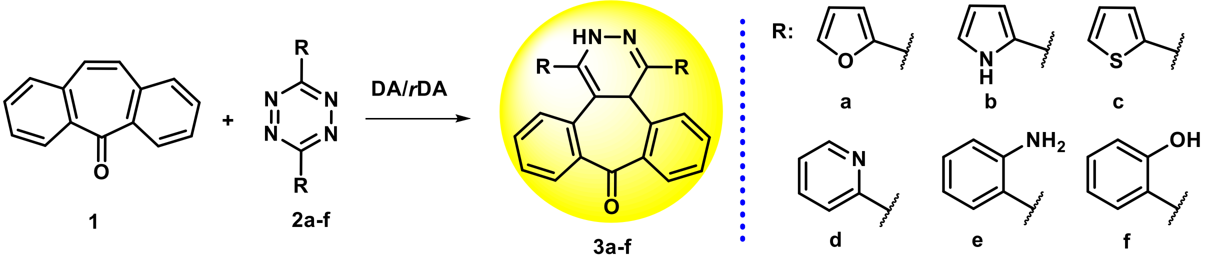
The widespread use of heavy metal ions in the industry results in serious environmental pollutions and human health problems, negatively affects agriculture, and destroys natural life [1]. Therefore, the development of fluorescence chemosensors for the determination of heavy and transition metal ions has attracted much attention in recent decades [2]. Dibenzosuberenone and polyconjugated derivatives exhibit photophysical properties such as photosensitizatione, fluorescence, and aggregation-indduced emission (AIE) [3]. Recently, our research group discovered a new class of dibenzosuberenone derived fluorescent dyes, and their photophysical and/or anion sensor properties were investigated [4,5]. In this study, various analogues of a new family of fluorophores based on derivatives dihydropyridazine-dibenzosuberenone were synthesized by inverse electron-demand Diels-Alder cycloaddition reactions between a dibenzosuberenone and tetrazines that bear various substituents (Scheme1). Then, the photophysical, heavy metal and multi-analyte sensor properties of these compounds will be investigated.



Scheme1. Derivatives dihydropyridazine-dibenzosuberenone.

Keywords: Fluorescence chemosensor, heavy metal ion, multi-analyte sensor, dibenzosuberenone, pyridazine.

Acknowledgments: This study was funded by the Scientific and Technological Research Council of Turkey (TÜBITAK) (Project No. 120R032). We thank TÜBITAK for its support.

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Geranium Essential oil and sun photoprotection

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Essential oils are volatile compounds that have been used since antiquity as local anesthetic, anti-inflammatory, antimicrobial, food flavoring agents and sedative [1]. Several herbs belonging to the genus *Pelargonium graveolens* are noted for their medicinal benefits in traditional system of medicine. This plant, *Pelargonium*, has various medicinal properties. They are rich source of monoterpenes, coumarins, sesquiterpenes tannins, cinnamic acids, phenolic acids, flavonoids, flavones and flavonols derivatives. *Pelargonium*-derived essential oil is used in perfumery, cosmetics, soaps, creams, aromatherapy products exhibit good antioxidant activity and has potential immune modulating effects no natural killer cells [2]. *Rose geranium* is a male-sterile cultigen and is therefore only propagated vegetatively. It is a popular plant due to its significant biological and pharmacological activities, including antiinfluenza, anticancer, antimicrobial, antioxidant, antineuroinflammatory, and antifungal activity [3]. The aim of this study is to investigate the photoprotection properties of *Geranium* essential oil in oil-in-water emulsions in the ultraviolet visible wavelength. The *Geranium* essential oil is mixed with the prepared emulsion. Thirty milligrams of emulsion exactly weighed were spread on PMMA plates over the whole surface (25 cm^2) using a finger coat to achieve a homogenous layer over the entire plate until a residual mass of 15 mg is obtained, a density of 0.6 mg/cm^2[4]. Three plates were prepared to be tested. Then, the transmission measurements were carried out using a Varian Cary 5000 UV/Vis/NIR Spectrophotometer. In this experiment, based on the results of UV absorbance, it shows that *Geranium* essential oil has UV absorbance in UVA = 12,70 ± 0.23 and in UVB = 9,41 ± 0.23. In this study, it finds that *Geranium* essential oil has the potential to use in sunscreen products.

***Keywords: Geranium* oil essential, photoprotection, sunscreen,skin**

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Microgram use of MOF-70 in a developed adsorbent-based analytical method for the preconcentration and extraction of pesticides from fruit juices

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Detection and quantitative determination of pesticides in beverages are of great importance [1]. Conducting this deed requires sample preparation methods inevitably [2]. The application of metal organic frameworks in this field can be so promising due to their inherently beneficial properties [3]. In the present research, a sample preparation method called dispersive micro solid phase extraction followed by dispersive liquid-liquid microextraction was developed based on MOF-70 as a highly efficient adsorbent for the extraction of seven pesticides including chlorpyrifos, haloxyfop-R-methyl, oxadiazon, diniconazole, clodinafop-propargyl, fenpropathrin, and fenoxaprop-P-ethyl from various fruit beverages (orange, pineapple, pomegranate, grape, and cherry beverages). In the first step, the pesticides are loaded on the MOF particles from the sample solution by vortexing and then settled down by centrifugation. Then, they are desorbed by acetonitrile from the MOF surface. In the next step, the obtained acetonitrile phase is mixed with µL-level of 1,1,1-trichloroethane and injected into deionized water. After the final centrifugation, the sedimented phase is collected and an aliquot of the obtained phase is injected into a gas chromatograph equipped with a flame ionization detector. MOF-70 is carefully synthesized and characterized using X-ray diffraction, Fourier transform infrared spectrophotometry, scanning electron microscopy, energy dispersive X-ray, and nitrogen adsorption/desorption analysis. After optimization of the process, satisfactory figures of merit were obtained such as high extraction recoveries (35-96%) and enrichment factors (175-480), low relative standard deviations (4.5-8.5%), wide linear ranges, and low limits of detection (0.20-0.76 µg L^{-1}) and quantification (0.65-2.47 µg L^{-1}). The developed approach can be introduced as a highly efficient analytical method based on MOF-70 for the analysis of various pesticides in juice samples.

Keywords: Metal organic framework; Gas chromatography; Fruit beverage; Diffusion-based synthesis; Pesticide analysis

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Colorimetric Ammonia Gas sensors by Mesoporous Silica Core-Shells: Studying the Effects of Various Metallic Species and Different Sensitive Organic Dyes

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This study presents an effective and simple colorimetric probe for sensing ammonia in gas phase based on reaction of a sensitive dye loaded onto the silica based core–shell Nano-structure. A core-shell nanostructure was designed and prepared via a sol-gel approach, and then a very simple impregnation method was employed to enrich it with a sensitive dye (Alizarin). Various analytical tools were used to characterize the structural and textural properties of prepared substrate which all of them proved the presence of a mesoporous system. A series of colorimetric and spectroscopic experiments using diffuse reflectance spectroscope (DRS) were employed to investigate the extent of the changes in dye response. Certain concentrations of ammonia were released into a closed chamber with certain volume via evaporating ammonia solution on a hot plate. Also all responses were detectable with naked eye as long as the ammonia concentration in the air was more than 50 ppm. [1,2].

Keywords: Core-shell, Gas-Sensor, Colorimetric, MCM-41, Ammonia

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Sonocatalytic degradation of a pharmaceutical pollutant on the Titanium Tin Carbide MAX phase

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In light of growing environmental concerns over antibiotic use, advanced technologies for removing antibiotics from pharmaceutical wastewater are required [1]. A new generation of efficient sonocatalytic water treatment systems could potentially solve such problems. In this study, we present a new type of nano-laminated material, titanium tin carbide (Ti_2SnC) MAX phase, that is prepared, characterized, and evaluated for its sonocatalytic activity. A variety of identification analyses including X-ray diffraction, scanning electron microscopy, and Fourier transform infrared were conducted to determine the physicochemical characteristics of the synthesized catalyst. The sonocatalytic degradation of oxytetracycline (OCT) in the aqueous solution with an initial concentration of 10 mg/L was investigated at various concentrations of the Ti_2SnC MAX phase. Among these, 1 g/L catalyst demonstrated high sonocatalytic performance and recyclability toward OTC degradation within 120 min at pH = 6.8 (natural) using an ultrasonic power of 150 W. Sonocatalytic performance of the catalyst was also investigated at pH ranges from 4 to 10. It was found to be primarily pH-independent, suggesting a wide range of catalytic activity. Ophenylenediamine was also used as a probe for determining the hydroxyl radical using a spectroscopic method. This work aims to develop an efficient and environmentally friendly wastewater treatment process using MAX-phase-based sonocatalysts.

Keywords: MAX-phase, Sonocatalysis, Antibiotic degradation

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New 1,2,3-triazole-methoxybenzylidene acetohydrazide hybrids as potent α-glucosidase inhibitors: synthesis, in vitro enzymatic and α-glucosidase inhibitors evaluations

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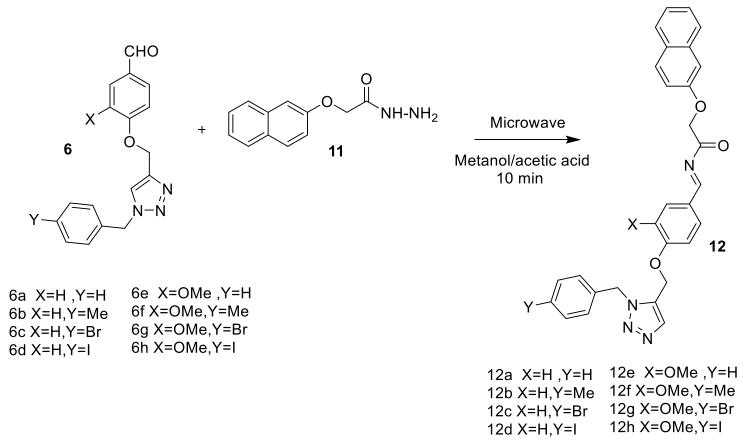
A novel series of 1,2,3-triazole-methoxybenzylidene[1] acetohydrazide derivatives **12a-h** were designed, synthesized, and evaluated for their in vitro α-glucosidase inhibitory activity leading to efficient anti-diabetic agents.[2] Eight 1,2,3-triazole-methoxybenzylidene acetohydrazide derivatives **12a-h** were synthesized into three main steps. In the first step, the 1,2, 3-triazole bearing aldehyde group moiety 6a-h wrer efficiently constructed via a click multicomponent reaction of 3 a,b with 5. In the second step the other starting material bearing hydrazine group was prepared from the reaction of **9** and **10**. In the last step in the presence of microwave reaction between aldehyde group moiety 6a-h and hydrazine groups moiety **11**, final products **12a-h** were produced The synthetic molecules were characterized *via* FT-IR,1H-NMR and ^{13}C-NMR spectroscopic techniques and elemental analysis and evaluated for their anti-hyperglycemic potential. Compounds **12a-h** exhibited good to moderate *in α*-glucosidase inhibitory activities in the range of IC50 values (2.01 ± 0.036 to 2.09 ± 0.08µM) as compared to the standard acarbose (IC50 = 1.92 ± 0.17 µM) and (IC50 = 1.99 ± 0.07 µM), respectively.

Keywords: Triazoles, acetohydrazide و α-Glucosidase inhibitors, Anti-hyperglycemic activity



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Encapsulation of herbal extract on lipid-based Nano/Microcarriers

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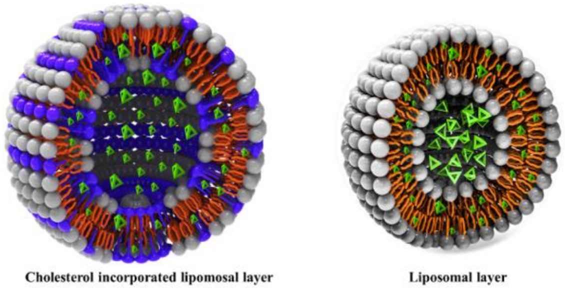
Food nutrients and herbals products play a fundamental role in human health quality, directly and indirectly preventing the risk of various human disorders. The physicochemical features of nutraceuticals often make it challenging to incorporate into different formulations, resulting in food ingredient instability (fast degradation and decomposition) [1]. The lipid-based formulation is an effective and safe carrier that delivers food nutrients and herbal extracts in an accurate pathway that simultaneously improves their health quality to the food and pharmaceutical industries. Liposomes have been proved to be an efficient strategy to improve the stability of food-based phytoconstituent, control their release, and enhance their functionalities. Natural product-loaded liposome was prepared by the thin film evaporation method. Meanwhile, the prepared nanocarriers are modified by bioadhesive layers and change the liposomal membrane surface by applying nanospray and electrospinning techniques, using the nanospray drying technique help to produce smaller particles, which improves the bioavailability and release of bioactive components and drugs. Chitosan and pectin biopolymers were added to liposomes to build up biopolymer-coated liposomes and convert them to powder by a nanospray dryer. Particle size and Z-potential of liposomes and modified liposomes were determined using dynamic light scattering (DLS). The primary liposome had diameters of approximately 134 nm, and coated liposomes were 300-500 nm. FT-IR spectroscopy confirmed the interactions associated with lipids hydrocarbon chains by herbal extracts. The loading ability was evaluated by calculating the encapsulation efficiency (EE%) over 85%, indicating herbal extracts' inserting ability into the liposomal membrane coated by biopolymers.



Cholesterol incorporated lipomosal layer

Liposomal layer

Keywords: Bioactive compounds; liposome; secondary layer; molecular docking; bilayer arrangement

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Extraction of work from motions related to the degrees of internal freedom of molecules

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Every thing thet happens in the universe, from the vital processes within a bacterium to the most complex computations in advanced upercomputers made by eletrons, atoms, molecules and their movements between energy levels, or energy level changes. It is done by analyzing the energy exchange between quantum systems and the einironment. Quantum thermodynamics has recently flourished, enhanced by highly controlled quantum experiments, the availability of powerful numerical methods, and the development of new theoretical tools such as unbalanced thermodynamics and quantum information theory that describe inequal oscillations which is used for the purposes such as better understanding of heat in quantum systems in the field of quantum and the design of new experiments, thermodynamic quantum exploration using nuclear rotation, molecular degrees of freedom and etc. Quantum states and energy levels belonging to molecular vibrations as well as inhibited rotation around chemical bonds can be used as a means of extracting or storing energy. The processes of extraction, transfer, and exchange of energy and heat in quantum motors designed based on degrees of internal molecular freedom can be used to transmit, store, and information process. Quantum motors designed based on the degrees of internal freedom of molecules can be used to transfer molecules and materials through interfacial space, thus model can be used to predict the equilibria phase of fluids and condensed matter. We can stimulate above processes and designed quantum motors by network methods and specify(identify) the critical states of the case-comment and use it them for their control.

Keywords: Quantum thermodynamics, Quantum machines, Work and heat, Internal degrees of freedom, Internal energy levels

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Biological Activity of Nano and Bulk Size Pb(II) Metal-Organic Frameworks, Branched-Tube and Sonochemical Assisted Synthesis

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New nanostructure lead(II) coordination polymer or MOFs $[Pb_5(\mu\text{-}L)_2]_n$ [L=4PCA=4-Pyridine Carboxylic Acid], has been synthesized by the reaction of a mixture lead(II) nitrate with 4PCA by Sonochemical method. Reaction conditions, such as temperature, time, concentration and initial reagents play important roles in the size, morphology and crystal growth of the final products. The PbO nanoparticles were prepared from the calcinations of the nanopowders of Nano-MOF at air atmosphere. The structure of the compound was determined by Single-Crystal X-ray crystallography, while nano-structural materials were characterized by X-ray powder diffraction (XRDP) and Scanning Electron Microscopy (SEM) [1]. Thermal stability of bulk and nano-sized particles of this Nano-Coordination-Polymer was studied and compared with each other. These CP, NCP and Lead(II) Oxide (LONPs) effects on the antibacterial activity *(against Staphylococcus epidermidis (Se) ATCC 14990, Bacillus subtilis (Bs) ATCC 6633, Bacillus cereus (Bc) ATCC 14579, Pseudomonas aeruginosa (Pa) ATCC 9027 and Escherichia coli (Ec) ATCC 25922 strains).*

Keywords: Nanopowder, Lead(II) Bromide, Lead(II) Oxide, Coordination Polymer.

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Indirect determination of diazinon using a chemiluminescence method based on the peroxidase-like property of molybdenum disulfide/zirconium-based metal-organic framework nanocomposite

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Organophosphate (OP) toxins, as the most familiar agents of neurotoxins, are widely used in public health, agriculture or by animal husbandry [1]. Global depletion of OPs into the environment threatens public health through widespread pollution of food and water [2]. An excess amounts of diazinon can lead to the dimness of vision, nausea, muscle tremors and, difficult breathing [3]. The application of new diagnostic systems to measure organophosphates has been an important issue for researchers. In this research, a sensitive analytical method provided for indirect determination of diazinon based on the peroxidase-like property of molybdenum disulfide/zirconium-based metal-organic framework nanocomposite (MoS_2 @ MIP-202 (Zr)). The inhibitory effect of diazinon on the enzymatic activity of acetylcholinesterase was used to obtain appropriate selectivity. In addition, MoS_2 @MIP-202 (Zr) nanocomposite, has a very effective peroxidase-like activity, and significantly increases the very poor emission resulting from the chemiluminescence reaction of the $NaHCO_3$-H_2O_2 system. In the presence of diazinon and its binding to acetylcholinesterase, the catalysis of acetylcholine to choline decreases and consequently, decreases the concentration of H_2O_2. So, the emission intensity of the chemiluminescence decreases linearly. The proposed system has a high sensitivity in diazinon measurement. The synthesized MoS_2@ MIP-202 (Zr) catalyst could be created a very effective diagnostic system using the green, cost-effective and easy method as well as the easy-to-use chemiluminescence system. A wide linear range of 0.2–200 ppb and the detection limit of 0.04 ppb obtained for the determination of diazinon using the method. The high repeatability of the method was confirmed by its application for environmental samples.

Keywords: Metal-organic frameworks, Optical sensors, Chemiluminescence, Molybdenum disulfide, Diazinon

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Ultra-high conductive Inorganic quasi solid state electrolyte containing Li ion

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Considering the energy crisis, the Scientists' attention has been attracted to high-efficiency energy conversion, storage systems, and more especially electrolyte as an essential part of this field area [1]. However, some critical factors such as leakage and volatilization have limited the long-term performance and practical usage of liquid electrolytes [2]. Therefore, the quasi-solid-state electrolytes could be a suitable alternative for liquid electrolytes [3]. But, compared to liquid electrolytes, the quasi-solid-state electrolytes have less ionic conductivity [4]. Hear in, by addressing this issue, preparation of an ultra-high conductive quasi-solid-state electrolyte based on a bismuth-titanium gel composite containing lithium ions is reported. The prepared material is characterized by the use of EDX and TGA instruments to confirm the ratio of the materials. The ionic conductivity performance was measured by electrochemical impedance spectroscopy (EIS). The utilized electrochemical system was an asymmetrical cell consisting of two flat graphite electrodes and as-prepared electrolytes. After optimization of the ratio amount of electrolyte materials, conductivity was achieved at 555 mS cm-1 at room temperature which hasn't been already reported [5]. In addition, this electrolyte has some other advantages such as non-flammability, environment friendly, and flexibility.

Keywords: quasi-solid-state electrolyte, inorganic materials, lithium ion, high conductivity

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An alternative magnetic semi-solid sorbent composed of modified magnetic nanoparticles & supramolecular solvent in removal of Direct Black EX 122 from aqueous samples

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In this study, a new and interesting magnetic semi-solid sorbent has been introduced.

In primary steps of this research, a compersion study on the extraction efficiency of three kinds of sorbents in dye remoal from aqueous solutions was performed.The three sorbents were: modified magnetic nanoparticle (modified-MNP), supramolecular solvent (SUPRA), and a sticky, viscose, and magnetic semi-solid phase composed of modified-MNP & SUPRA. Modified-MNP & SUPRA were prepared in our Lab, which have been reported before [1, 2, 3, 4]. The results of primary experiments showed that the magnetic semi-solid sorbent composed of modified-MNP & SUPRA, could act better than those of two other sorbents in dye removal. Since azo dyes are environmental pollutants and their removal also has been considered by all scientists [5], so the extraction conditions for the removal of Direct Black EX 122 from aqueous samples, were optimized. Direct Black EX 122 is an azo dye and used in textile industry. The effective variables such as: pH of dye solution, temperature, the amount and kind of the sorbent (both of modified-MNP & SUPRA), extraction time, the volume and concentration of dye solution were investigated. Under optimal condition, high extraction efficiency, facile removal, and low time-consuming separation of azo dye from water samples was observed.

Keywords: magnetic, nano particle, supramolecular solvent, semi-solid, sorbent.

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Direct Formation of Persistent Hydrogen-Bonded Organic Framework Radical for Enhanced Photothermal Conversion

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Synthesis of materials with photoresponse in the shortwave near-infrared region (SWIR) is a scientific challenge but highly desired. Herein, we demonstrate creating radical compounds as a convenient and economical solution. In this work, viologen radicals were generated during the self-assembly process and in-situ stabilized into a hydrogen-bonded organic framework (HOF), giving rise to a persistent radical compound (**PFC-26R**) with photoresponse in Ultraviolet-visible and SWIR region. The highly-ordered arrangement guarantees an effective shielding effect to protect radicals from bleaching, therefore **PFC-26R** exhibits outstanding stability in various solvents and ambient conditions for as long as three months. IR thermal camera recorded a drastic temperature rise of **PFC-26R** from 25°C to 214°C in 53s under simulated one-sun irradiation (1 W/cm^2), ranking state-of-art photothermal conversion performance relative to other reported materials. Thanks to the easy processibility of HOFs and the persistent radical nature, a seawater evaporation device based on **Cu@PFC-26R** thin film was fabricated, which presents an effective platform for capturing solar energy to provide freshwater from seawater with excellent salt rejection performance and a high evaporation rate of 2.85 kg/m^2·h, which is among the top values reported in this field. This research makes an important step toward the direct synthesis of ultra-stable radical materials for safe and efficient solar energy technologies.

Keywords: Hydrogen-Bonded Organic Frameworks. UV–SWIR Absorption. Photothermal Conversion. Persistent Radical. Seawater Desalination

Synthesis of NiS nanoparticles and their application for determination of amoxicillin and cefazolin by using a chemiluminescence method

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Chemiluminescence (CL) reactions are chemical reactions releasing energy as electromagnetic emission. Analytical approaches based on CL reactions are usually convenient, economical, and exhibit good figures of merits such as wide linear concentration range and high sensitivity [1]. NiS nanoparticles (NPs) have many utilizations in diverse fields of advanced research like catalysts, cathodes of rechargeable lithium batteries, solar cells, and supercapacitors [2]. In this work, a new and sensitive CL method was proposed for determination of amoxicillin (AMX) and cefazolin (CFZ) in pharmaceutical preparations. The CL method is based on enhancing effect of AMX and quenching effect of CFZ on the NiS NPs-luminol-O_2 chemiluminescence (CL) reaction in a strongly alkaline medium. NiS synthesized by hydrothermal synthesis method by X-ray diffraction (XRD), scanning electron microscopy (SEM), and Fourier-transform infrared spectroscopy (FTIR) methods. The effects of various chemical reagents, involved in the CL reaction, on the CL emission intensity were also investigated and optimized. Under the optimum conditions, a linear relationship was obtained between the CL intensity and the concentration of CFZ and AMX in the range of 1.00×10^{-5}-1.00×10^{-3} mol L^{-1} and 1.00×10^{-6} – 8.00×10^{-4} mol $L^{-1}$with limit of detections of 4.5×10^{-6} and 2.5×10^{-7} mol L^{-1}, respectively. The mechanism of CL system was also discussed, briefly.

Keywords: Amoxicillin, Cefazolin, Luminol, NiS Nanoparticles

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Functionalized HMS as efficient mesoporous catalyst for synthesis of tetrahydrobenzo[b]pyran and 1,4-dihydropyrano[2,3-c]pyrazole derivatives

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Mesoporous compounds are the most popular materials, due to their structural characteristics, such as high surface areas and pore volumes and have found variety applications, such as adsorbents, catalyst supports, drug delivery systems and biosensors [1]. Among theme, hexagonal mesoporous silica (HMS) with wormlike mesoporosity, uniform and narrow pore size distribution, high surface area and pore volume, short channel, thermal stability, easily synthesis and functionalization has found promising applications as a support for synthesis of heterogeneous catalysts [2]. Pyranopyrazole and benzopyran derivatives, have become important due to their pharmacological and biological properties such as anti-inflammatory, antioxidant, anti-bacterial, in perfumes and cosmetics and in food as additives [3,4]. The present study describes the synthesis, characterization, and investigation of catalytic activity of xanthine-Ni complex incorporated into functionalized HMS (HMS/Pr-Xa-Ni) in synthesis of tetrahydrobenzo[b]pyran and 1,4-dihydropyrano[2,3-c]pyrazole derivatives.

Keywords: HMS, Mesoporous, Pyranopyrazole, Benzopyran

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Enrichment natural pigment from pomegranate juice: isolation by macroporous resin and characterization adsorption/desorption process

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Color plays an important role in human life and different industries, including food, cosmetics, and pharmaceuticals. Synthetic pigments in spite of providing variety in color, high yield and low price, always being a concern in different industries. For this purpose, natural pigments, due to their biologically and environmentally safe feature, attracting a considerable attention to using them in the food products [1]. Anthocyanins (ACNs) are water-soluble natural pigments responsible for producing various colors in flowers, fruits, and vegetables. Pomegranate juice (PJ) is a beverage rich in ACNs compounds that shows high antioxidant activity compared to other fruit juices and beverages. This study aimed to separate the ACNs as natural red pigment from PJ using LXA-10 macroporous resin in a batch system [2]. All adsorption and desorption processes on the resin have been optimized for maximum separation efficiency. The ACNs maximum adsorption condition (contact time: 40 min, pH: 2.5, a PJ to resin ratio: 30 ml/0.7 g), and ACNs maximum desorption (contact time: 8 min and a 6-bed volume solvent) were obtained as optimum operating conditions. In which the maximum of 94.0% adsorption and 93.3% desorption percentage of ACNs were achieved. The different adsorption isotherms models were tested which results concluded that Freundlich model with R2 = 0.96 fitted adequately with the experimental data. A kinetic study was carried out that showing the ACNs adsorption data correctly adjusted by an equation corresponding to a pseudo-second-order chemical reaction with R2 = 0.99. The constituents and the contents of the purified products were analysed, and the antioxidant activities were determined using FRAP test. The purified product contained five major ACNs in PJ and showed strong antioxidant activity (8.8 mmol Fe (II)/L sample) in comparison with initial PJ (1.4 mmol Fe (II)/L sample). In conclusion, purification by LXA-10 macroporous resin was a highly efficient and economical method for purification red natural pigment from PJ.

Keywords: Macroporous resin, FRAP, Anthocyanins, Batch system

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On chip electromembrane surrounded solid phase microextraction of antidepressants using PEDOT-GO nanocomposite coating

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Tricyclic antidepressants (TCAs) are commonly used for clinical treatment of major depressive disorder, anxiety and certain personality disorders as well as chronic pain. Amitriptyline, nortriptyline, imipramine, desipramine, maprotiline and sertraline are known as the most conventional class of antidepressants. However, some adverse health effects have frequently occurred such as mind confusion, dry mouth, and constipation. In addition, due to the relatively narrow therapeutic/toxic index and low therapeutic window of TCAs, monitoring the concentration of these compounds in biological fluids is imperative [1]. Sample preparation has always been one of the most challenging steps for the analysis of different analytes from various complex matrices. In the recent few decades the perspective of these methods has been focused on miniaturization and minimization of the organic solvent usage and lowering the limits of detection. In order to achieve these goals, electromembrane surrounded solid phase microextraction (EM-SPME) has been introduced as proper and effective extraction method. It is stated that this method overcame the drawbacks of direct immersion SPME and the limitations of EME. High cleanup ability, appropriate extraction efficiency, high preconcentration and coupling with gas chromatography are some advantages of EM-SPME for extraction of compounds from complicated matrices in low concentrations [2].

In the present work, EM-SPME on chip was developed to extract antidepressant drugs from various complex matrices. Therefore, poly(3,4-ethylenedioxythiophene)-graphene oxide (PEDOT-GO) nanocomposite was electrochemically synthesized on SPME fiber as a conductive polymer. Consequently, the SPME holder has been injected in acceptor phase and the fiber has played the negative electrode role during the extraction. Likewise, after electromembrane extraction, thermal desorption was applied to transfer the drugs in to the column in gas chromatography-mass spectrometry. Effective parameters on extraction efficiency were investigated and optimized. Under optimum conditions, the limits of detection of the analytes were in the range of 0.005-0.025 µg L^{-1}. Linearity of the method was obtained within the range of 0.010-500 µg L^{-1} for imipramine and sertraline, 0.025-500 µg L^{-1} for amitriptyline, nortriptyline and desipramine, and 1.000-250 µg L^{-1} for maprotiline with coefficients of determination better than 0.9984. Moreover, the precision of the method is suitable with relative standard deviations lower than 6.2%. The method was applied for extraction of the mentioned drugs from biological fluids such as bone marrow aspirate, urine and plasma samples; and satisfactory relative recoveries between 96 and 105% were obtained.

Keywords: Electromembrane extaction, solid phase microextraction, on chip, antidepressants.

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Progress in CO_2 Utilization: from homogeneous to heterogeneous catalysts

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With modern industry development, carbon dioxide (CO_2) has attracted more and more attention as its unignorable influence on the greenhouse effect. While in the aspect of synthetic chemistry, CO_2 is considered as an ideal C1 source for its merits, such as nontoxicity, economy, renewability, and abundance. Based on this, the transformation of CO_2 into organics using homogeneous catalysts has become a highly promising area in modern green and sustainable chemistry. Up to now, numerous strategies have been developed to effectively utilize CO_2 for the synthesis of valuable chemicals. Moreover, also heterogeneous catalysts are intensively investigated for the utilization of carbon dioxide, especially Metal-Organic Frameworks (MOFs). MOFs are non-conventional porous materials having a broad spectrum of applications. The catalytic use of MOF-based materials is cutting-edge in the field of scientific and technological developments. Recently, MOFs are being investigated as promising catalysts for synthesizing of industrially important cyclic carbonates under solvent-free ambient conditions. A wide variety of terminal and internal substrates are converted efficiently with high selectivity. MOFs as heterogeneous catalysts are remarkably stable and have structural rigidity, hence recycled for subsequent use with almost the same activity. Therefore, MOF-catalysts are highly efficient for the cycloaddition of CO_2 to epoxides into cyclic carbonates.

Posters

Novel Schiff Bases with Diamondoid Adamantane Moiety

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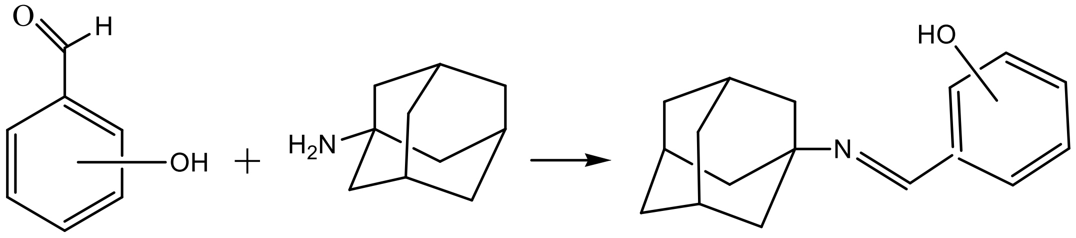
Schiff bases, named after Hugo Schiff, are formed when any primary amine reacts with an aldehyde or a ketone under specific conditions [1]. Schiff bases with the general structure $R_2C=NR'$ ($R' \neq H$) are found to be a versatile pharmacophore for design and development of various bioactive compounds. Many aromatic Schiff base compounds have developed as antibacterial, antitumour and antivirotic drugs in recent years [2]. In chemistry, diamondoids are variants of the carbon cage molecule known as adamantane ($C_{10}H_{16}$), the smallest unit cage structure of the diamond crystal lattice. Diamondoids also known as nanodiamonds or condensed adamantanes may include one or more cages [3]. A diamond combines several very useful properties, such as extreme mechanical hardness, stability against chemical reagents, broad optical transparency, wide band gap, high radiation hardness, and high thermal conductivity [4]. Diamondoids, also have many properties of diamond, therefore molecules with diamondoid moiety contain modified properties. Thus, we have attempted to prepare Schiff bases with diamondoid adamantane moiety. For this purpose, salicylaldehyde derivatives **1** was treated with amantadine (1-amino adamantane) **2**, as the primary amine, to obtain amantadine- Schiff base hybrids **3** (Scheme 1).



1 **2** **3**

Scheme 1. Synthesis of amantadine- Schiff base hybrids

Keywords: Schiff base, Adamantane, Diamondoid, Nanodiamond

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Synthesis of 2, 2, 2-trifluoro-1- (2- (2-oxo-2-phenylethyl) - 1H-benzo [d] imidazole-5-yl) ethane-1-one

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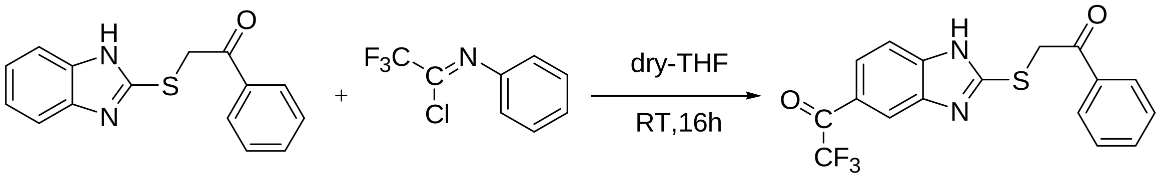
Fluorine has unique properties that altering organic molecules physicochemical and biological properties. Nowdays 20% of all pharmaceuticals are containing fluorine atoms. The trifluoromethyl group (CF_3) is one of the most common fluorinated substituents in medicinal compounds because it offers simultaneously high lipophilicity, an elevated electron density that especially at aromatic positions, play an important role in the design of new potential drugs and crop-protection agents [1-3]. In this investigation, firstly, we have synthesized 2-((1H-benzo [d] imidazole-2-yl) thio)-1-arylethane-1-ones, then these intermediates have been used for synthesis a new series of 2, 2, 2-trifluoro-1-(2-(2-oxo-2-phenylethyl)-1H-benzo[d]imidazole-5-yl) ethane-1-one using acetymidoyl chlorides in THF solvent at room temperature. All of the product's structure have been characterized by ^{1}H-NMR, ^{13}C -NMR, ^{19}F -NMR and IR spectral.



(a) (b) (c)

Yield =90%

Yellow Solid

Keywords: Trifiuoroacetimidoyl chloride,Benzoimidazolo-2-thioacetophenone

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Synthesis and Application of Metal Organic Framework based on High Nitrogen Ligand 4,5-Di(1*H*-tetrazole-5-yl)-2*H*-1,2,3-triazol (H_3dttz) for Removal of A Hazardous Azo dye (Basic Red 46) from Aqueous

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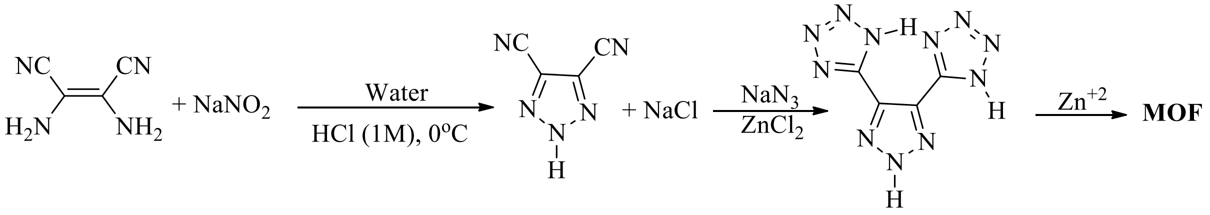
Environmental pollution is one of the major threats to human life. Among the different types of pollution, wastewater stream is one of the major problems due to a large amount of water used in our daily life. Waste water containing dye is the major source of water pollution [1]. During the past years, several methods such as coagulation, flocculation, ion exchange, membrane separation and advanced oxidation have been reported and attempted for the removal of dyes from effluents [2]. In this study, Basic Red 46 (BR 46) was used as a model compound. It is a synthetic azo dye which is used widely in the textile industry. The porous metal-organic framework based on 4,5-di(1*H*-tetrazole-5-yl)-2*H*-1,2,3-triazol (H_3dttz) was synthesised [3,4] and used for dye pollutant removal. The results indicated that the MOF adsorbent could effectively remove the BR-46 dye from the solution.



Keywords: Textile dye; Tetrazole; Triazole; H_3dttz; Basic Red 46

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Synthesis and Characterization of 5,5′-Bistetrazole in the Presence of Inorganic Catalyst

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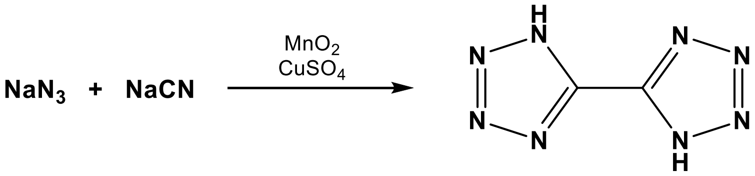
The aim of this study was to synthesize and identify the high nitrogen composition of 5,5′-bis tetrazole, which has been used as a copper sulfate catalyst to improve the synthesis process at two hours. 5,5′-bistetrazole has been regarded as a green energy substance due to its high nitrogen capacity [1]. Synthetic composition of the reaction of azide and cyanide salts in the presence of manganese oxide has a path similar to click chemistry [2]. Copper sulfate catalyst has been used to increase the reaction rate and hydrochloric acid to convert manganese bistetrazole salt to 5,5′-bistetrazole [3,4]. FTIR, ^{1}HNMR and ^{13}CNMR Identification methods have been used to confirm the structure that demonstrates the success of synthesizing this compound.



Keywords: Tetrazole, Catalyst, Bistetrazole, High Nitrogen Components

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Study on the synthesis of chromene-indole and pyridopyrimidine-indole hybrids as bilogically active structural frameworks

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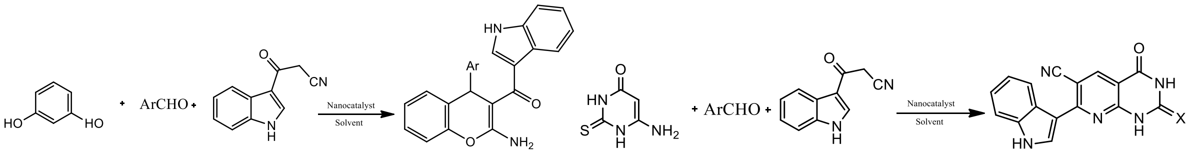
Indole derivatives have been reported to exhibit a wide range of biological activities. Indole nucleus occupies a unique position in heterocyclic chemistry due to its noticeable pharmacological properties and thus stands as an important scaffold in drug design. On the other hand, chromene derivatives are important group of heterocycles with diverse biological properties and therapeutic application which have attracted many attentions. The natural chromenes also display a diverse range of valuable biological properties such as antimicrobial and antiviral activities [1-4]. Hybrid heterocycles play a vital role in bioactive compounds and drugs. Chromenes and pyridopyrimidines, which are widely found in natural compounds, have a variety of biological and medicinal properties. Biological properties of chromene derivatives and pyridopyrimidines are well known they show antimicrobial, influenza virus inhibition, antitumor properties and effect on nervous system, Alzheimer's treatment, hypertension and convulsion [5]. At present study, a novel method for the synthesis of 2-amino-4*H*-chromenes and pyridopyrimidines using three-component reaction of 3-cyanoacetylindole, resorcinol (or 6-amino-2-thiouracil) and various arylaldehydes in the presence of nanocatalyst is described.



Keywords: Pyridopyrimidine, Indole, Chromene, Aminochromene

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Porous nanostructures from MOFs, COFs and SBA-15, to PMO microporous and mesoporous nanoreactors: 14 years with ONG

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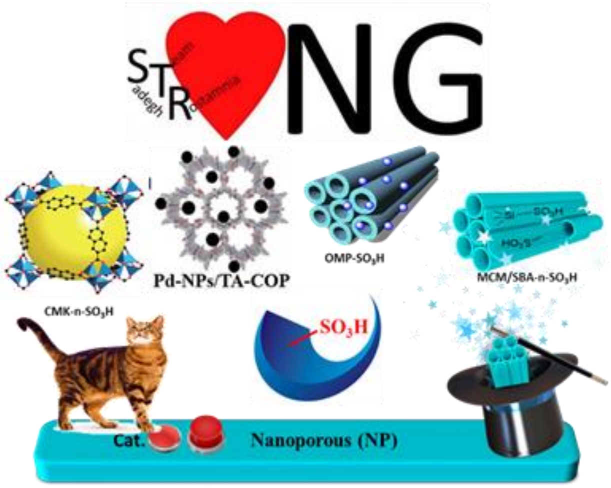
Within the feld of materials, chemistry, catalysis, energy, drug-delivery and even industry the nanostructures as a nanoreactor has possessed much attention. Normally, the synthesis of these materials are based on supramolecular and self-assembly phenomna in solvothermal condition [1]. Post-synthetic modification synthesis of these materials have main role in our group for desighned meta-organic frameworks (MOFs), covalent organic frmaeworks (COFs) for vrious application. Furthermore, these porous materials, from MOFs, COFs and SBA-15, to PMO, can be an excellent candidate for the stabilization of metal nanoparticles in their pore cages that it is our goal in Oganic and Nano Group (ONG) at IUST [2-4].



Keywords: Metal-organic frameworks, Covalent organic frameworks, Nanoreactors.

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Synthesis and characterization of amphiphilic invertible polyurethane

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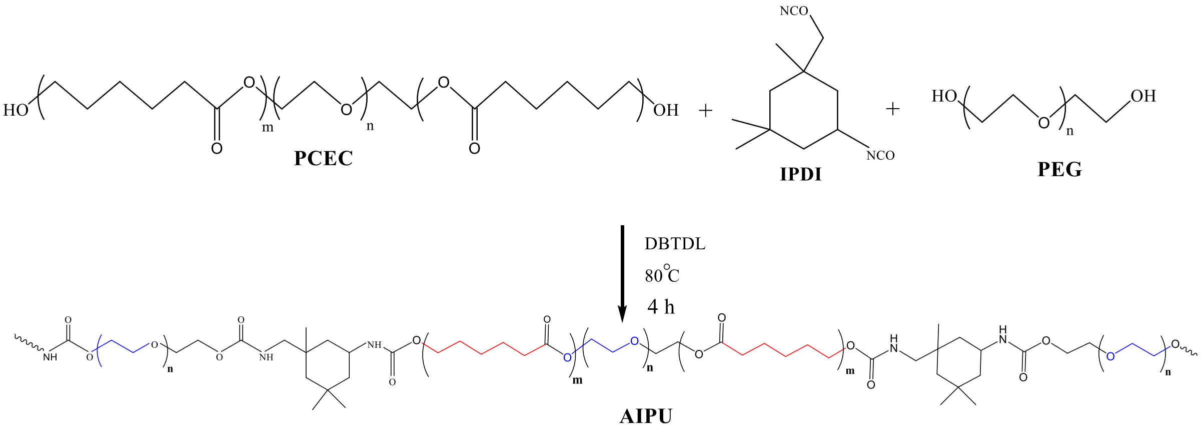
Amphiphilic invertible polymers (AIP)s are very important kinds of polymers due to their versatility and unique characteristics making suitable for applications in the various fields of science and technology. Possesing hydrophilic and lipophilic moieties, AIPs display environment-dependant capability of arrangement of thier molecules as micellar or inverse micellar assemblies [1-2]. AI-polyurethans (AIPU)s can be synthesized via polycondensation reaction between diisocyanates and diols with short lipophilic and hydrophilic constituents that are alternately or randomly distributed along the polymer backbone [3].

In this work, The PCL-PEG-PCL (PCEC) triblock copolymer was synthesized using a ring-opening polymerization of ε-caprolactone in the presence of PEG as a macroinitiator and stannous octoate as a catalyst and applied as a chain extender in the preparation of amphiphilic random polyurethane. AIPU was prepared by the reaction of poly ethylene glycol, isophorone diisocyanate (IPDI), PCEC and one drop of dibutyl tin dilaurate (DBTL) as a catalyst. The chemical structure of PCEC and AIPU was verified by FT IR and ^{1}H NMR spectroscopies. AIPU showed self-assembled structures in nonpolar organic media by direct dissolution method. The morphologies of these nanoparticles were investigated by field emission scanning electron microscopy (FE SEM), atomic force microscopy (AFM), dynamic light scattering (DLS), ^{1}H NMR spectroscopy and water contact angle (WCA) measurement.



Scheme1: Structure of amphiphilic invertible polyurethane

Keywords: Amphiphilic polymer, Invertibility, Self-assembly, Nanoparticles.

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Study on an innovative synthesis of thiazole-5-one using magnetic supported copper nanocatalyst

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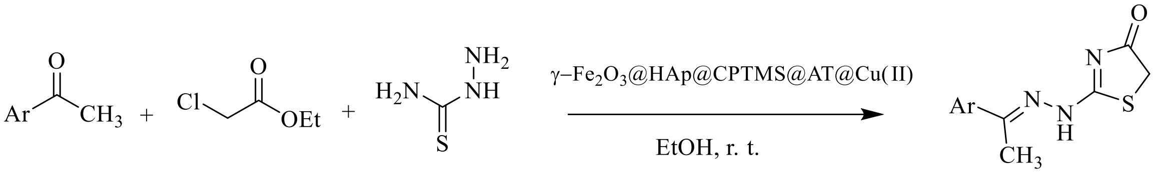
Thiazole as an important heterocyclic scaffold is the main constituent of numerous medicinal and biologically important compounds and has attracted many interests. The one-pot reaction can apply to a multi-step reaction, method, or synthesis. It is effective because several synthetic transformations and bond-forming steps can be carried out in a single pot, while avoiding several purification procedures at the same time. One-pot procedure can thus minimize chemical loss, save time, and simplify practical aspects [1-3]. Focusing our research interest on the evolution of innovative catalysts and submitting practical methods in organic synthesis, we wish to report a straightforward, efficient, and green protocol for the one-pot synthesis of ((phenylethlidene)hydrazinyl)thiazol-4(5*H*)one derivatives using a cyclocondensation reaction of acetophenone derivatives, active methylene ethyl acetoacetate and semicarbazide in the presence of γ-Fe_2O_3@HAp@CPTMS@AT@Cu(II) as a novel magnetically recyclable heterogeneous acidic nanocatalyst in ethanol at room temperature. Following our continued studies in the benign synthesis of biologically important heterocycles, we have investigated a facile method for the green synthesis of novel derivatives of thiazole-5-one in the presence of an efficient magnetic nanocatalyst (γ-Fe_2O_3@HAp@CPTMS@AT@Cu(II)). The γ-Fe_2O_3@HAp@CPTMS part of the catalyst was synthesized according to the literature reports [3-5] and supported by Cu (II). The catalyst was employed in the synthesis of a series of novel thiazoles. In this study, a novel three-component reaction of various acetophenone (1), thiosemicarbazide (2) and ethyl chloroacetate (3) in EtOH at room temperature to afford some novel derivatives of triazoles (Scheme 1).



1 **2** **3** **4a-j**

Ar: C_6H_4, 4-MeC_6H_4, 3-$_2$ONC_6H_4, 4-HOC_6H_4, 4-MeOC_6H_4, 2-HOC_6H_4, 4-BrC_6H_4, 2-ClC_6H_4, 4-$_2$ONC_6H_4, 3-MeC_6H_4

Scheme 1. Synthesis of thiazole derivatives (**4a-j**).

Keywords: γ-Fe_2O_3, Hydrazinyl-thiazole, Hydroxyapatite, One-pot, Green synthesis

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A Temperature-sensitive Nanofibrous-based Hydrogel Thin Film for Breast Cancer Therapy

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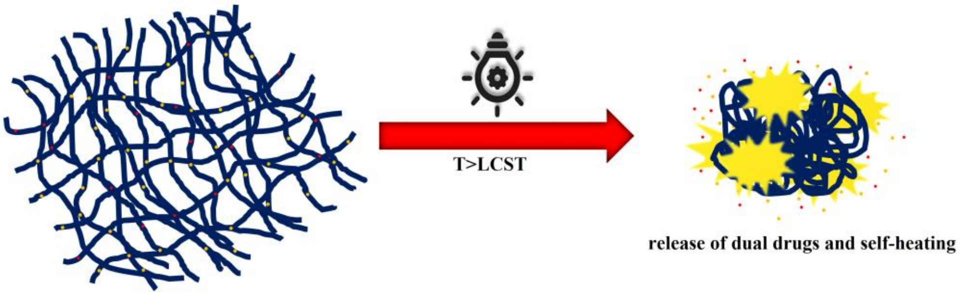
With the high rate of mortality, breast cancer treatment has attracted much attention globally. We designed a thermally cross-linked electrospun composite nanofiber with temperature sensitivity, local administration, and controlled release of dual drugs. A simultaneous heat generation with the tunable release of drugs was observed in response to visible light radiation. For this aim, the modified gold nanoparticles (Au NPs) were synthesized and loaded with curcumin (Cur). Poly(N-isopropyl acrylamide-co-N-methylolacrylamide) (poly(NIPAAm-co-NMA)) was prepared through redox copolymerization of N-isopropyl acrylamide (NIPAAm) monomer and N-methylolacrylamide (NMA) crosslinker. The electrospun composite nanofiber was fabricated through the blend electrospinning of a mixture of Cur-loaded modified Au NPs, paclitaxel (PTX) drug, and poly(NIPAAm-co-NMA). A nanofibrous hydrogel thin film was obtained after thermally crosslinking of the electrospun composite nanofiber. Since the hydrogel thin film is containing Au NPs, conversion of light to heat occurs under visible radiation [1]. Moreover, a swell and deswell behavior is observed below and above its LCST resulting in the controlled release of dual drugs [2]. The cytotoxicity of composite nanofiber was evaluated over the breast cancer cells (MCF-7) and fibroblast normal cells (L929) within 24h and 48h in both conditions with/without light radiation. The smart hydrogel thin film can be implanted directly on the surface of the skin at the place of the breast tumor or can be used for post-surgery by implanting the film on the tumor empty site after tumor resection to prevent tumor recurrence.



Keywords: Temperature-sensitive, Electrospun composite nanofiber, Hydrogel thin film, Dual drugs, Chemo-thermal therapy

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An Antibacterial Nanofibrous Mat Based on Copper-based Metal Organic framework-embedded Polyacrylonitrile

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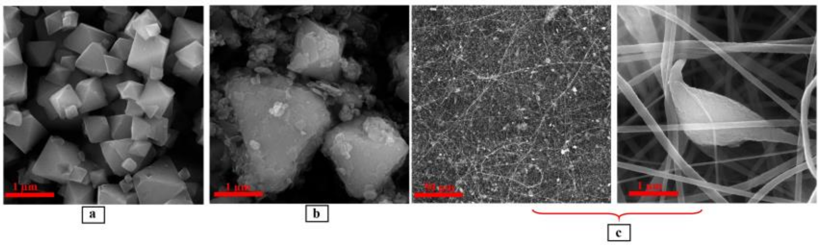
Bacterial contamination is becoming a big concern in the health issues threatening human life around the world. Metal-organic frameworks (MOFs) are introduced as the antibacterial coordination polymers whose antibacterial activities are affected by their intrinsic features such as their specific surface area, porosity, the release rate of metallic ions, pore structure, and their biodegradability and biocompatibility [1]. The construction of MOFs with metallic ions possessing intrinsic antibacterial activity such as copper (Cu) metal results in a bactericidal MOF with durable antibacterial activity [2]. To avoid toxicity, MOFs with increased stability and controlled release of copper ions over a prolonged time are required. This aim can be achieved through post-surface modification of MOFs [3]. In this study, we prepared an antibacterial nanofibrous mat composed of water-stable Cu-based MOF embedded in polyacrylonitrile polymer through blend electrospinning. Polyvinylpyrrolidone (PVP)-assisted strategy was used to synthesize Cu-MOF with a regular octahedral morphology without agglomerations and a successive post-synthetic modification was carried out with L-Cysteine (Cys) through the interaction of its thiol groups with unsaturated Cu sites of the Cu-MOF. The characterization was carried out with different analytical methods such as XRD, FTIR, TGA, SEM/EDAX, CHNS, UV-Vis, BET/BJH, and zeta-potential. The cytotoxicity of the nanofibrous mat was investigated on L929 cells and its antibacterial activity was evaluated on both *Gram-positive* and *Gram-negative* bacteria. This nanofibrous mat with controlled release of copper ions and easy fabrication and handling is a good candidate for antibacterial applications.



Schem 1. SEM images of Cu-MOF (a), Cu-MOF@Cys (b), and nanofibrous mat (c)

Keywords: Copper-based metal organic framework, Polyarylonitrile, Nanofibrous mat, Antibacterial performance, Post-synthetic modification

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Polydopamin and Poly(2-hydroxy ethylmethacrylate) coating on silicon surfaces for medical devices applications

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Formation of bacterial biofilm is a severe danger for the public health and global economy. Biofilm can be detected on numerous surfaces initial from plaque on teeth through food packaging materials to water purification filters, medical devices, and oil pipelines [1]. In particular, permanent urinary catheters are widely used in medicine to help people who can not urinate alone. Statistics show that about 15% to 25% of hospitalized patients receive urinary catheters during their stay[2]. Urine catheters are usually made of flexible hydrophobic polymeric materials such as silicone rubber or polyurethane, however, such materials serve as a surface for the growth of urinary pathogens to adhere, followed by colonization and biofilm formation[3,4]. Hydrogels have been considered as antibiofilm materials, a hydrogel raises the hydrophilicity of the surface by forming a hydration layer and prevents the absorption of non-specific proteins. [5]. In the present work, dopamine was polymerized on silicone surfaces and after reactivation of polypopamine with α-Bromoisobutyryl bromide; 2-hydroxyethyl methacrylate monomer was polymerized on the silicone surface. The synthesized compounds were verified by FT-IR, 1H-NMR, XRD, SEM, and TGA. Antibiofilm and antibacterial properties of the prepared coating were investigated.

Keywords: Polydopamin, Poly(2-hydroxy ethylmethacrylate), Silicon, Antibacterial coating.

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Synthesis of Oxazine derivatives under mixed metal oxide magnetic nanocatalyst

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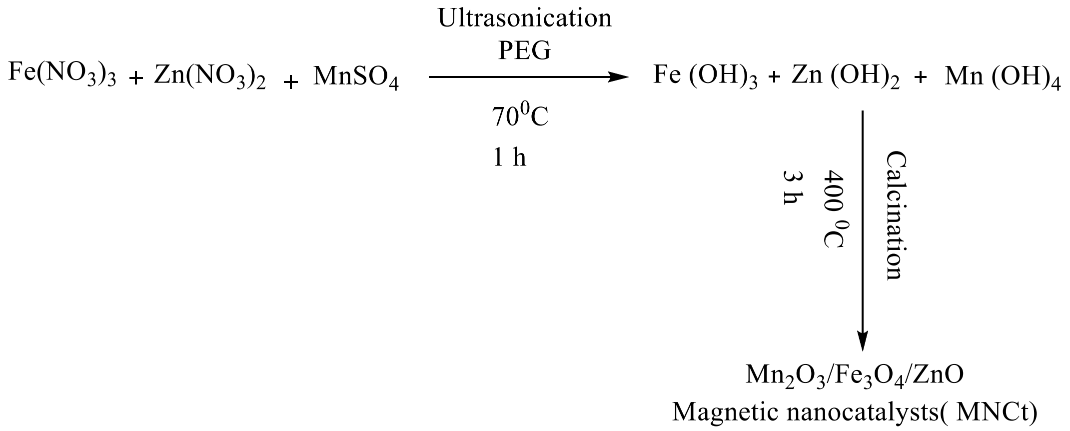
In the present study, mixed metal oxide nanocatalyst have been explored as an efficient, cost-effective, and recyclable nanocatalyst for environmentally protocol and efficient synthesis of pharmaceutically interesting Naphtho [1,2-e] [1,3] Oxazine derivatives through a one-pot three-component condensation of aromatic aldehydes, β-naphthol and urea under green conditions in water solvent and short reaction time with excellent yields. The structure of products was approved by FT-IR, ^{1}H-NMR spectroscopy and melting point. The results of SEM imaging of nonacatalyst showed that all compounds have a spherical morphological structure with mean diameter of 16.50 ± 3.94. These nanoparticles are important in organic reaction with their ability to be easily separated and recycled by magnetic field.



$$Fe(NO_3)_3 + Zn(NO_3)_2 + MnSO_4 \xrightarrow[70^0C,\ 1\ h]{\text{Ultrasonication, PEG}} Fe\,(OH)_3 + Zn\,(OH)_2 + Mn\,(OH)_4 \xrightarrow[3\ h]{\text{Calcination, } 400\ ^0C} Mn_2O_3/Fe_3O_4/ZnO$$

Schem 1. Structural formula for the synthesis of manganese oxide / iron oxide / zinc oxide nanocatalysts

Keywords: Magnetic Nano Catalyst, Ultrasonic, Oxazine, Aqueous medium

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Use of povidone-iodine as an efficient catalyst in the one-pot oxidative cyclization of new 1,2,4-triazolo[4,3-a]pyridine derivatives

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Triazolopyridines are an important fused-ring heterocycle several important medicine e.g. Nefazodone and Trazodone have triazolopyridine ring. The 1,2,4-triazolo[4,3-a]pyridine structure extensively exists in many compounds with various pharmaceutical properties, e.g. anti-antiproliferative, antibacterial, inflammatory, antithrombotic, antidepressant/ antipsychotic, and antiviral activities [1]. In all syntheses of [1,2,4]triazolo[4,3-a]pyridines the electron-withdrawing substituents on the pyridine ring can cause Dimroth rearrangement of the initially formed compounds into derivatives of [1,2,4]triazolo[l,5-a]pyridines. In this abstract simplistic and organized approach to synthesis 1,2,4-triazolo[4,3-a]pyridines and related heterocycles has been completed via one-pot condensation of readily available 2-hydrazineylpyridine with corresponding aldehydes monitored by I_2-sources facilitated oxidative-cyclization [2]. This one-pot MCRs is appropriate to a variety of aromatic, aliphatic, bis-, tris-, and a,b-unsaturated aldehydes, and can be suitably conducted on the gram scale. Here for the first time in contribution to our previous interest [3], we have developed a short and efficient synthesis of *N*-fused 1,2,4-triazoles using a mild and straightforward one-pot oxidative cyclization method using (6 mole %, $PVPI_3^-$ which is a commercially available reagent, 0.5 mmol of each starting materials at RT and in 1-4 h. A variety of substituents are tolerated allowing the synthesis of diverse products in good to excellent yields. The main improvement of this procedure is to access *N*-fused 1,2,4-triazoles in high yields and short reaction time. The newly developed synthetic route is believed to be valuable for the construction of building blocks and also for medicinal chemistry studies comprising *N*-fused 1,2,4-triazole moiety.

Keywords: 1,2,4-triazolo[4,3-a]pyridines, one-pot multicomponent oxidative cyclization, I_2-sources **(**$PVPI_3^-$ **)**

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Tandem and oxidative synthesis of oxazolines and benzoxazoles from Aminoalcohols and different aldehydes using potassium cyanide

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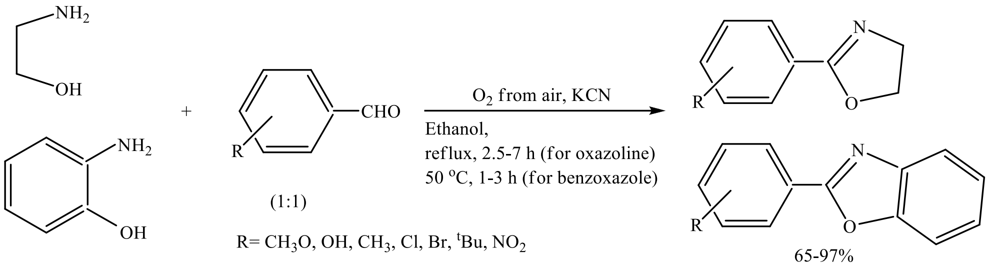
A lot of important biological active compounds and drugs contain oxazoline or benzoxazole cores in their structures.[1] Thus, the preparation of these valuable heterocycles has established an important synthetic strategy specially from the point of view of medicinal chemistry.[2] However, some method synthesizing these important compounds have some disadvantages such as high temperature, long reaction time, acidic condition, using unavailable reagent or catalyst, using a strong or specific oxidant, low yields, and so on.[3] Here, in an innovative way, the tandem and oxidative synthesis of these compounds is introduced from the reaction of aldehydes with 2-aminoethanol and *o*-aminophenol respectively using oxygen from air and potassium cyanide (Figure 1). Various aromatic aldehydes containing electron withdrawing or donating groups are efficiently converted to their corresponding oxazolines or benzoxazoles in this way. Reusability of potassium cyanide, using oxygen from air as a green and the simplest available oxidant together with the tandem nature make the present method in accordance with green chemistry principles. Good to excellent yields, relatively short reaction times, easy work-up and also excellent chemoselectivity are considered as other advantages of each of these conversions.



Keywords: Aldehyde, Oxazoline, Benzoxazole, Potassium cyanide, Tandem synthesis.

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Conductive electrospun nanofibers based on PVA/graphene/cellulose nanocrystals as wound healing

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An perfect wound healing has properties such as antimicrobial activity, non-toxicity, gas exchange ability, constant drug release in the wound, biocompatibility, and ease of removal [1]. Colonization of Bacterial in the wound environment leads to lasting inflammation and delayed wound healing[2]. The use of appropriate antibiotics is essential to prevent infection and bacterial growth. Antimicrobial compounds include honey, silver, iodine, and antibiotics such as gentamicin, metronidazole, and neomycin used in wound healings. [3] Curcumin has been extensively used in wound healing because of antibacterial, anti-inflammatory, and antioxidant activity [4-5]. In the present work, electrospun nanofibers based on PVA, aminated graphene and oxidized cellulose nanocrystals were prepared and crosslinking of nanofibers was performed at room temperature according to Schiff-base reaction and different proportions of curcumin were used to prepare nanofibers. The synthesized compounds were verified by FT-IR, 1H-NMR, SEM, and TGA. and the mechanical properties,morphology, conductivity, contact angle, and antibacterial properties of the prepared nanofibers were investigated.

Keywords: PVA, Graphene, Cellulose nanocrystals, Curcumin, Wound healing.

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One-pot synthesis and antibacterial evaluation of 2-(4-(14H-dibenzo[a,j]xanthen-14-yl)phenyl)-4,5-diaryl-1H-imidazole using choline chloride.2 $ZnCl_2$ as catalyst

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A novel, and simple way for synthesis of imidazole derivatives bearing dibenzo[a,j]xanthene moiety, in one-pot four-component reaction from 2-naphthol, terephthalaldehyde, benzil derivatives, and ammonium acetate in presence of Choline chloride.2 $ZnCl_2$ as a green and reusable catalyst are described. These original compounds were established by spectral methods ^{1}H NMR, ^{13}C NMR, FT-IR, and elemental analysis. The antibacterial assay of the synthesized compounds was also evaluated. The minimum inhibitory concentration was determined for the test compounds as well as for reference standards.

Keywords: Deep-Eutectic Solvents, Imidazole, One-Pot reaction, Dibenzo[a,j]xanthene.

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Novel electrically conductive nanofibrous scaffolds-based polyaniline-*grafted* tragacanth gum and investigation of their performances in skin tissue engineering application

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Tissue engineering (TE) is a multi-disciplinary science that introduced as a powerful strategy for regeneration or repair of failed tissues/organs[1,2]. This relatively new science is the base of living cells, signal molecules, and scaffolds. The aime of this study was to design and development of novel electrically conductive nanofibrous scaffolds based on tragacanth gum (TG), polyaniline (PANI), and poly(vinyl alcohole)[3,4]. For this purpose, the TG was functiionalized with *p*-antanilic acid, and then anilne monomer was grafted onto the functiionalized TG *via* an oxidation polymerization approach to afford a TG-*g*-PANI copolymer. The TG-*g*-PANI/PVA nanofibrous scaffolds with differne weight ratios were fabricated *via* co-electrospinning technique. The fabricated scaffolds showed porous morphology with interconnected 3D structure according to scanning electron microscopy (SEM) image. Some physicochemical (*e.g.,* electerrical cnductivity and hydrophilicity) as well as biological (*e.g.,* biodegradability, cytocoptability, cells adhesion and prolifration capability) features of developed scaffolds were investigated[5]. As the results, it was found that the TG-*g*-PANI/PVA nanofibrous scaffolds have acceptable potential for especial types of TE (*e.g.,* skine, nerve, and bone) that require electroactivity, owing to significant effect of electrical conductivity on cell's adhesion, migration and differentiation, as well as DNA synthesis and protein secretion.

Keywords: Natural polymers, Tragacanth gum, Electrospinning, Polymeric scaffolds, Tissue enginering

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Iodine Functionalized Magnetic Graphene as a New and Efficient Nanocatalyst for Acetylation of Sugar Derivatives

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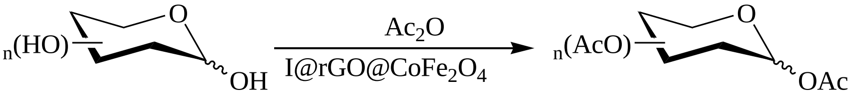
Per-*O*-acetylation is an important organic reaction used for the initial protection of hydroxyl groups. Acylation of sugars is conducted in both acidic and basic catalysts. Catalysis plays a key role in the chemical processes that could not only promote chemical reactions but also reduce toxicities, unwanted products, and enhance the selectivity of desirable products, especially those that could be new approaches to green chemistry [1]. The supported magnetic nanocomposite retains the desirable properties of both homogeneous and heterogeneous systems. Increasing the catalytic activity, the possibility of separation by magnetic field without the use of centrifugation, filtration, and also the possibility of recycling the catalyst in the next reaction is the reason for the expansion of these compounds [2-3]. In this study, environmentally friendly, iodine-based magnetic nanocomposites were synthesized by a three-step simple process. Iodine was loaded by deep eutectic solvent (DES) as a reducing agent of graphene oxide (GO) and simultaneously, immobilizing iodine as a new and effective nanocatalyst for synthesis of acetylation reactions of various sugar derivatives (Fig 1). The X-ray diffraction (XRD) pattern of magnetic nanocomposite identified the orthogonal structure of the $CoFe_2O_4$ and the nanoparticles were well reduced on the GO, and scanning electron micrographs (SEM) showed that iodine and $CoFe_2O_4$ were uniformly dispersed on the graphene oxide sheets. I@rGO@$CoFe_2O_4$ nano-crystallites were also characterized by the thermogravimetric analysis (TGA), Fourier transform infrared spectroscopy (FT-IR), and vibrating sample magnetometer (VSM). After determining the optimal reaction conditions with the solvent-free for the synthesis of per-*O*-acetylated glucose, several native mono and disaccharides reacted well with high yields in the presence of I@rGO@$CoFe_2O_4$. This reaction was successful for the disaccharides like sucrose and lactose. Per-*O*-acetylation of mannose and mannitol under similar conditions at room temperature showed the least time among other sugars. While the best yields at room temperature belonged to glucose within 10 minutes.



Schem 1. Synthesis of per-*O*-acetylation of cabohydrates

Keywords: Per-*O*-acetylation, Sugar, Magnetic nanocomposite

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Antibacterial and cytotoxicity evaluation of poly (*N*-vinyl imidazole)/ graphene oxide nanocomposite hydrogels

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Hydrogels represent an important class of biomaterials in biotechnology and medicine because many hydrogels exhibit excellent biocompatibility, causing minimal inflammatory responses, thrombosis, and tissue damage. N-vinyl imidazole (VI)-based hydrogels have attracted considerable attention in biomedical applications since they show antibacterial activity, biocompatibility, and improved biodegradability [1]. Functional nanocomposite VI-based hydrogel systems have received great interest in the preparation of new hydrogels with improved physical and mechanical properties [2]. The applications of graphene-based composite hydrogels as promising materials for biomedical applications have been exhaustively studied [3]. Graphene oxide (GO), one of the most important derivatives of graphene, has also attracted considerable attention in recent years. Two series of pH-sensitive poly (N-vinyl imidazole)/GO nanocomposite hydrogels (PVI/GO) were synthesized successfully via an in-situ polymerization approach. In the first series, the polymerization was carried out with different feeding ratios of VI and MBA (N, N′- methylene-bis-acrylamide) in the presence of GO (0.3-1.0 wt%) (PVI/GO-1). The second series was prepared using VI and DIL (3, 3′ -divinyl-1, 1′ (1, 6-hexanediyl) di-imidazolium dibromide) (PVI/GO-2) as an ionic liquid crosslinker in the presence of GO. PVI/GO-1 hydrogels become stiffer and more brittle than less-strength elastic PVI/GO-2 hydrogels. The prepared PVI/GO nanocomposite exhibited significant antibacterial activity against Gram-negative bacteria. In addition, the results showed that GO and ionic DIL cross-linker have improved the antibacterial activity of PVI/NGQD hydrogels. Finally, cell proliferation and cytotoxicity studies represented that these nanocomposite hydrogels can be considered as a potential candidate for biomedical applications. The synthesized PVI/GO nanocomposite hydrogels were characterized by FT-IR, TGA, XRD, EDS and SEM.

Keywords: Nanocomposite hydrogels, Graphene oxide, N-vinyl imidazole, Antibacterial, Cytotoxicity.

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Synthesis and characterization of melamine-based porous polyamides

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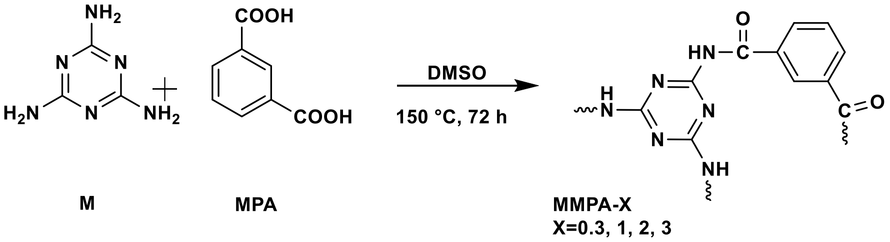
Porous organic frameworks/polymers (POFs/POPs) are an attractive class of porous materials due to their distinctive features including simple synthesis, permanent and tunable porosity, high specific surface area, good thermal stability and low density. They have been recently received increasing attention and research interest mainly due to their wide variety of potential applications such as gas storage, catalysis, pollutants adsorption, molecular separations, etc. [1]. Among the different classes of POPs, covalent triazine-based polymers (CTPs) are a promising type of materials containing nitrogen-rich porous frameworks with high potential adsorption materials [2]. Reversible bond formation, pre-orientation, and reduction of conformers can lead to crystalline covalently connected materials. The present study aims to synthesis and characterization of nitrogen-rich porous polyamides by catalyst free one-pot polycondensation under mild condition. CTPs are constructed from melamine (MA) and m-phthalic acid (MPA) with different molar ratios. As the mole ratio of MA:MPA was adjusted to 3:1, 2:3, 1:1 and 1:3 the corresponding MMPA was named MMPA-3, MMPA-2, MMPA-1, MMPA-0.3, respectively (Fig. 1). The obtained MMPAs have been characterized by FTIR, TGA, XRD, BET and FE-SEM. The effect of molar ratio of MA/MMPA on the thermal stability, crystallinity, porosity and morphology of MMPAs was systematically examined. Among synthesized MMPAs, only the sample with lower amount of melamine (MMPA-0.3) had crystalline structure.



Schem. 1 Schematic representation of the synthesis of MMPA

Keywords: Porous organic polymers, Triazine-based polymers, Melamine, m-Phthalic acid

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Synthesis of a new derivative of tetrazolo(1,5-a)pyrimidine

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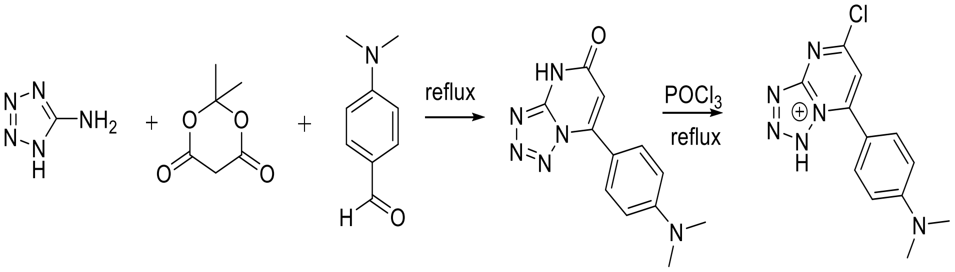
The high biological activity and low toxicity of tetrazole have made this compound a biochemical and pharmacological target [1]. Since the structure of pyrimidine is a nuclear structure that is biologically important and shows the effects of cytotoxicity against different classes of cancer cells [2]. Tetrazole with pyrimidine as a key unit, have special drug importance that has been well studied, and biological applications [3]. Tetrazole (1,5-a) pyrimidines, which have multifaceted properties and various derivatives of them have been studied, which can be used in medicine. In this paper, the synthesis of a new derivative called 4,(5-chlorotetrazolo(1,5-a) pyrimidine-7-yl)-n,n-dimethyl aniline) in a single container method in a facial multi-component reaction with high efficiency was reported. The final product of synthesis is in the form of yellow powder with melting point of 176 °C (figure 1). Since according to previous studies, different derivatives of this structure have antimicrobial power, so it is expected that the new compound as an antibacterial agent will bring good results further study of drug.



Schem 1. synthesis of 4,(5-chlorotetrazolo(1,5-a) pyrimidine-7-yl)-n,n-dimethyl aniline)

Keywords: 5-Amino-1H-tetrazole, Tetrazolo(1,5-a)pyrimidine, Biological properties, Antibacterial

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Preparation and characterization of fluorescent melamine-formaldehyde resin microspheres

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The melamine-formaldehyde (MF) resin is prepared from the polycondensation of melamine and formaldehyde. MF microspheres have been synthesized by different synthetic methods with various types of catalysts and surfactants [1]. Abundant pores and a high amount of nitrogen functionalities endow MF microspheres as a promising and low-cost absorbent, pollutants in water, heavy metal ions adsorption, acid dyes and carbon dioxide capture [2], etc. We have successfully synthesized weekly cross-linked MF colloidal microparticles with relatively monodisperse size by dispersed polycondensation and subsequent pH adjustment with acetic acid. Additionally, a variety of microspheres has been doped during formation, by incorporating fluorescent graphene quantum dot (GQD) nanoparticles [3] into the microspheres and then further polymerization and cross-linking. The obtained MF-GQD microspheres with luminescent properties have been characterized by Fourier-transform infrared spectroscopy (FTIR), thermal gravimetric analysis (TGA), X-ray diffraction (XRD), dynamic light scattering (DLS), UV–vis absorption and scanning electron microscopy (SEM). The effects of the GQDs amount (2-10 wt%) have been investigated on the various properties such as morphology, particle size and fluorescent emission of MF-GQD microcapsules. By adjusting the amount of GQDs added, the amount of encapsulated GQDs in the water-soluble MF microspheres, and consequently their fluorescent emission, was effectively regulated. The prepared microspheres may present potential applications in the fields of optoelectronic devices, bio-imaging, medical diagnosis, and the packing structural functional composites.

Keywords: Melamine-formaldehyde microsphere, Graphene quantum dot, Fluorescent, Composite

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Surface modified silica-coated manganese ferrite nanoparticles as efficient adsorbents for heavy metal removal from wastewater

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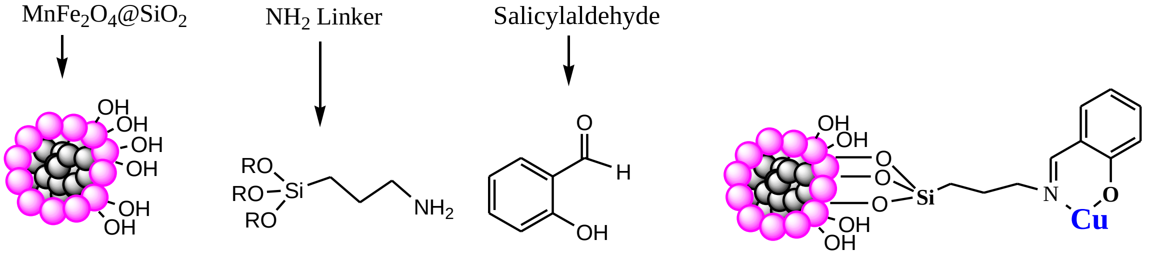
Copper is widely used in many industries, such as electroplating, paint, metal finishing, electrical, fertilizer,woodmanufacturing and pigment industries. In recent years, for the treatment of Cu (II)-rich effluents, considerable attention has been concentrated on the removal of Cu^{2+} ions by adsorption method because it is simple, relative low-cost, 0effective and flexible in design and operation[1]. Recently, extensive researches have been focused on the development of adsorption methods. The development of improved adsorbents for the removal of toxic heavy metal ions from wastewater remains a continuing research objective for environmental pollution control processes[2]. Magnetic nanoparticles have continued to draw considerable interests because of their great potential applications in magnetic fluids, catalysis, biotechnology/biomedicine, magnetic resonance imaging and magnetic recording devices in view of its paramagnetism, biocompatibility and safety. There are researches on the application of adsorption in the environmental area by magnetic nanoparticles. Specifically, the adsorptions of heavy metal ions onto mesoporous magnetic nanoparticles possess intriguing features for the adsorption of heavy metal ions, such as easy recover, large surface area, high pore volume, ordered porous channels, uniform and tunable pore structure, and great diversity in surface functionalization[3]. In the present study, amine-functionalized silica-coated magnetic nanoparticles have been reported in the adsorption of Cu heavy metal ion from wastewater. The adsorption data obeyed the Langmuir equation. The copper ions can be desorbed from this Nano-particles with 47% desorption efficiency and the Surface modified silica-coated-MNPs exhibit good recyclability.



Keywords: Manganese ferrite, Nanoparticles, Heavy metal, Wastewater.

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Synthesis and characterization of melamine-based covalent organic framework

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Covalent organic frameworks (COFs) are an emerging class of porous covalent organic structures whose backbones were composed of light elements (B, C, N, O, Si) and linked by robust covalent bonds to endow such material with desirable properties, i.e., inherent porosity, well-defined pore aperture, ordered channel structure, large surface area, high stability, and multi-dimension [1]. As COF can be crystalline and are porous polymers with predictable/tunable structures, they provide great potential in many fields of applications such as separation and gas storage, electronic devices and catalysis. Interestingly, COFs were reported for use as catalyst in two ways; as size selective catalysts, and as a template for catalytically active nanoparticle preparation [2]. In this study, we report the synthesis and characterization of melamine-based COFs using a dibromoalkane with different molar ratios of 1:1, 1:2 and 2:1 melamine to dibromoalkane via solvothermal method.The structure of the synthesized melamine-based COFs was characterized by scanning electron microscopy (SEM), Fourier transform infrared spectroscopy (FT-IR), thermaogravimetric analysis (TGA) and X-ray diffraction (XRD). The porosity analyses were also done via BET measurements and fluorescent properties were studied by fluorescence spectrometer. Furthermore, the effect of molar ratio of melamine/dibromoalkane on the porosity, thermal stability, solubility, crystallinity and optic properties of the prepared COFs was examined.

Keywords: Covalent-organic frameworks, Porous polymers, Melamine, Dibromoalkane

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Novel 1,2-aminopropanthiols substituted derivatives as selective carbonic anhydrase,acetylcholinesterase and α −glycosidase enzymes inhibitors

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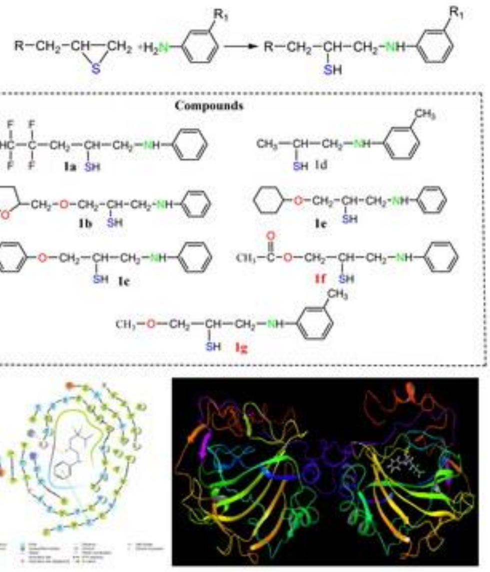
Aminothiol derivatives exhibit a wide range of biological activites and can function as potential medicinal molecules in the development of a drug.In recent years, due interes has been allocated to them in connection with their versatile use in medicine as well as intermediates of organic synthesis.Aminothiols constitute an important class of compounds for medicinal and synthetic chemistry.Some of them (e.q. cysteine, homocysteine) are used as drugs in medicine.The synthetic aminothiol ,amifostine, was originally developed as a radioprotector and has been extensively used as a chemical radioprotector for the normal tissues in cancer radiotherapy and chemotherapy.Aminothiols and their derivatives also exhibit a variety of other physiological activity.These compounds can be used to create blockers,autoimmunomodulators, antiseptics and hypomicimic agents.They can serve as key compounds for the synthesis of various nitrogen and sulfur-containing heterocyclics,allowing them to be widely used as drugs in pharmacological practice.Aminothiols are the sinton for fine compounds in the making physiologically active compounds[1,2]



***Keywords**:* 1,2-aminopropanthiol,enzyme,inhibition,molecular docking

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New 1,2,3-triazole-methoxybenzylidene acetohydrazide hybrids as potent α-glucosidase inhibitors: synthesis, in vitro enzymatic and α-glucosidase inhibitors evaluations

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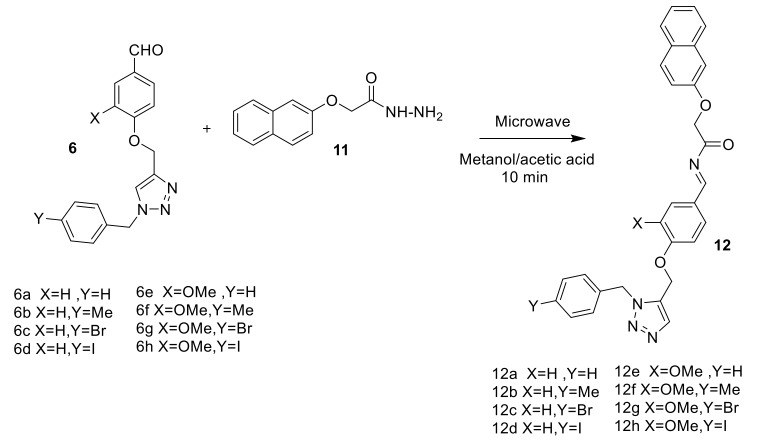
A novel series of 1,2,3-triazole-methoxybenzylidene[1] acetohydrazide derivatives **12a-h** were designed, synthesized, and evaluated for their in vitro α-glucosidase inhibitory activity leading to efficient anti-diabetic agents.[2] Eight 1,2,3-triazole-methoxybenzylidene acetohydrazide derivatives **12a-h** were synthesized into three main steps. In the first step, the 1,2, 3-triazole bearing aldehyde group moiety 6a-h wrer efficiently constructed via a click multicomponent reaction of 3 a,b with 5. In the second step the other starting material bearing hydrazine group was prepared from the reaction of **9** and **10**. In the last step in the presence of microwave reaction between aldehyde group moiety 6a-h and hydrazine groups moiety **11**, final products **12a-h** were produced The synthetic molecules were characterized *via* FT-IR,1H-NMR and ^{13}C-NMR spectroscopic techniques and elemental analysis and evaluated for their anti-hyperglycemic potential. Compounds **12a-h** exhibited good to moderate *in α*-glucosidase inhibitory activities in the range of IC50 values (2.01 ± 0.036 to 2.09 ± 0.08µM) as compared to the standard acarbose (IC50 = 1.92 ± 0.17 µM) and (IC50 = 1.99 ± 0.07 µM), respectively.



Keywords: Triazoles, acetohydrazide, α-Glucosidase inhibitors, Anti-hyperglycemic activity

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Synthesis of 5-((1-H-Tetrazol-5-yl)-2-aminophenyl) methanol) as novel fluorescent dye

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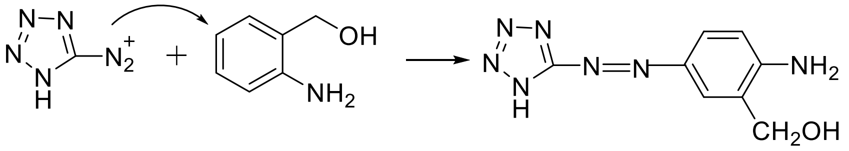
The growing interest in the use of fluorescent pigments has been partly brought about by an increasing awareness of safety considerations, and also because pigments in either paints or inks provide a striking contrast to the normal range of paints on which they may be superimposed. This feature can be utilised in advertising posters where eyecatching appeal can be particularly rewarding. The main feature of fluorescent pigments in comparison with luminescent pigments is that they only emit light on excitation, such as with natural or ultraviolet light. In contrast, luminescent pigments have the property of absorbing light which falls upon them and re-emitting it over a period of time on a different wavelength[1]. In this article, we synthesized a fluorescent dye based on 5-aminotrazole and 2-amino benzyl alcohol. 0.17 g of 5-amino-1H-tetrazole was added into a balloon containing 5 ml of a mixture of water and added two drops of 98% sulfuric acid to the reaction mixture. Then 0.137 g of sodium nitrite was added to the reaction mixture. After completion of the reaction, in the next step, 0.2 ml of 2-amino benzyl alcohol was added dropwise to the reaction mixture to obtaine the brown fluorescent product. The synthesis of this substance was investigated and proven by FTIR and 1H NMR and 1C NMR devices.



Keywords: 5-Aminothiazole, 2-Amino benzyl alcohol, Fluorescent dye, Diazonium salt

Reference

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Doped-boron nitride nanostructures as a potential removal of rimantadine from environment: A DFT study

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When a drug is released in large quantities into the environment and nature, it is dangerous and requires removal where the drug accumulates, for example in water and soil. Therefore, design of a device to removal the accumulated drugs in environmental is very important. The rimantadine drug (Rd) can be one of those drugs that needs to removal the amount in environment [1]. The purpose of this computational study is to measure and evaluate the interaction of rimantadine drug with boron nitride and its doped nanostructures. The BN nanoparticles have a wide range of attractive properties such as stability, high temperature strength, low dielectric constant, high thermal conductivity and oxidation resistance, which leads to a number of potential applications as electronic materials [2].

In this work, we studied that replacing the Al, Si and Ga atoms instead of a boron atom in boron nitride nanosheet (BNNSh) is a useful way to removal of Rd from environment. We studied the interaction between Ge-, Si- and Ga-doped-BNNSh and the Rd drug to determine which one of the doped nanostructures is better to removal of Rd using the B3LYP method with a basis set of 6-31G(d) by Gaussian software 09. A poor energy interaction between the Rd drug and the boron nitride nanoparticle was observed. The results show that the Ga-doped BNNSh is the best nanostructure for removal of Rd drug.

Keywords: Boron nitride nanostructures, Removal, Rimantadine, Environment, DFT

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Magnetic Mesoporous Organosilica Nanoparticle with Pyridine-Dicarboxamide Units: Application as Catalyst Support for CO_2 Fixation

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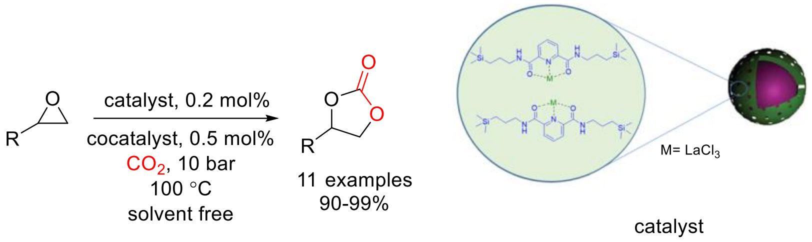
The unwanted CO_2 emmision from the use of fossil fuels and industrial activities causes global warming and its subsequent concerns. Although the limitation in the generation of CO_2 is defined as the first protocol for solving this issue, the capture and then CO_2 utilization as C1 feedstock has drawn more and more attentions from sustainability and green chemical synthesis point of views[1]. Among various types of CO_2 conversion pathways, direct coupling of carbon dioxide with epoxides resulting in the corresponding cyclic carbonates has been very interested due to atom-economical, scalable and industrially [2]. To date, various types of mesoporous materials comprising either metal or organocatalyst were developed for this important transformation[3]. Herein, we would like to describe magnetic mesoporous organosilica structures with the pyridine-dicarboxamide framework as a solid ligand for immobilization of lanthanum catalyst for CO_2 cycloaddition to various types of epoxides under relatively mild reaction conditions. Thanks to the high surface area, uniform and adjustable pore diameter, and significant pore volume, the presented catalyst shows good to excellent activity for the titled carbon dioxide conversion. The catalyst could also be reused for at least five reaction cycles without any remarkable decrease in activity and selectivity.



Keywords: CO_2 fixation, Cyclic carbonates, Mesoporous organosilica nanoparticle, Heterogeneous catalysis

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Efficient CO_2 Fixation Catalyzed by Ionic Liquid Supported on the Magnetic Yolk-Shell Mesoporous Silica

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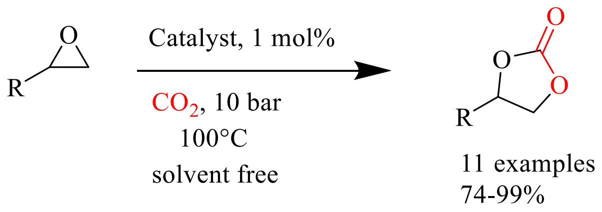
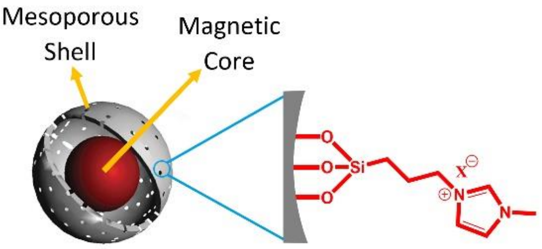
During the past 30 years, excessive use of fossil fuels, deforestation, urban development and industrialization have drastically increased the CO_2 concentration on the atmosphere. Global warming, melting polar glaciers and climate change are among the most important consequence of this phenomenon.[1] To address these issues, much research has been devoted to CO_2 capture and storage (CCS) and subsequent its conversion to value-added chemicals.[2] Among various ways of CO_2 valorisation, its conversion to cyclic carbonates *via* direct coupling of CO_2 with epoxide has received more attention.[3] However, CO_2 is thermodynamically stable and this kind of transformation inherently needs suitable either metal or organocatalyst. Porous materials are considered as good candidate to design novel catalyst for conversion of CO_2 to cyclic carbonates due to their large surface area, high pore volume and tuneable pore size. [4] Herein, we wish to disclose ionic liquid grafted on the magnetic yolk-shell mesoporous silica (IL@MYS) as recoverable, durable and efficient catalyst for conversion CO_2 to cyclic carbonates. Our studies revealed that due to porous shell with short channels, hollow region, a large surface area, high conversion of various type of epoxide under relatively mile reaction condition was achieved. The catalyst was also simply recovered by using external magnet and reused for several times without remarkable loss of activity and selectivity.





Keywords: CO_2 fixation, Mesoporous silica, Yolk-shell, Ionic liquid, Magnetic nanocatalyst

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A new strategy to intercalate metal particles between two-dimensional polymers

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Two-dimensional polymers (2DPs) with planar structures have attracted a great deal of attention, due to their extraordinary mechanical, physical, optical and chemical properties [1],[2]. In contrast to the conventional linear, dendritic and network polymers with a wide variety of synthetic procedures, synthesis of two-dimensional polymers is challenging owing to the problems related to the confining monomers in sheet like structures [3],[4]. Herein, we report a new strategy to synthesize conjugated 2DPs based on triazine under mild conditions. Reaction between nucleophiles and triazine was promoted by special factors to force polymerization in two-dimensions and construction of 2D polymers. This reaction was directed in two dimensions by formation of porous nanopolymers in the presence of a strong base. This study provides a general guidance for the design and construction of new two-dimensional polymers with different geometry. We have studied the mechanism of reactions in detail to find and control the parameters that affect the strcture of the final product. We have used coordination chemistry as well as aromaticity as two main factors to drive polymerization in certain topologies and orientations, then we used a new strategy to intercalate metal particles between two-dimensional materials. The synthesized polymer was characterized by FT-IR, SEM, XRD and TGA. SEM images show surface morphology with a medium-sized layer structure in the micrometer range.

Keywords: Two-dimensional polymers, Triazine, Sheet-like

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Use of magnetic recyclable bionanocomposite catalysts in the synthesis of benzo[*g*]thiazolo[3,2-*a*]quinolines based on nitroketene acetal

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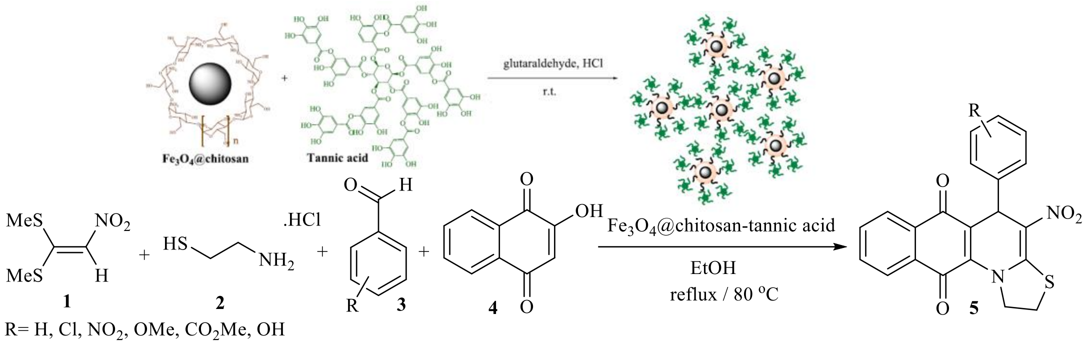
An important issue to discover biological structures is the design of sustainable, safe, clean, cost-effective, and excellent efficient synthetic reactions to provide compounds with interesting biological properties.[1] Among sulfur-nitrogen containing heterocycles, thiazolo[3,2-*a*]pyridines are an important class of compounds with two different fused heterocycles, which are found in a broad range of compounds with a variety of biological activities.[2] Due to the essential demand for the production of small molecules containing bioactive heterocycles with green approach and in order to improve efficiency and reaction time, here a novel method has been developed to prepare a series of heterocycles containing thiazole and benzo-fused quinoline rings from one-pot four-component reaction of nitroketene dithioacetals, cysteamine hydrochloride, 2-hydroxy-1,4-naphthoquinone and aromatic aldehydes in presence of Fe_3O_4@chitosan-tannic acid as a heterogeneous nanocatalyst in excellent yields and shorter reaction time than other methods (Scheme 1). This novel magnetic bionanocomposite was synthesized with chitosan and tannic acid as a natural material with unique properties, including high performance, easy separation from the reaction mixture by an external magnet, and recyclability.[3] The synthesized bionanocatalyst and the structures of all the synthesized compounds were characterized by essential analysis.



Scheme 1. Catalytic activity of Fe_3O_4@chitosan-tannic acid in the synthesis of thiazolo quinolines

Keywords: Nitroketene acetal, Thiazolo quinoline, Bionanocomposite, Magnetic catalyst.

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UV resistant Smart UV-curable Polyurethane Acrylate Nanocomposite Reinforced with Graphene Quantum Dots

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This project focuses on synthesis of smart biofriendly UV-curable polyurethane acrylate nanocomposites reinforced with graphene quantum dots (GQDs) and investigates the UV protective property of the resultant product. Polyurethanes are used in production of transparent and flexible coatings, adhesives, and multiple purposes owing to distinguished features such as high mechanical, chemical and thermal resistance. lately, usage of UV-curable polyurethanes has interested industrialists and researchers due to biocompatibility, removing of hazardous organic solvents, high speed curing at low temperature and economizing on energy consumption [1]. GQDs have many applications because of some features including solubility in water, biocompatibility and terrific optical features such as ability to absorb UV rays [2]. Smart coatings possess photo-responsive properties [3]. Use of GQDs in synthesis of polymer nanocomposites could be a good idea to produce smart coatings with fluorescence property and ability to protect from UV rays.

On this basis, GQDs were synthesized using pyrolysis of citric acid and the preparation steps were performed as described in the previous works [4,5]. Afterwards, GQDs 0.5 wt% were added to UV-curable polyurethane acrylate resin and then graphene quantum dots/polyurethane acrylate nanocomposite (GQDs 0.5 wt%/PU) was achieved. UV resistance property and fluorescence feature of the nanocomposite film were confirmed through photoluminescence and UV-visible spectroscopies. The results proved that the synthesized nanocomposite absorbed about 90% of UV radiation. This coating with specific abilities could be used in aircraft, automotive, building, electronic, and drugs and foods packaging industries.

Keywords: UV-curable, Polyurethane acrylate, Graphene quantum dots, UV resistant

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Preparation and characterization of hydrogel based on graphene and chitosan for waste water treatment

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Nowadays, due to the growing environmental awareness and concerns over the increasing use of dyes in the synthesis, printing, textile and food, it is necessary to resolve environmental problems [1,2]. Up to now, a wide range of biological and physicochemical approaches, including chemical oxidation, biodegradation, electrolysis, photo-catalytic degradation, membrane separation and adsorption have been developed to treat dyeing wastewater. Among these methods, adsorption is the most broadly used method owing to its easy and safe operation, high efficiency and comparatively low cost [3]. Chitosan is a non-toxic, biodegradable and biocompatible polysaccharide. Several researchers have reported the graphene or chitosan composite hydrogels as efficient adsorbents for water purification [4].

Graphene oxide, a modifed graphene material, contains various oxygen containing functional groups, such as epoxides, hydroxyls, and carboxyls in its basal plane or at dges. Specifcally, these oxygen groups can bind to positively charged organic compounds via electrostatic interactions. However, the contribution of GO to dye adsorption can be attributed to the π–π stacking interactions between the aromatic ring of the dye and the basal planes of GO [5]. The objective of this work is to generate a hydrogel based on graphene and chitosan for their use as dye sorbents in liquid media. The surface morphology and chemical structure of the nanocomposite hydrogel were characterized by FTIR, TGA, Raman, XRD and SEM. The UV/Visible absorption spectrum revealed that the obtained porous nanocomposite hydrogel can efficiently remove anionic dyes from wastewater with high absorption power.

Keywords: Graphene, Chitosan, Hydrogel

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Wastewater Treatment by Phytoremediation in constructed wetlands as a green technology

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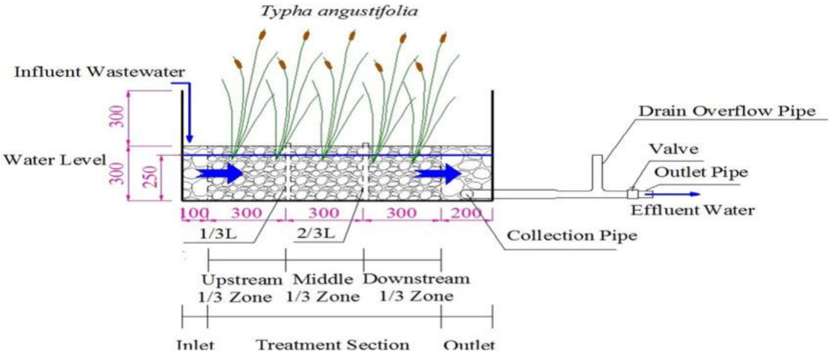
Water is an exceptionally essential source for the presence of life on the earth. The water quality has seriously affected because of the overgrowth of the population, human activities, and unskilled utilization of natural water resources [1]. Constructed wetland (CW) systems are used worldwide for removing pollutants from several types of wastewater. Their construction is relatively simple and their operational and maintenance costs are lower than conventional wastewater treatment technologies [2]. Plant metabolism can help to remediate or clean up contaminated sites. The pollutants enter the plant primarily via the roots, which contains many detoxifying mechanisms, provides surface area for adsorption and accumulation of water and nutrients that promote growth. These pollutants when absorbed by the plant, may be stored in the roots, stems, or leaves; changed into less harmful chemicals within the plant; or changed into gases that are released into the air as the plant transpires [3]. In this study, plants were selected and exposed to contaminated water. After a specified time, the output water was tested and the percentage of contaminated material was calculated. Then different parts of the plant were tested.



Keywords: Phytoremediation, Industrial and textile wastewater, Heavy metals, Pigments, Environment.

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Removal of heavy metal ions in industrial wastewater using Graphene oxide–ferro oxide nanocomposites

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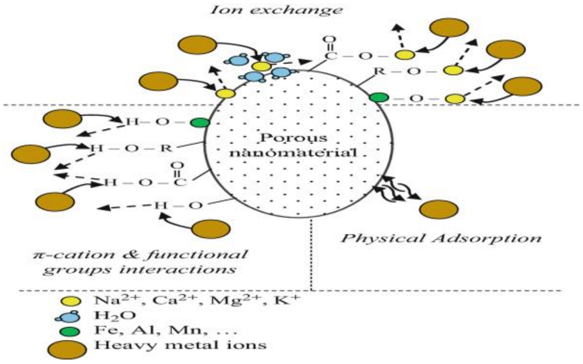
Removal of contaminants in wastewater, such as heavy metals, has become a severe problem in the world. The endless introduction of toxic heavy metals through industrialization has worsened the heavy metal pollution in the environment. Up till now, numerous technologies have been developed to solve this problem, including chemical precipitation, ion exchange, adsorption, membrane filtration, electrochemical treatment, and so on. As an emerging technology, nanotechnology has been gaining increasing interest and many nanomaterials have been developed to remove heavy metals from polluted water, due to their excellent features resulting from the nanometer effect. Heavy metals such as Pb, Zn, Cu, Hg, etc. could pose a severe threat to human's health because they can be accumulated biologically in the food chain. In this work, novel nanomaterials, including graphene oxide-based nanomaterials, and nanocomposites, and their applications for the removal of heavy metal ions from wastewater were systematically reviewed. Their efficiency, limitations, and advantages were compared and discussed [1]. Nano size graphene is known to possess large surface area and some promising properties in terms of mechanical, electrical, chemical and magnetism. Hence, graphene oxide-based nanomaterials are discovered to be useful in the application of heavy metal removal from wastewater [2].



Keywords: Graphene, Nanomaterials, Heavy metal, Industrial wastewater.

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Preparation of anti-corrosion and wear resistant nanocomposites using the graphene oxide functionalized with metal elements

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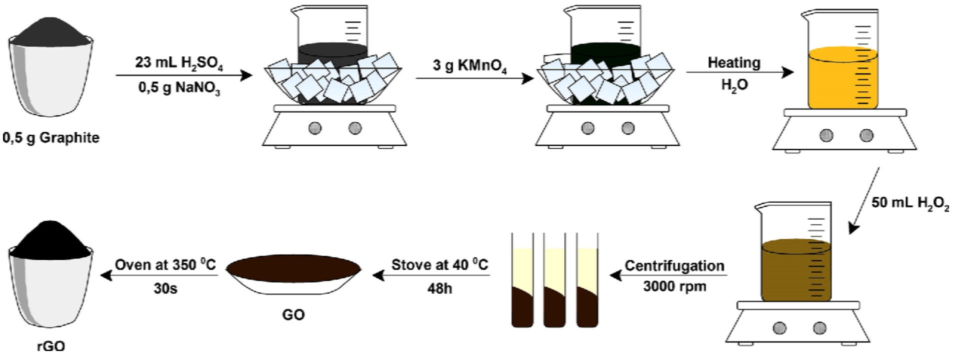
Graphene oxide nanocomposite laminates with high degree of graphitization and little structural damage were found to be highly impermeable to all gases, liquids and aggressive chemicals[1].Therefore, the nanocomposite sheets used in the present work can effectively prevent the penetration of corrosive media such as Cl ions and dissolved oxygen. Micro pores are the fast diffusion paths of corrosive media in coatings. In the present work, the proper addition of nanocomposites effectively decreased the number and size of the pores.



Keywords: Graphen, Graphene oxide, Corrosion, Nano composite

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Green synthesis of substituted thiazine derivatives using an efficient Cadmium nanocatalyst

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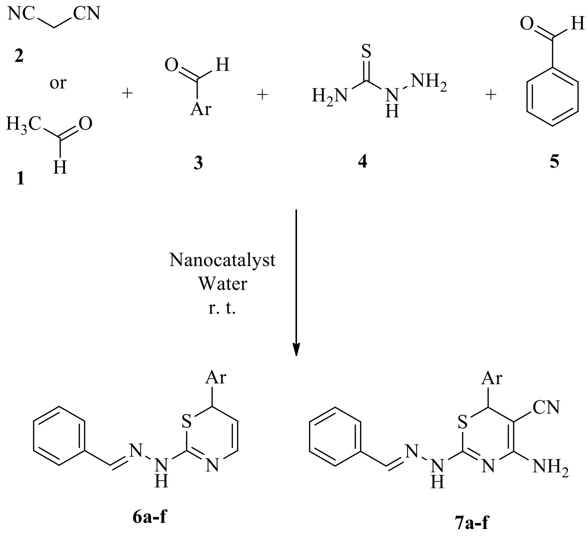
In current report, γ-Fe_2O_3@FAp@Cd [1-3] was used in the synthesis of novel derivatives of polysubstituted thiazines by the reaction of diverse aryl aldehydes, acetaldehyde or malononitrile, benzaldehyde and thiosemicarbazide in water at room temperature. This method provided a novel approach for the green synthesis of thiazine in excellent yield (85–95%) and reasonable reaction time (60–80 min). The structures of prepared compounds were confirmed by analytical methods.



Ar: 4-Cl. 4-NO_2, 2-NO_2, 4-OH, 2-Br, 4-Me, 4-MeO

Scheme 1. Synthesis of substituted thiazine derivatives (**6a-f**) and **(7a-f)**

Keywords: γ-Fe_2O_3@FAp@Cd, γ-Fe_2O_3, Thiazine, Nanocatalyst, Green synthesis

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Preparation of Nanocomposites Based on Reduced Graphene quantum dot And It's Study in the Removal of Water Pollutants

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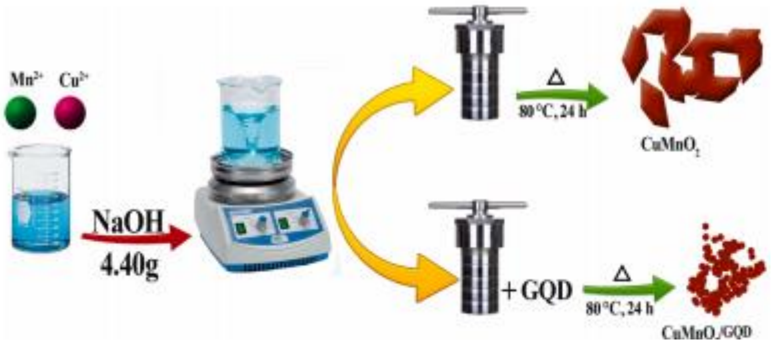
Graphene quantum dots (GQDs) have attracted increasing attention due to their unique properties such as high-water solubility, photoluminescence activity, good biocompatibility, physical, chemical, and electrical properties which makes them appropriate candidates for use in a variety of bio applications, sensors, and photocatalysts [1]. The synthesis of quantum dot graphene was carried out by hydrothermal method, and citric acid was used as a precursor to carbon as well as urea. Nanocomposites made from $Cu\ (NO_3)_2\cdot 3H_2O$ and $Mn\ (NO_3)_2\cdot 4H_2O$ accelerate and improve pollutants such as paint by doping on quantum dot grapheme [2].



***Keywords*:** Nanocomposites, Graphene, Graphene quantum dot, Reduced Quantum Dot Graphene

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Preparation of some new Macrocycle as Nano machine

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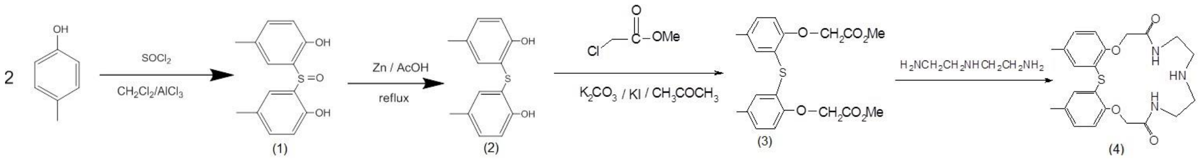
Crown ethers and their compounds have the property of complexing with metals, which is interesting in many fields and in topics such as environmental chemistry, metal extraction and separation, water treatment, nanotechnology, etc. Our aim of this research work is to prepare new diamidic macrocyclic compounds based on dibenzosulfide as receptors for metals, cations and also as components of nanomachines. Prepared macrocycles can bond with metal ions due to having O and N atoms. Crown ethers have the ability to form strong bonds with cations and form complexes, and this is due to the oxygen donor atoms being co-ordinated with the cation inside the ring. Crown ethers are effective in phase catalytic transfer because the outer surface of the ring is hydrophobic [1]. Their selectivity depends on the relative size of the cavity, the diameter of the cation, the number of donor atoms in the crown ring, the relationship between the donor atoms to the cation, and the cation charge [2]. These compounds can also be used as dumbbells and as components of nanomachines. In this research work, we wish to report the preparation some of new constructive component nano machines as diamide macrocycles and related larite. For this purpose, first sulfoxide (1) was prepared by the reaction of thionyl chloride with paracresol with 65% efficiency, then by reduction combination (1) was prepared with zinc powder and bisphenol acetic acid (2). Due to the reaction of bisphenol and methyl chloroacetate in the presence in dry acetone, methyl diester (3) was obtained by reflux with 98% efficiency. Diamide macrocycle (4), with efficiency 70% was prepared by amidation of methyl diester (3) and diethylene triamine and was crystallized by dry methanol. And Larith Ether due to the reaction of macrocycle of diamide with pentanoyl chloride in the presence of triethylamine and in dry dichloromethane solvent reflux was achieved with a yield of 74%.



Schem 1. The prepared compounds were identified by IR spectra, HNMR, CNMR, mass spectrum

Keywords: Crown ethers, Water purification

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Design, synthesis, and application of semicarbazide- pyridoyl-sulfonic acid-based nanocatalyst for the preparation of pyranopyrazole derivatives

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Semicarbazide (SC) is a derivative of urea that is of remarkable interest because of its chemistry to form stable chelates with essential metal ions and potentially beneficial biological activities, such as antitumor, anti-bacterial, antiviral, and antimalarial [1]. Magnetic nanoparticles (MNPs), a type of alternative support or catalyst-supported material, have been recently explored extensively [2]. Among iron oxide magnetic nano-particles, sulfonic acid-functionalized magnetic nanoparticles (SAMN), known as the recoverable solid strong acid, have attracted much attention due to economically important and environmentally benign features [3]. Pyranopyrazoles have received considerable attention due to the wide range of biological activities such as anti-cancer, antileishmanial, antimicrobial, anti-inflammatory, lactamase inhibitor, *etc* [4-5]. In this study, a novel, efficient, and recoverable nanomagnetic catalyst bearing the semicarbazide linkers, namely, FSiPSS was designed, synthesized, and characterized by the use of various techniques such as FT-IR, EDX, elemental mapping analysis, XRD, SEM, TEM, TGA/DTA, BET, and VSM. Then, the catalytic capability of the novel prepared nanomagnetic FSiPSS catalyst was successfully investigated in the synthesis of diverse pyranopyrazoles through a one-pot four-component reaction from commercially available starting materials with the help of ultrasonication in very short reaction time, good to high yields and easy work-up.

Keywords: Semicarbazide, Pyridoyl, Sulfonic acid-based catalyst, Nanomagnetic, Four-component, Pyranopyrazole.

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The Palladium-anchored multidentate SBA-15/tetra-urea: a highly efficient reusable nano-catalyst for Mizoroki-Heck and Suzuki-Miyaura cross-coupling reactions

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Urea and its derivatives have found numerous applications in organic, analytical, and medicinal chemistry, polymer sciences, agriculture, and industry [1]. Nowadays, the heterogenization of metal complexes with catalytic activity within inorganic matrixes (such as SiO_2, MCM-41, SBA, clay, zeolite, etc.) is a field that has advanced due to the combination of high reactivity and chemical selectivity with facile separation of the catalyst [2]. Among them, SBA-15 is endowed with some remarkable properties such as thicker walls, larger pores, and dual pore as well as the highly hydrothermal and thermal stabilities [3]. The immobilization of organic frameworks on/into the mesoporous and microporous materials surface/pores would lead to the materials hydrophobic and hydrothermally stable and thus furnish them with improved catalytic activities in applications for organic synthesis [4]. Therefore, in order to expand the applicability as well as stability of Pd-decorated SBA-15 materials in air and in aqueous media, it is necessary to enhance the surface using organic functional groups by appropriate organic ligands as linkers between SBA-15 silica and Pd [5].

In this study, the surface of mesoporous silica SBA-15 was modified by using a tetra-urea-based ligand which is an inherent air- and moisture-stable ligand. Subsequently, palladium ions were anchored within the multidentate SBA-15@tetra-urea (SBA@TU) pore channels with the help of this ligand. The SBA@TU@Pd nano-structure catalyst was characterized by various techniques. The catalytic activity of the SBA@TU@Pd nano-catalyst was successfully evaluated for Mizoroki-Heck and Suzuki-Miyaura cross-coupling reactions under mild conditions with a minimal amount of Pd. The synthesized mesostructure exhibits advantages such as high stability and activity catalyst, short reaction times, high yields of products, simple recovery, and maintenance of catalytic activity for at least five sequential runs.

Keywords: SBA-15, Tetra-urea-based ligand, Mizoroki-Heck, Suzuki-Miyaura, Cross-coupling reaction.

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Bio-based epoxy thermosets of vanillin-derived epoxy monomer: effect of epoxy monomer functionality on thermal properties

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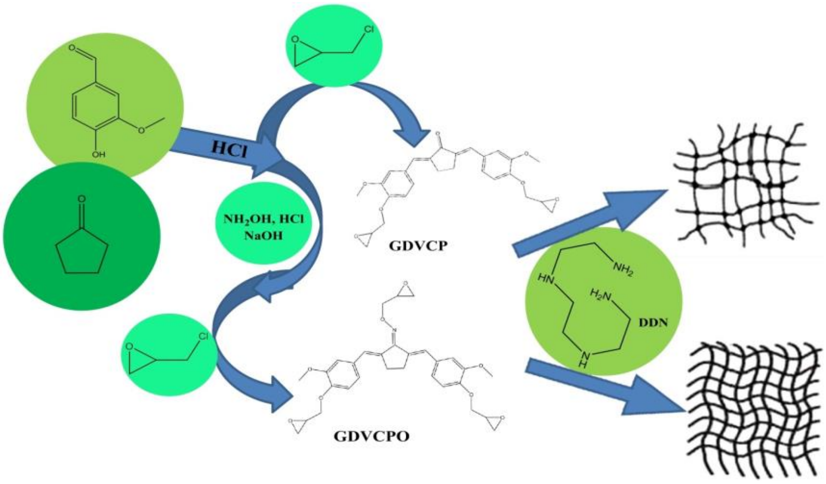
Tri-functional vanillin-derived epoxy monomer (GDVCPO) was developed through the synthesized di-functional reagent (GDVCP) via oximation and cured with a same type of hardener (amine based) to evaluate thermal properties of the resultant epoxy thermosets [1]. At 30 °C, the polymers were all glassy and the progress of curing process was followed by evaluation of the most significant band in FT-IR and DSC thermogram. The number of monomer functionality was found to develop thermal properties of the resultant products to higher value [2] (from 97 to 140 °C). According to the obtained results, increasing the number of functional groups in monomer, increased the cross-linking density and T_g [3] of EDVCPO-DDN comparing with EDVCP-DDN network (140 °C and 97 °C, respectively).



Keywords: Epoxy monomer, bio-based resin, vanillin, functionality

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Study on thermal properties of synthesized vanillin-based epoxy thermoset resins: effect of different hardener

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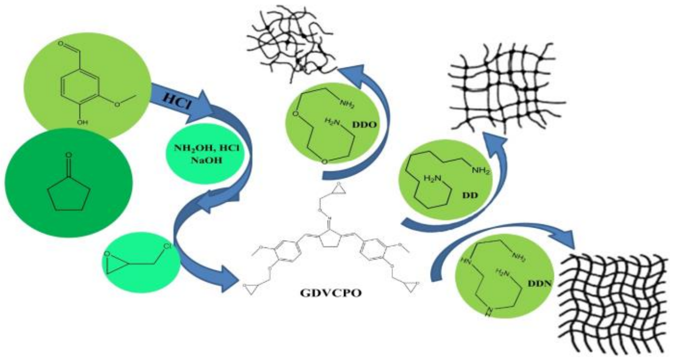
A new bio-based tri-functional epoxy resin was prepared with glycidation of tri-hydroxyl precursor which was synthesized via oximation of a two-functional material derived from vanillin [1]. Various types of amine based hardeners (such as DDN, DD and DDO) were used. Thermal analysis (performed by DSC) of the resulted epoxy-amine products showed the glass transition temperatures (T_g) ranging from 105 to 140 ˚C. For instance, the epoxy network containing DDN (EDVCPO-DDN) displayed higher T_g value (140 ˚C) as compare to the other samples. The behaviour could be due to the higher number of hardener functionality and rigid structure formed inside the network [2]. However, with changing the structure of the hardeners (by atoms), T_g of the resultant thermoset resins decreased to the lowest value [3]. Therefore, the obtained thermoset resins using DDO (as a hardener), possibly diminishing the overall cross-linking and T_g to the lowest value (105 ˚C) among the analogue samples prepared with EDVCPO.



Keywords: Epoxy thermoset resin, Amine based hardener, Cross-linking, Functionality, Glass transition temperature

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Cu-doped into porous-hollow carbon spheres derived from soybean waste; as an efficient nanocatalyst for the Synthesis of 1,2,3-Triazole Derivatives

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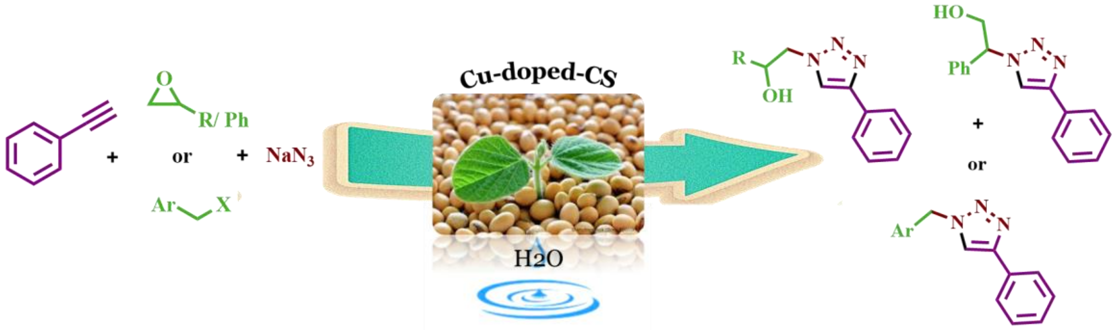
In the present work, Cu doped into porous-hollow carbon spheres prepared by a facile, green, and up-scalable route in two steps. In the first step, the hollow carbon spheres were derived from ground soybean waste by hydrothermal carbonization (HTC) process [1] through controlable high-temperature heat treatment. The second step was completed with copper doping into activated hollow carbon spheres to improve the catalytic performance. The structure of the as-prepared nanocatalyst characterized by a series of measurement techniques, including XRD, FE-SEM, and ICP-OES. The as-prepared copper-rich nanocapsule demonstrated superior activity in selective 1,2,3-triazole derivatives [2-4] in the presence of water as an environmentally benign solvent *via* azide-alkyne cycloaddition reaction.



Keywords: Soybean waste, Carbon spheres, Nanocatalyst 1,2,3-Triazole, Green chemistry.

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Preparation of Magnetic Superabsorbent Nanocomposites Based on Reduced Graphene Oxide with some Metal Elements in order to Remove Lead from the Environment

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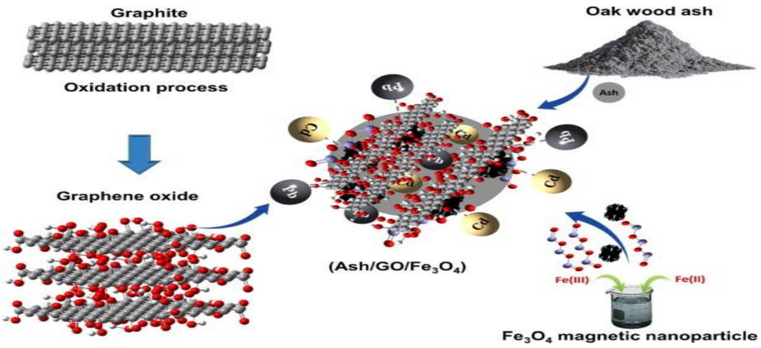
Heavy metals are among the environmental pollutants which humans can encounter through water and food Cause dangerous chronic and acute poisoning. Water pollution with heavy metals, an existing and evolving problem is in the world. Heavy metals such as lead, copper, cadmium, zinc and nickel, Are among the most common pollutants in Industrial wastewater is found [1]. Various methods for removing heavy metals from solutions is used, including ion exchange, Adsorption, reverse osmosis, electrodialysis, concentration evaporation, Bio removal, solvent extraction, clotting and separation process Constantly pointed. Currently for economic and technical reasons, these methods are often not accepted in the country and abroad [2]. Among the adsorbents, graphene oxide nanoparticles due to their potential high absorption capacity and high specific surface area for removal heavy metals are used from water [3].



Keywords : Graphen, Graphene oxide, Magnetic Superabsorbent, Nano composite

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Green Synthesis of Chromeno[2,3-d]pyrimidines with GO-SO$_3$H catalyst

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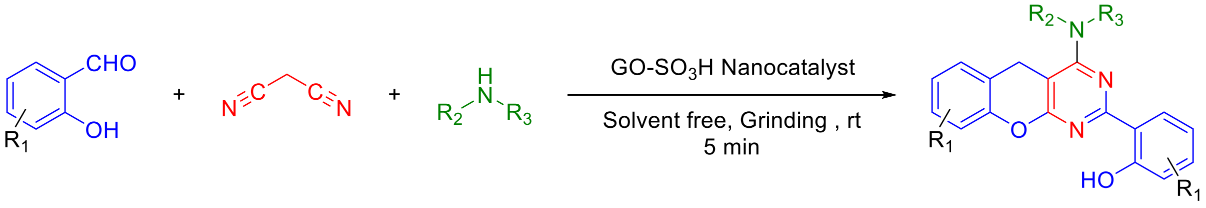
Multicomponent reactions (MCRs) have emerged as invaluable tools in the drug discovery process in a one-pot synthetic operation. MCRs include two or more steps without any isolation of intermediates, which reduce time and save both energy and raw materials. These techniques permit fast, automated, economical, and highthroughput synthesis of the libraries of pharmaceutical and organic compounds [1]. Chromeno[2,3-d]pyrimidines are attracting much attention due to their wide range of pharmacological and biological activities such as in vitro anti-aggregating activities, and also in pharmacological activities such as antiviral, antimicrobial, antifungal, antioxidant, antileishmanial, antitumor, hypotensive, antiproliferation, local anesthetic, antiallergenic, central nervous system (CNS) activities and effects, as well as treatment of Alzheimer's disease and Schizophrenia disorder [2, 3]. In addition, these molecules exhibit excellent photophysical properties but detailed study has not been carried out so far [4]. Chromeno[2,3-d]pyrimidine was first synthesized by O'Callaghan from the condensation reaction of 2-iminocoumarin-3-carboxamides with aldehydes following a complex multi-step protocol [5]. we hereby report functionalized Graphene Oxide as a novel, diversified, recyclable and reusable catalyst for the synthesis of Chromeno[2,3-d]pyrimidine derivatives via a one-pot, pseudo four-component condensation of salicylaldehydes 1a, malononitrile 2a, and secondary amines 3a under solvent free condition at room temperature in 5 minutes.

Keywords: Multicomponent reactions, Knoevenagel condensation, Nanocatalyst, Graphene Oxide, Chromeno[2,3-d]pyrimidines.



1a 2a 3a 4a-4l 45-94%

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Boosting the quaternary ammonium halides catalyzed CO_2 coupling with epoxides on the hollow mesoporous silica sphere

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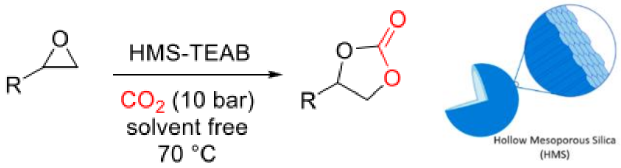
In the present century, the expansion of industrial units, the indiscriminate use of fossil fuels, and population growth have led to the inevitable entry of significant amounts of CO_2 greenhouse gases into the Earth's atmosphere. Considering the essential processes that lead to the production of this greenhouse gas in developing countries such as Iran, it seems that the best way to deal with this crisis is to manage the recovery and intelligent efficiency of CO_2 gas with development. Methods based on green chemistry.[1] Among the various forms of CO_2 conversion to valuable chemicals, the coupling reaction of this gas with epoxides and the formation of five-membered ring carbonates have received much attention.[2] Due to their large surface area, high pore volume, and adjustable pore size, porous materials are good candidates for designing a new catalyst to convert CO_2 to cyclic carbonates.[3] Herein, we want to reveal that mesoporous silica hollow (HMS) with tetraethylammonium bromide (TEAB), could effectively convert CO_2 and various types of epoxides to the corresponding cyclic carbonates under mild reaction conditions. The results show that a hollow region inside the catalyst increases the local concentration and retention time of CO_2 in the catalyst pores, in which tetraethyl ammonium bromides can lead to high conversion of CO_2 molecules through a confinement effect. The catalyst was quickly recovered and reused in 6 consecutive reaction runs during the coupling of styrene oxide and CO_2 with a slight decrease in reactivity.



Keywords: Hollow mesoporous silica sphere, Quaternary ammonium halide, CO_2 Fixation, Cyclic carbonate, Confinement effect

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Novel synthesis metal organic frameworks with sulfonic acid tags Co-MOF-71/Imidazole/SO_3H as catalyst: Its application for the synthesis of new pyrazolo[3,4-*b*]pyridines via a cooperative vinylogous anomeric based oxidation

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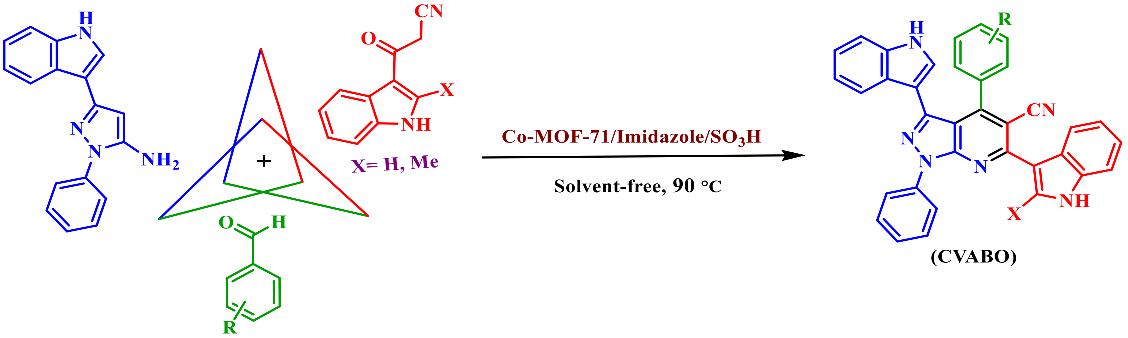
Over the past decade, metal-organic frameworks (MOFs) are known as a porous material that has attracted the attention of many researcher groups and industries. These materials consist of multifunctional organic materials bind to metal or metal clusters through coordinated components such as carboxylates to form crystalline materials with high surface area and high thermal stability. Due to their high design capability in their structures, that is many applications in separation, storage, magnetic resonance imaging (MRI), adsorption and desorption, catalytic, drug delivery and power save [1-2]. Multi-component reactions (MCRs) have been considered as a suitable method for the preparation of many organic and pharmacologically highly biologically active compounds [3]. However, some of these methods are associated with limitations such as the use of expensive raw materials, harsh reaction conditions, long reaction times, and low efficiencies. Therefore, the development of an efficient and versatile catalyst is still needed. Compounds with *N*-SO_3H bonds have been used as efficient catalysts and/or reagents in synthesis of organic molecules [4]. According to the strategy for developing of biologically active compounds, we wish to report Co-MOF-71/Imidazole/SO_3H as metal-organic frameworks as catalyst for the synthesis of novel pyrazolo[3,4-*b*] pyridine derivatives under solvent-free and green conditions *via* CVABO mechanism (Scheme 1).



Scheme 1: Preparation of novel pyrazolo[3,4-*b*] pyridine derivatives using Co-MOF-71/Imidazole/SO_3H.

Keywords: Anomeric effect, Co-MOF-71, Multicomponent reactions, Pyrazolo[3,4-*b*] pyridine.

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Synthesis of Novel Propranolol Derivative Incorporating a Diamondoid Adamantane Motif

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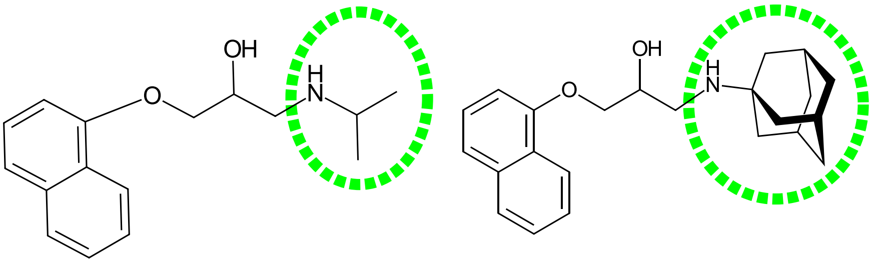
Beta-blockers are a class of medications that prevent endogenous catecholamines from acting on beta adrenergic receptors in the sympathetic nervous system. Propranolol is a beta-adrenergic receptor antagonis, a first-generation beta-blocker that is commonly used to treat heart arrhythmia, hypertension. Additionally, propranolol is an efficient and safe medication for the treatment of migraine headaches, essential tremors, anxiety disorders, and infantile hemangiomas.[1] Diamondoids are a class of hydrocarbon cage molecules that simulate the lattice structure of a diamond. Adamantane is the smallest member of the diamondoid group, consisting of a single cage-shaped diamond crystal unit.[2] Amantadine (as anti-Influenza A), Rimantadine (as anti-Influenza A), Tromantadine (as anti-Herpes simplex agent), Memantine (as anti-HIV), Adapalene (as anti-acne), Saxagliptin and Vildagliptin (as inhibitor of dipeptidyl peptidase IV (DPP-IV inhibitor) for the treatment of type 2 diabetes mellitus (T2DM)) are adamantyl-based compounds which have been introduced to pharmaceutical market and successfully utilized clinically. Amantadine and Memantine are also used for treatment of neurodegenerative disorders. Amantadine gives symptomatic benefits in Parkinson disease, and Memantine are used for the treatment of moderate to severe stages of Alzheimer disease. On the other hand, nowadays adamantane scaffold is used for the modification of known pharmacophors.[3] The adamantane modifications were chosen to enhance lipophilicity and stability of the drugs, thereby improving their pharmacokinetics. In this work, we replaced the isopropyl side chain in a popular Propranolol drug with adamantane moiety. Adamantane is not a magic bullet, but it certainly is more than just a lipophilic add-on.



Keywords: Propranolol, Adamantane, Diamondoid, Nanodiamond, Lipophilic Bullet

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Application of Magnetic Iron Oxide Nanoparticles Modified with GQD/Cu-Ni for Controlled Release of the Anticancer Drug Methotrexate

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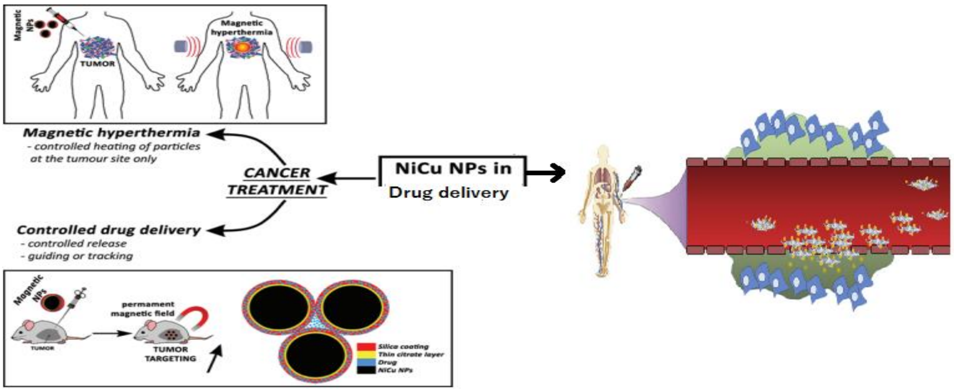
The advanced drug delivery systems, combining the ability to improve the therapeutic efficacy and to reduce side effects of drugs represent a challenge for medicine. Nanotechnology offers a wide range of new strategies to produce innovative nanomaterials, suitable for the development of a large number of smart drug delivery systems, ranging from carbon based nanomaterials (CBNs) toward metallic nanoparticles and nanobiocomposites (NBCs) materials. Among all nanostructures, carbon based nanomaterials seem to be eligible as nanovector of drugs and therapeutics. Graphene exhibits ananosheet structure that makes easier the translocation of the nanocarrier across the cellular membranes and the cellular compartments. Graphene and graphene derivatives exhibit excellent antibacterial and antimicrobial properties, fundamental aspect to avoid/to minimize the bacterial and microbial infections that could occur during therapeutics deliveries [1]. Drug delivery systems are essential components of drugs controlled release [2]. In this articel, the application of graphene quantum dot nanocomposite (GQD)/Cu-Ni coated with magnetic iron oxide nanoparticles was investigated and the synthesized nanocomposite was evaluated as a nanocarrier of the anti-cancer drug methotrexate.



Keywords: Drug delivery, Controlled drug release, Drug nanocarriers, Graphene quantum dots, Methotrexate

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Preparation of Magnetic Iron Oxide Nanoparticles Modified with GQD/Cu-Ni

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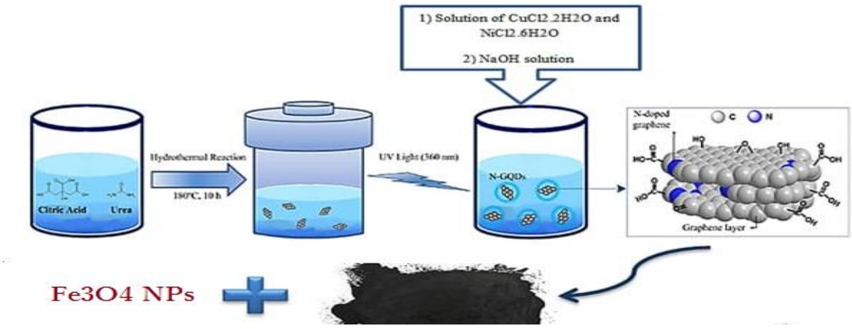
Graphene quantum dots (GQDs), a kind of carbon based quantum dots, are small pieces of graphene sheets with lateral sizes of less than 20 nm and thicknesses of about 0.4-2.0 nm [1]. Graphene quantum dots (GQDs) have attracted increasing attention due to their unique properties such as high water solubility, photoluminescence activity, good biocompatibility, physical, chemical, and electrical properties which makes them appropriate candidates for use in a variety of bioapplications, sensors, and photocatalysts [2]. GQDs possess lower cytotoxicity, large surface area and potential for surface functionalization that bring about as more effective drug loading carrier. Furthermore, the recent developments are carried on the combination of GQDs with metallic or polymeric nanomaterials for imaging and drug delivery aspects [3]. In this study, we synthesized iron oxide nanoparticles modified with GQD / Cu-Ni graphene nanocomposites and tested as a drug nanocarrier. In this study, copper (Cu) and nickel (Ni) metals with excellent magnetic properties and improved nanocarrier performance played a significant role. In synthesized nanocarriers, the presence of magnetic nanoparticles provided the possibility of easy and fast separation and detection.



Keywords: Graphene, Iron oxide nanoparticles, Graphene quantum dots, Drug nanocarriers

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Effect of silica nanoparticles on shear strength of moisture curing silyl-modified polyether sealant

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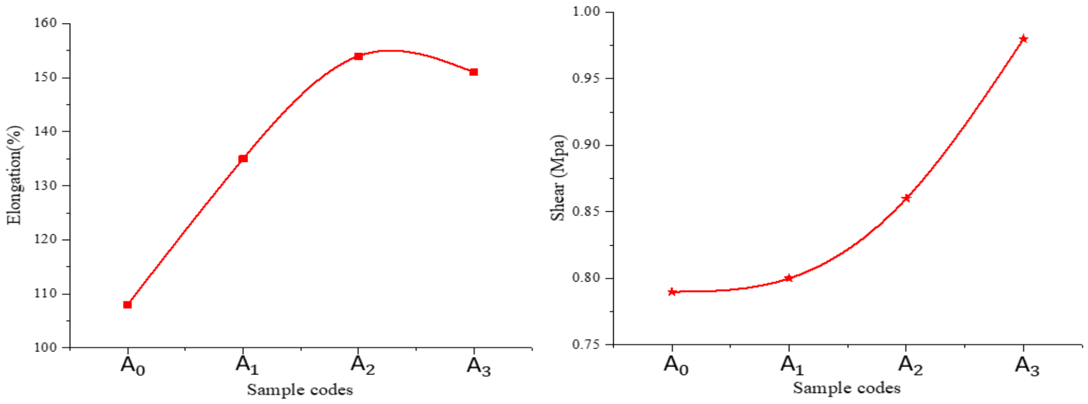
Silyl modified polyether (MS polymer), defined as polymers typically featuring alkoxysilyl functional groups. Curing is a two-step process involving the conversion of the alkoxysilane to silanol and the condensation of −Si−OH and −Si−OR to form siloxane linkages upon elimination of ROH. In this study the influence of quantity (A_0:0%, A_1:0.3%, A_2:0.6% and A_3:0.9% by weight) of nano-silica on the mechanical properties of the formulated silyl-modified polyether sealant have been examined. Studies have shown that with addition of nano-silica (0.9 wt%), shear strength (0.79 Mpa to 0.98 Mpa) and elongation (108% to 151%) were improved 24.05% and 39.81%, respectively, compared with the sample without nano-silica.



(a) (b)

Keywords: Silyl modified polyether, Nano silica, Shear strength, Moisture cure, Sealant.

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The effect of mixing ratio hardener to polymer on shear strength and percentage of elongation in the formulation of two-component adhesives based on MS polymer

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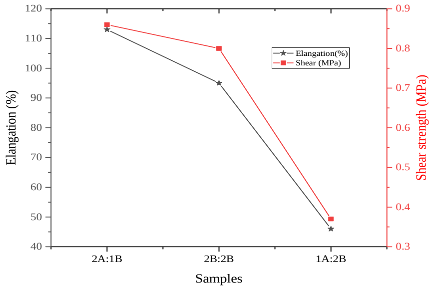
Modified silyl-terminated polyether (MS Polymer) as a widespread material in adhesive and sealant industries may offer advantages over two-component polyurethane adhesives. MS polymer has a polyether backbone that carries methoxysilyl groups, which can crosslink by moisture from the air at ambient temperatures. The silyl-terminated systems are also isocyanate-free systems. They also can provide better stability and low-temperature extrudability than silicone-based systems. The prepared two-component silyl modified polyether sealant includes component A and component B, and the two components react to cure. The mixing ratios for the prepared sealant are 2:1, 2:2 and 1:2 parts by weight. Component A is based on MS polyether polymer and formulated by plasticizer, filler, coupling agent and carbon black. Component B is produced by plasticizer, filler, UV absorber, pigment, adhesion promoter and a catalyst. Studies have shown that by reducing the component B to component A ratio, shear strength and percentage of elongation were improved.



Keywords: MS polymer, Sealant, Shear strength, Two-component, Elongation.

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Efficient Synthesis of Adamantane-Containing Thioureas with Potential Anti-cancer Activity

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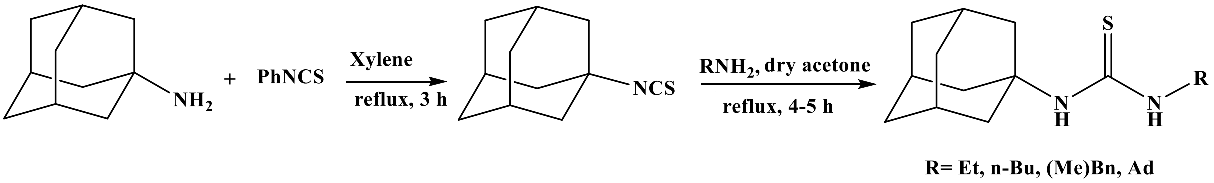
Cancer is emerging as one of the fastest-growing diseases in the world and a leading cause of death following cardiovascular diseases. Cancer is the world's second-largest cause of death; accounting for 9.6 million deaths in 2018 [1]. Currently marketed anticancer medications have increasing problems of various toxic side effects and development of resistance to their action. So, there is an urgent clinical need for the synthesis of novel anticancer agents that are potentially more effective and have higher safety profile [2]. Adamantane, the simplest of the diamondoid structures, is a stable, rigid, symmetrical and bulky tricyclic hydrocarbon. Adamantane derivatives have numerous applications especially in medicinal chemistry. There are eight adamantane-based drugs in pharmaceutical market. Additionally due to the remarkable physico-chemical properties of adamantane, such as size, rigidity, stability, biocompatibility, and unique lipophilicity, this scaffold is used as an "add-on" for known pharmacophors for modification of drugs. The adamantane modifications were chosen to enhance lipophilicity and stability of the drugs, thereby improving their pharmacokinetics. There are many drug candidates containing adamantane scaffold [3]. Hence, in this work we synthesized potential biologically active thioureas containing adamantane moiety and then studied their anti-cancer properties**.** Reaction of amines with isothiocyanates is among the most widely used procedures for the preparation of thioureas. Due to the bimolecular nature of this reaction, the adamantane moiety can be introduced in to the molecule of thiourea either with adamantyl amine or with adamantyl isothiocyanate. We firstly prepared adamantyl isothiocyanate then it was undertaken with different amines for preparation of adamantane-containing N,N-disubstituted thioureas (Scheme 1).



Schem 1. Synthesis of adamantane-containing thiourea derivatives

Keywords: Adamantane motif, Diamondoid, Anti-cancer, 1,3-Disubstituted thioureas.

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Mesoporous silica nanoparticle supported iron catalyst for CO_2 cycloaddtion to epoxides

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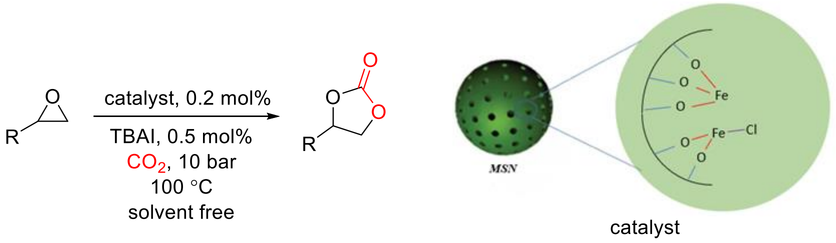
In recent decades, the global climate condition has been adversely affected by the rapid increase in carbon dioxide emissions from fossil fuel combustion related to transportation, industrialization, and other human activities. The concentration of CO_2 has reached an alarming level (415.34 ppm), and to address this issue, the development of inexpensive, eco-friendly, and sustainable approaches for CO_2 capture and subsequent conversion into valuable products have drawn more attention [1]. Among various types of CO_2 valorizations, the reaction between epoxides and CO_2 which is resulted in five-membered cyclic carbonates is paid attention due to its products being extensively used as a polar aprotic solvent in battery electrolytes and intermediates or precursors in the production of polycarbonates and pharmaceuticals [2]. Porous materials are appropriate candidates for designing a new catalyst for the conversion of CO_2 to cyclic carbonates because of their large surface area, large porosity, and adjustable porosity.[3] Herein, the direct coupling of carbon dioxide with epoxides in the presence of the catalytic amount of iron immobilized on mesoporous silica nanoparticles (MSN) in combination with tetra-n-butylammonium iodide (TBAI), under relatively mild reaction conditions has been described. We demonstrated that CO_2, along with various types of epoxides, could be effectively and selectively converted to cyclic carbonates at 100 °C within a short reaction time. The catalyst was also recovered and reused in four consecutive reaction runs with a slight decrease in reactivity and selectivity.



Keywords: Mesoporous silica nanoparticles, Iron catalyst, CO_2 Conversion, Cyclic carbonate, Heterogeneous catalysis.

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Coupling of CO_2 with Epoxides by Periodic Mesoporous Organosilica with Ionic Liquid Frameworks under Solvent and Metal-Free Conditions

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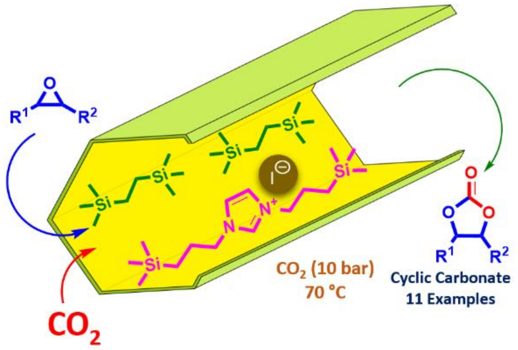
Over the past two decades, human activities have drastically increased the concentration of carbon dioxide in the atmosphere, a major problem that results in intense greenhouse effects. Although some strategies have been developed to reduce or retard CO_2 pollu, nowadays, capturetion and utilization of CO_2 in value-added products are considered the main challenging projects to moderate CO_2 environmental impact.[1] The catalytic formation of cyclic organic carbonates *via* direct coupling epoxides with CO_2 has received significant attention.[2] The imidazolium-based ionic liquids are considered eco-friendly organocatalysts for this important transformation.[3] It was well-documented that incorporation of ionic liquid into the porous materials not only provides the possibility of using them in a more effective pathway and the recovery of ionic liquid, but the porous networks could also potentially help to increase the retention time of CO_2 around catalyst, thus improving the efficiency of CO_2 capture and utilization. Herein, bifunctional periodic mesoporous organosilica with ionic liquid and ethylene frameworks (BFPMO-IL) were used as efficient support for immobilizing iodide ions as an efficient and straightforward organocatalyst for the preparation of cyclic carbonates from carbon dioxide with various types of epoxides under solvent, additive and metal-free reaction conditions.



Keywords: Periodic mesoporous organosilica, Ionic liquid, CO_2 Conversion, Cyclic carbonate.

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Synthesis and characterisation of 2-Alkoxy-8-methyl-6-(pyrrolidin-1-yl)-4*H*-[1,2,4]triazolo[5,1-*f*]purine: A novel heterocyclic framework

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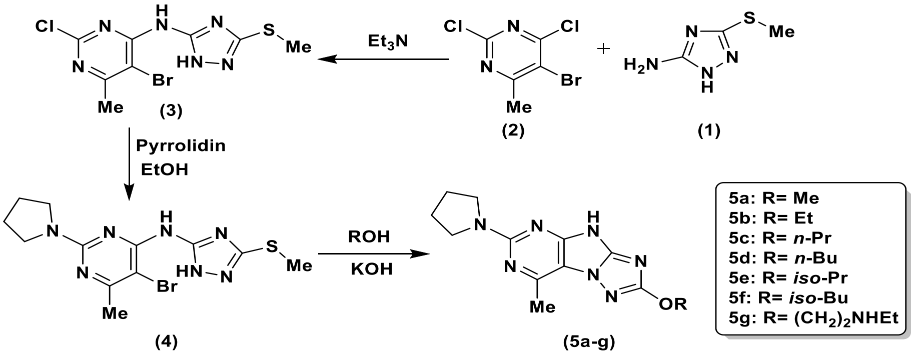
Purine, a natural spread heterocyclic core, plays an important role in life cycles of human, flora, and fauna. Purine-based compounds are currently used in the treatment of a wide range of diseases such as cancers, viral diseases, neuropsychiatric disorders, neurodegenerative diseases, inflammatory diseases, tuberculosis, or impotence [1] The interest in synthesis of purines springs from the biological and pharmaceutical importance of naturally occurring purines such as antibacterial [2], anti-inflammatory [3] activities, as well as efficacy in photodynamic therapy [4]. They also have agrochemical properties including herbicidal and soil fungicidal activity; thus, they have been used as pesticides and insecticides [5]. In the present work, initially the reaction of 5-amino-3-(methylthio)-1*H*-1,2,4-triazole (1) with 5-bromo-2,4-dichloro-6-methylpyrimidine (2) in refluxing Et_3N gave 5-bromo-2-chloro-6-methyl-*N*-(3-(methylthio)-1*H*-1,2,4-triazol-5-yl)pyrimidin-4-amine (3) which were subsequently underwent S_NAr reaction with pyrrolidine in boiling EtOH to yield quantitatively the corresponding pyrrolidine-substituted compound (4). Further reaction of the latter compound with different alcohols in the presence of KOH under reflux condition was resulted in the synthesis of various derivatives (5a-g) having novel [1,2,4]triazolo[5,1-*f*]purine heterocyclic core via cyclocondensation.



Keywords: Purine, Purine-based compounds, [1,2,4]Triazolo[5,1-f]purine, Heterocyclic core

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Synthesis of new derivatives of a novel [1,3]selenazolo[5,4-*e*][1,2,4]triazolo[1,5-*c*]pyrimidine heterocyclic architecture via Dimroth rearrangement

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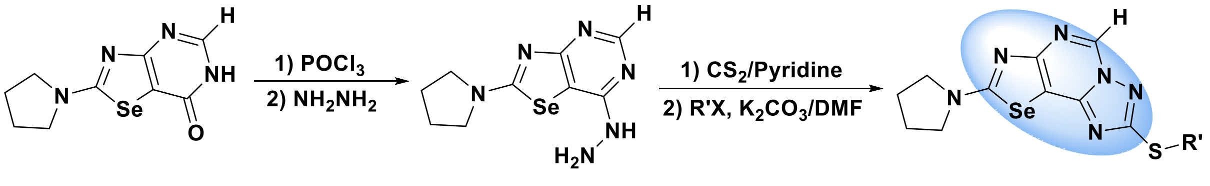
Amongst heterocyclic organoselenium cores, 1,3-selenazole skeleton has received much attention from medicinal chemists. The worldwide high profile of 1,3-selenazoles is not only because of the presence of the selenazole moiety in many pharmacologically active substances such as selenazofurin and amselamine, but also biological properties include antioxidant [1], anticancer [2], human carbonic anhydrase IX inhibitory [3], antimicrobial and anticonvulsant [4] activities. Based on the broad spectrum biological activities of selenazoles and aiming to synthesize novel fused heterocycles containing Se in their scaffold, in the present protocol, 2-(pyrrolidin-1-yl)-[1,3]selenazolo[4,5-*d*]pyrimidin-7(6*H*)-one **(1)** was synthesized as a starting material and subsequently treated with $POCl_3$ and hydrazine hydrate to give 7-hydrazinated selenazolo[4,5-*d*]pyrimidines **(2)**. The heterocyclization of compound **(2)** with CS_2 via pyridine base-catalyzed Dimroth rearrangement yielded a novel tricyclic [1,3]selenazolo[5,4-*e*][1,2,4]triazolo[1,5-*c*]pyrimidine framework which was subsequently converted to the desired *S*-alkylated derivatives **(3a-f)** on treatment with various alkyl halides in the presence of K_2CO_3/DMF in good yields.



(1)

(2)

(3a-f)

(6a): R'= Me; (6b): R'= Et; (6c): R'= *n*-Pr; (6d): R'= *n*-Bu; (6e): R'= Bn; (6f): R'= CH_2CO_2Et

Keywords: Selenazole, [1,3]selenazolo[5,4-e][1,2,4]triazolo[1,5-c]pyrimidine, Base-catalyzed Dimroth rearrangement, Selenazolo[4,5-d]pyrimidine

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Carbon cage adsorbent synthesized with graphene quantum dot composite for methylene blue removal

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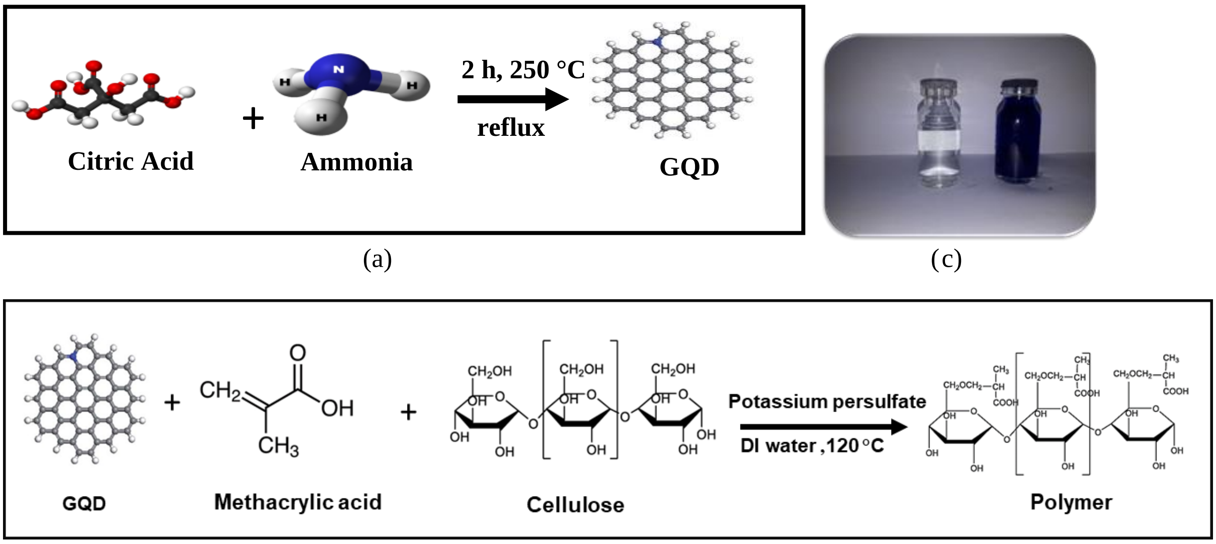
Graphene based materials, including graphene and derivatives such as graphene oxide and graphene quantum dots, have considerable potential as key components in next-generation membrane technologies. Their tunable size, surface chemistry, and structure can be engineered for a spectrum of aqueous filtration purposes ranging from ultrafiltration to reverse osmosis [1]. Membrane-based separation technology has been introduced in dyes removal treatment and is well known for its advantages. Previously various techniques such as nanofiltration, photodegradation, oxidation, biological treatment, adsorption and liquid membrane separation have been developed for the degradation and removal of toxic dyes from contaminated water [2]. In this work we have fabricated a GQD based polymer adsorbent. In a typical synthesis, GQD was synthesized through carbonization of citric acid and ammonia. The synthesized GQD was modified with methacrylic acid and (acrylamidomethyl)- cellulose acetate butyrate to form polymeric adsorbent. The synthesized adsorbnet was charactrized by FT-IR, XRD, FE-SEM and TGA to prove the correctness of the synthesis method. The different concentration of methylene blue solutions prepared and concentration of each solution before and after filtration was determined by UV spectrometer.



(a) (c)

(b)

Schem. 1 Schematic synthesis of (a) GQD, (b) schematic synthesis of polymeric adsorbent and (c) filtered methylene blue

Keywords: Graphene Quantum Dot (GQD), Adsorbent, Polymer, Wastewater, Methylene blue

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Synthesis and modification of super lipophilic magnetic graphene oxide as an oil additive

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Friction and wear are the two major reasons for energy and material losses in mechanical processes. Lubrication is a principal issue to improve energy efficiency and mechanical durability. Irrespective of the finishing of any metal surface, it contains ridges, valleys, asperities and depressions [1,2]. The dispersion of graphene in nonpolar media, such as polyethylene, can be improved by the modification of the graphene surface with nonpolar materials. Some research groups have functionalized graphene with long alkyl groups by the reaction of GO and long alkyl amines and subsequent chemical reduction and improved lipophilicity via the reaction of long alkyl compounds with the remnant oxygen-containing groups on the graphene. As an oil additive, modified graphene must be able to form a uniform and stable dispersion in fluid, promising features to achieve good electrical, thermal, and tribological (friction and wear). The high electrothermal conductivity of graphene is much focused on as a lubricating material, and it presents the role of high thermal conductivity and cooling effect in the lubricant. Graphene and its derivatives have been considered as one of the most promising and attractive lubricating nanomaterials and hold potentials in tribological applications. They were employed not only as solid lubricants to form protective membranes on certain substrates, but also as reinforcing phases in various polymers, ceramics and lubricating additives in various base oils [3,4]. In this research, a simple, industrial and fast exfoliation technique for the production of graphene using sodium azide and graphite in a water solvent without the need for a specific device has been presented following by lipophilizing with octylamine and only with Fe (II). Magnetic nanoparticles were applied on graphene surface, and simultaneously the graphene surface was both lipophilic and magnetic. The method used for graphene production is unique up to now and also it does not oxidize in production procedure. Performed analyzes demonstrate non-destructive properties without any changes in surface functional groups.

Keywords: Graphene, Exfoliation, Lipophile magnetic graphene, Tribology, Oil additive

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Synthesis of crystal-based graphene quantum with novel morphology by triammonium citrate

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Graphene quantum dots (GQDs) that consist of nano meter-scaled graphene particles with sp^2-sp^2 carbon bonds are expected to show specific properties like size dependent general quantum dots (QDs) [1, 2] or chemically modified quantum dots with sp^2-sp^2 carbon bonds. In contrast to graphene, most applications of GQDs have been focused on the photoluminescence (PL)-related fields since GQDs show a PL. Recent studies clears that, additional properties of GQDs such as high transparency and high surface area have been discussed for energy and display applications [3]. N-doping into graphene was highly effective in modulating its band gap to achieve new properties for device applications [4]. Due to the considerable quantum confinement and edge effects of GQDs, direct substitution with nitrogen in GQDs lattice can drastically modulate the chemical and electronic properties and offer more active sites, thus leading to unexpected phenomena which could be extensively applied in various fields. Recently, N-doped GQDs (N-GQDs) have been synthesized through hydrothermal or electrochemical methods which are based on slicing graphene oxide (GO) and its reduction. However, synthesis of GO typically takes several days and requires lots of strong chemical acid and oxidant in a series of chemical treatments of the bulk graphite powder [5]. In this research work, first, triammonium citrate crystal (TAC) was synthesized in pure form with new angles and crystallography with a new method and the structure was determined which was used for synthesizing nitrogen doped- graphene quantum dot. Therefore, we have reported a facile hydrothermal method for synthesis N-GQD. Synthesized N-GQD has special morphology, fluorescence and viscosity. Compared with other nitrogen compounds that is necessary for N-GQD synthesis, ammonia is much more suitable due to low toxicity and stability.

Keywords: Triammonium citrate crystal, Nitrogen-doped graphene quantum dot, Crystallography

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Room Temperature and Metal-Free Thiocyanation of Aromatic Heterocycles and Enamines

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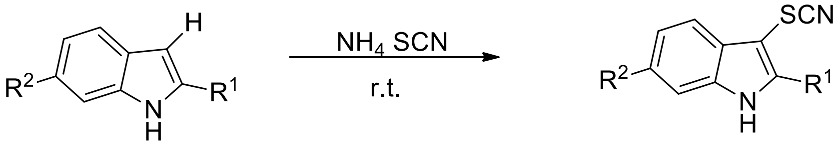
A one-pot, rapid metal-free method for thiocynation of heterocycles and aromatic compounds have been developed. The thiocyanate moiety in aromatic and heteroaromatic compounds is critical in organic synthesis and pharmaceuticals[1]. Most applications of the thiocyanate motif have been regarded when used as an active group on *N*-bearing (hetero) arene compounds. Nitrogen exists in all living organisms, mainly amino acids, proteins, and nucleic acids (DNA and RNA). Although the conveyed methods are efficient, some have disfavors, including low yields, intensely acidic conditions, prolonged reaction times, high temperatures, and costly and toxic reagents or solvents [2]. So, designing new protocols for the thiocyanation of organic compounds is yet in demand. The salient features of this method are the use of an eco-friendly oxidant, reaction tunability to access various products, broad substrate scope, and good to very good yields [3].

In this project, an efficient room temperature,and metal-free procedure has been developed for thiocyanation of indole, isatin and its derivatives in a one-pot and mild manner.



Keywords: Thiocynation, Heterocyle, Arylheterocycles

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Synthesis of ZnGlu MOF/Mesoporous Silica SBA-16: as an Eco-Friendly Highly Efficient Nanocomposite for Solvent-Free Chemical Fixation of Carbon Dioxide with Epoxides

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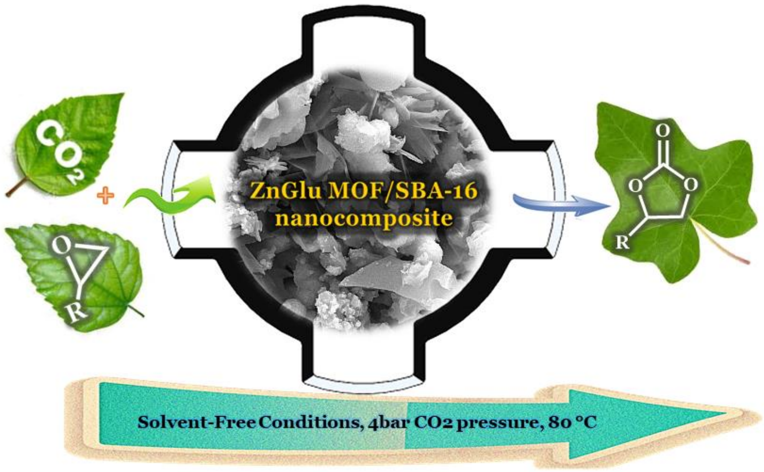
In this study, ZnGlu metal-organic framework/ordered mesoporous silica SBA-16 (ZnGlu MOF/SBA-16) has been successfully introduced as a novel efficient, and eco-friendly nanocomposite with excellent chemical stability for the solvent-free chemical fixation of carbon dioxide under 4bar CO_2 pressure. The structure of the as-prepared nanocomposite was characterized by a series of measurement techniques, including FT-IR, XRD, BET, TEM, FE-SEM, EDX, EDX-mapping, and ICP-OES. From the standpoint of green chemistry, ZnGlu MOF/SBA-16 nanocomposite demonstrated superior catalytic activity for the conversion of CO_2 and various epoxides towards the preparation of cyclic carbonates [1,2] without using any toxic metal and reagents. This novel efficient catalytic system can be expediently recovered using simple filtration, and its satisfying catalytic activity was kept after five recycle runs under the same reaction. It's notable that ZnGlu MOF/SBA-16 with exemplary potential can be applied for industrial purposes as a green nanocatalyst.

Keywords: CO_2 Fixation, SBA-16, MOF



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Synthesis of Phosphoroamidates via Atherton–Todd Reaction under oxidative Conditions

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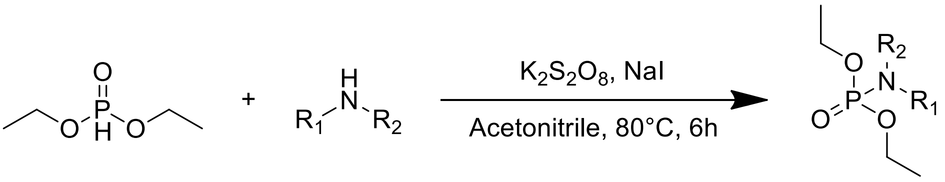
The Atherton–Todd reaction is one of the most characteristic reactions of diesters of H-phosphonic acid. The reaction is widely used in situ under mild conditions for the synthesis of a large number of biologically active compounds such as phosphates and Phosphoroamidates. Both P and N atoms are key physiological elements present in genetic material, energy transfer, enzymes, and other biomolecules and are required for various life processes. As such molecules containing P-N linkages are found in a large array of biologically active natural products [1,2].

Iodine-mediated oxidative cross-coupling methods offer better routes to P-N compounds by eliminating toxic halogenating agents such as CCl_4 in the synthetic processes. The method also uses inexpensive oxidants wothout additives and generates water or alkanol as stoichiometric waste. However, the synthetic routes are prone to the formation of many undesired side products, suffer from low yields, and sometimes have limited applicability [3].

In this work an efficient and simple cross-dehydrogenative coupling (CDC) procedure for the synthesis of phosphoroamidates via an Atherton–Todd coupling reaction of amines with dialkyl H-phosphite using $K_2S_2O_8$ as an oxidant and NaI as a catalyst has been developed (Scheme1). This method is easy to conduct, and various phosphoramidates were obtained in moderte to excellent yield.



Schem1. Synthesis of Phosphoramidates

Keywords: Phosphoramidate, Atherton–Todd reaction, H-phosphonate, Dialkyl phosphite

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Synthesis of boron based additives and application in lubrication

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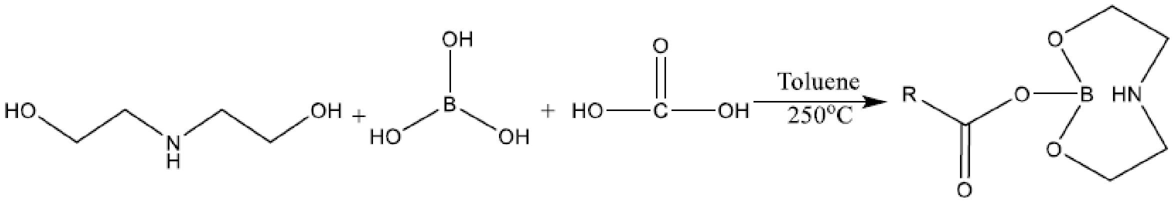
Lubricating oil is a functional material applied for separating two surfaces. During the last decades, additives have been added to the lubricants to give them special properties and improve their lubrication performance [1]. Boron and boronate compounds are widely used in a range of tribological applications such as friction modifiers, antioxidants, antiwear additives, and in many cases as environmentally friendly lubricants oils and fuels. To improve the hydrolytic stability of borate esters, the addition of some amine compounds to produce additional molecular coordination is used [2]. added of electron-rich groups (such as nitrogen atom) into borate ester, to stabilize the electron-deficient of boron atom, and that can reduce the possibility of attack by some nucleophiles. More importantly, it can enhance antiwear performance for the synergetic effect between boron and nitrogen element [3]. Herein, we report the synthesis of boron ester-containing additives to improve the performance of a lubricating oil from the reaction between fatty acids and boric acid with secondary amine in toluene solvent at 250 °C. Finally, a reddish viscous liquid was obtained. It has the ability to dissolve in oil, as well as its antioxidant properties and viscosity. All synthesized compounds are stable materials whose structure is based on their mass spectra, 1H and 13C-NMR and IR spectroscopy data.



Schem. 1 Schematic synthesis of boron ester-containing additives

Keywords: Boron ester, Antiwear, Antioxidant, Lubricant, Additives

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Synthesis and application of synthetic oils

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Lubricants have been used in various industries, such as drilling, aviation, automotive, factories, and food processing The food grade lubricants that are available in the market are mostly produced from refined naphthenic mineral oil or white oil, which are not promisingly safe based oils Mineral oil based lubricants are harmful to human beings and the environment, and also there is another issue of its poor biodegradability and toxicity which has led to health problems on a long term basis Synthetic polyol esters are used as environmentally acceptable base fluids in high performance lubricants A very good low temperature behaviour, high thermo oxidative stability of some types, very high viscosity index, good anti wear and low evaporation properties have led to their use in many lubricants Compromise between viscosity, volatility and cost influences the choice of base stocks for their effective ecofriendly formulations Generally, ester based biolubricants can be prepared via esterification reactions between polyhydric alcohols with fatty acids in the presence of acid catalyst.

Keywords: : Synthetic oils, Synthetic esters, Bio lubricants, Polyol ester

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Preparation and characterization of hydrogel based on graphene and chitosan

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A hydrogel is a 3D molecule, composed of cross-linked network-like soft materials. According to current preparation methods, there are two broad classes of hydrogels: physical hydrogels and chemical hydrogels. Structurally, physical hydrogels mainly display molecular interactions including ionic cross-linking, hydrogen bonding and hydrophobic interactions. In contrast, chemical hydrogels are characterized by covalent bonding between constitutive molecules. Importantly, chemical hydrogels cannot be destroyed by water molecules[1].

Hydrogels can be prepared from synthetic or natural materials such as chitosan, sodium alginate, hyaluronic acid, cellulose, PEG, PVA, etc[2].

In particular, chitosan is a natural aminopolysaccharide with widespread resources and does not induce acute cytotoxicity. The large number of amino and hydroxyl groups in chitosan provide functional groups for chemical reactions[3].

Graphene, an sp^2 hybridized, hexagonally arranged, covalently bonded chain of polycyclic aromatic hydrocarbon arranged in a single sheet of atomic thickness in a honeycomb crystal lattice with a unit cell of two carbon atoms has unique properties owing to its structural and chemical morphology such as high surface to volume ratio, excellent transparency, unmatched conductivity and high mechanical strength[4].

The objective of this work is to generate a hydrogel based on graphene and chitosan by low-toxic and cost-effective precursors in mild condition under 60 second time. The formation of hydrogel was evinced by FT-IR, XRD, SEM and EDX.

Keywords: Graphene, Chitosan, Hydrogel

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Design, synthesis and molecular docking simulation of new quinazoline derivatives as potential anticonvulsant agent

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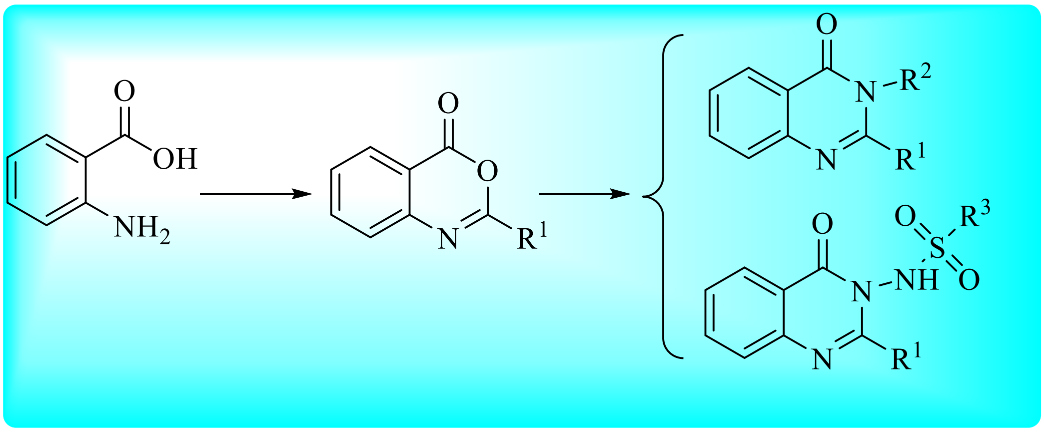
Epilepsy is a common neurological condition, affecting 0.5-1% of the population worldwide [1]. Epilepsy is a family of neurologic disorders, if not treated, is associated with progressively impaired cognition and function, brain damage, and other neurologic deficits. Conventional drugs like phenobarbital, primidone, phenytoin, carbamazepine, ethosuximide and benzodiazepine are widely used but exhibit an unfavorable side effect profile and failure to adequately control seizures [2]. Thus, new concepts and original ideas for developing antiepileptic drugs are urgently needed. Quinazoline moiety is an important scaffold of many reported anticonvulsants [3]. In the other hand, cyclooxygenase-2, an enzyme synthesizing the pro-inflammatory mediators, prostaglandins, has widely been reported to be induced during seizures and is considered to be a potential neurotherapeutic target for epilepsy management [4]. In view of above-mentioned we design and synthesis new quinazoline derivatives with cyclooxygenase-2 inhibitory and anticonvulsant activity to control (prevent) seizures.



Keywords: Quinazoline, Synthesis. Anticonvulsant

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Synthesis, characterization and biological evaluation of 1,2,4- oxadiazole derivatives containing kojic acid moiety

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The chemistry of heterocyclic compound is known to be useful as a key starting material for their application as active pharmaceutical ingredients. Amongst them 1,2,4-oxadiazole and its derivative are known to be important in the development of medicinal chemistry [1]. Furthermore, kojic acid is an organic acid which produced by many species of fungi and bacteria and have attracted much attention of organic chemists because their various biological activities [2,3]. Thus, we became interested in the synthesis of hybrid molecules containing kojic acid coupled to oxadizole. In this work, we report the synthesis of novel 3,5-disubstituted oxadiazoles containing kojic acid moiety. For this purpose, kojic acid **1** was converted to 5-benzyloxy-2-(hydroxylmethyl)-4*H*-pyran-4-one **2** by the reaction with benzyl chloride. The oxidation of compound **2** using activated manganese (IV) oxide in 1,4-dioxane gave the desired aldehyde, which was converted to the corresponding aldoxime **3** by treatment with hydroxylamine hydrochloride. Aldoxime was transformed to the corresponding hydroximoyl chloride using *N*-chlorosuccinimide. Oxadizole derivatives were synthesized in good yields by the cycloaddition reaction of nitrile oxide, generated in situ from the corresponding hydroximoyl chloride, with various nitrile in the presence of tetrahydrofuran under reflux conditions(scheme1). The structures of oxadizoles were characterized by FT-IR, ^{1}H-NMR and ^{13}C-NMR spectra.

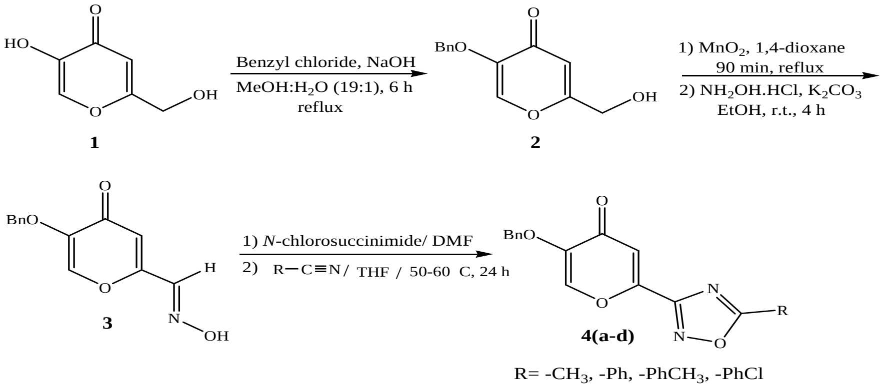

Fig. 1: Synthesis of 3,5 - disubstituted oxadiazoles contianing of kojic acid moiety

Keywords: Oxadiazole, kojic acid, cycloaddition reaction.

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Utilization of phenyl isothiocyanate for the synthesis of multi-functionalized derivatives of 4-imino-7-cyano-3-phenyl-6-(pyrrolidin-1-yl)-2-thioxo-1,2,3,4-tetrahydroselenopheno[3,2-*d*]pyrimidine

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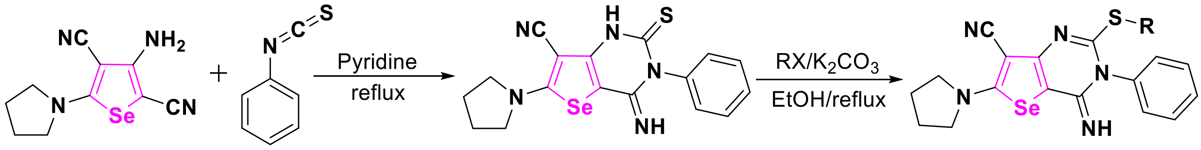
Selenophene is a 5-membered cyclic compound containing one Se atom and two double bonds. Among chalcogenophenes, selenophene plays an important role in organic synthesis because of its electrical property and stability. Selenophene has drawn the attention of researchers in view of its interesting biological activities such as anti-inflammatory [1], anti-convulsant and anti-oxidant [2], hepatoprotective [3], antihyperalgesic and anti-nociceptive and anticancer effects[4]. Herein, we wish to report a facile procedure for the synthesis of potential pharmacologically active derivatives **3(a-g)** of a novel selenopheno-condenced heterocyclic system. The heterocyclization of 3-amino-2,4-dicyano-5-(pyrrolidin-1-yl)selenophene **1** with phenyl isothiocyanate in the presence of pyridine under reflux condition afforded selenophenopyrimidine **2**. In the following step, compound **2** treated with several alkylhalides in K_2CO_3/EtOH to obtain 2-(alkylthio)-7-carbonitrile-4-imino-3-phenyl-6-(pyrrolidin-1-yl)-3,4-dihydroselenopheno[3,2-*d*]pyrimidines **3(a-g)** in good to excellent yields. The structural assignments of all newly synthesized compounds are based upon spectroscopic and microanalytical data.



R: Me, Et, *n*-Pr, *n*-Bu, Bn, CH_2COOEt, CH_2CN

Keywords: Selenophenopyrimidine, Phenyl isothiocyanate, Selenium-containing compounds

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Synthesis of benzimidazoles by Ni-catalyzed hydrogen transfer reduction of nitroarenes with alcohols

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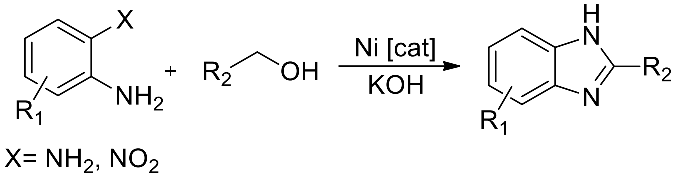
In the present years, nanocomposite and catalysis are the most attractive combination, which inspires the scientific community to apply both the technology concurrently, because as the particle size of the metal catalyst decreases the relative number of surface metal atoms increases, and consequently the activity increases. The nanoparticle catalysts can also be easily separated and recycled with retention of high catalytic activity. Because of advantges of these nanocatalysts, many researchers have synthesized and characterized through the different analytical techniques followed by application studies in the synthesis of various heterocycles like benzothaizole, benzoimidazole, benzooxazole and other heterocycles. In this section, we have discussed about the application of nanocatalysts for the synthesis of benzimidazoles [1-2].

Benzimidazole and its derivatives represent an important class of N-containing heterocyclic compounds, which have received considerable attention in recent years due to their potential applications as anticancer, antibacterial, antiulcer, antiviral and antihistamine agents. In addition, they could also be applied in other fields, such as chemosensing, dyes, fluorescence and corrosion science. Owing to the potential biological and other technical interest in benzimidazole compounds, a number of synthesis strategies have been developed [3]. herein we report a simple and efficient synthetic method of benzimidazoles by the reaction of ortho-nitroanilines and primary alcohols a nickel-catalyzed direct. This catalytic system afforded products with good yields.



Keywords: Heterogeneous Nanocatalyst**,** Nickel, Primary Alcohols, Benzimidazole

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Synthesis of Biodegradable Hydrogels to Remove Pb^{2+} Ions from Industrial Effluents

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Hydrogels are a class of wet and soft materials, constituted by weakly cross-linked polymers that are composed of a hydrophilic three-dimensional network [1]. Weakness in mechanical strength and lack of thermal stability of hydrogels have led to limitations in their widespread use in various industries. The growing need of the industry to solve this problem and to obtain specially improved hydrogels has led to the design and production of Nanocomposite hydrogels. The polymer network of nanocomposite hydrogels has improved elastic and rheological properties in comparison with conventional hydrogels. Another point that adds to the importance of structural studies of nanocomposite hydrogels is the high strength of these materials against the application of external forces as well as maintaining its structural stability [2]. In this study, hydrogels are synthesized which, in addition to their biodegradability, are nanoscale and therefore offer high efficiency in terms of water treatment as well as the absorption of pollutants such as paints and metal ions from industrial effluents.

Keywords: Hydrogel, Industrial effluents, Nanocomposite hydrogels

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Immobilized Cu(I) Nanoparticles on Montmorillonite -Modified with Benzalkonium Chloride (MMT-BAC@Cu(I)) and Their Catalytic Activity as an Eco-Friendly and Heterogeneous Nano-Catalyst for Facile Synthesis of 5-Substituted-1*H*-Tetrazoles in Deep Eutectic Solvent

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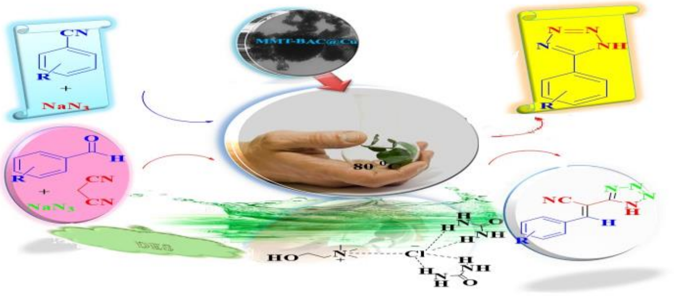
We have synthesized Immobilized Cu(I) Nanoparticles on Montmorillonite -Modified with Benzalkonium Chloride (MMT-BAC@Cu(I)). We used a green nanoclay catalyst with the MMT-BAC@Cu(I) structure in this work. Since clay [1] and clay minerals are the major constituents of the earth's crust, the advantages of availability, low cost, non-toxicity, and biocompatibility of clay were our focus in synthesizing this nanoclay catalyst in the project, which was used as a heterogeneous and green catalyst for synthesis of 5-substituted-1H-tetrazoles. The structure of the catalyst was detected and confirmed using XRD, EDX, ICP, TEM, SEM, and IR techniques. We also tried to create green conditions in this work by using a new generation of green solvents like deep eutectic solvents (DESs) [2] as green alternatives to hazardous organic solvents. DESs are composed of two or more components with the capability to establish hydrogen bonds with important advantages such as non-toxic, inexpensive, and having high solubility. The method's advantages include good to excellent product yields, green conditions, easy work up, and short reaction time.



Schem 1. MMT-BAC@Cu (I) as nano-catalyst for facile synthesis of 5-substituted-1*H*-Tetrazoles in deep eutectic solvent

Keywords: Montmorillonite, Heterocycles, Nanoclay, 5-substituted-1H-tetrazoles, DES

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Application of metal-organic frameworks containing sulfonic acid groups (MOFs-SO_3H) for the synthesis of chromeno[4,3-*d*]pyrimidin derivatives *via* cooperative vinylogous anomeric based oxidation concept

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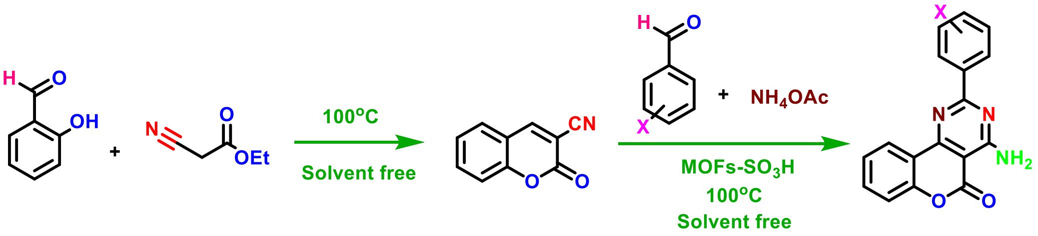
Metal-organic frameworks (MOFs) have come to be regarded as a promising novel framework in the last century due to the presence of nanoscale channels and hole a pore structure similar to the zeolites found [1]. The structure of the materials is composed of metal or metallic cluster coordinated by polyhedral organic ligands [2]. Increasing or increased in quantity of level area, pore volume and flexibility of architecture of metal-organic frameworks has revealed a new field in research that is mainly aimed at preparing a new framework of materials and research their applications in catalytic processes, gas separation, adsorption and drug delivery [3]. Synthesis of *N*-heterocycle compounds *via* Hantzsch method are includes a wide range of materials with biological activity, which are used to treat dangerous diseases such as antimicrobial, cancer, malaria, anticonvulsant, antifungal, HIV, anti-tumor, antioxidant, antihypertension and urinary incontinence treatment [4-5]. In order to further investigate the applications of catalysts, we have decided to design and synthesize metal-organic frameworks containing sulfonic acid groups (MOFs-SO_3H) as heterogeneous catalyst for the one-pot synthesis of chromeno[4,3-*d*]pyrimidin derivatives (Scheme 1).



Schem. 1: Synthesis of chromeno[4,3-*d*]pyrimidin derivatives using MOFs-SO_3H

Keywords: Anomeric effect, Chromeno[4,3-*d*]pyrimidins, Heterogeneous catalyst, Metal-organic frameworks (MOFs).

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Cu-Ni Alloys Nanoparticles Supported on Magnetic Montmorillonite - Modified with Benzalkonium Chloride (MMT-BAC@Fe3O4@CuNi): As an Eco-Friendly and Recyclable Nano-Catalyst for Facile Synthesis of Benzimidazole Derivatives under solvent-free conditions

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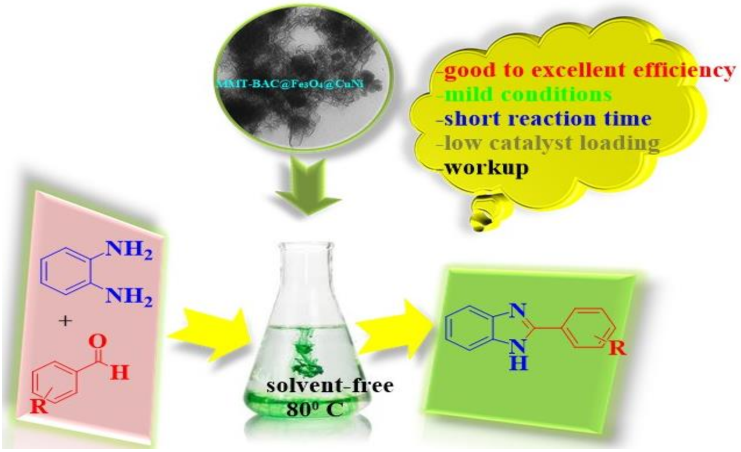
In this paper, we have successfully synthesized Cu-Ni Alloys Nanoparticles Supported on Magnetic Montmorillonite -Modified with Benzalkonium Chloride (MMT-BAC@Fe3O4@CuNi). Since clay [1] is an inexpensive, non-toxic, and biodegradable substance, so it is widely used as a green catalyst, and montmorillonite is used as a substrate in catalyst construction thanks to its large surface area and outstanding adsorption capacity. The structure of the MMT-BAC@Fe_3O_4@CuNi catalyst was detected and confirmed using XRD, EDX, ICP, TEM, SEM, and IR techniques and used in the synthesis of benzimidazole derivatives[2] from the raw materials of various aldehydes and 1,2–diaminobenzene, as highly active pharmaceutical compounds in solvent-free conditions[3]. The employed method includes good to excellent efficiency, short reaction time, mild conditions, non-hazardous organic solvents, low catalyst loading, and easy work up.



Schem 1. MMT-BAC@Fe_3O_4@CuNi as an eco-friendly catalyst for facile synthesis of benzimidazole derivatives under solvent-free conditions

Keywords: Montmorillonite, Heterocycles, Benzimidazole derivatives, Solvent-free

References

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Highly efficient, catalyst-free synthesis of novel pyrazolyl-containing dihydropyridines

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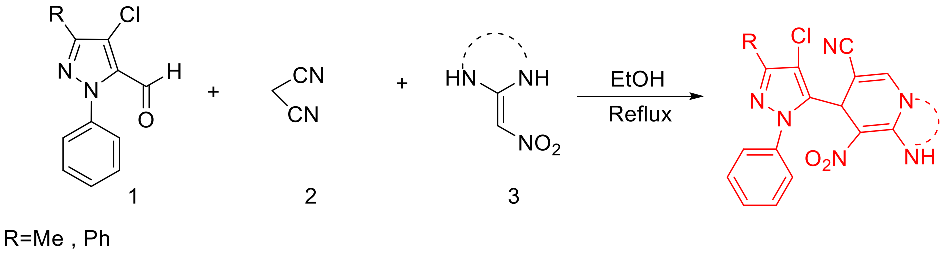
Pyrazole derivatives constitute an important family of compounds due to their applications as pharmaceuticals, agrochemicals and dyestuffs.[1] Derivatives of dihydropyridine are studied as novel compounds with anticancer activity based on proapoptotic mechanisms.[2] Different heterocyclic motifs in a single molecule can be incorporated to produce molecules with enhanced biological properties.[3] Having these facts in mind and in continuation of our studies on synthesis of biologically important heterocyclic compounds,[4] herein we would like to report an efficient method for synthesis of new pyrazolyl-containing dihydropyridines by using pyrazole-5-carbaldehydes (**1**), malonitriles (**2**) and different type of keteneaminals (**3**).



Keywords: Pyrazole, Dihydropyridine, Synthesis.

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Synthesis of mesoporous phosphorous-doped carbon spheres which supported palladium nanoparticles for Solvent-Free Chemical Fixation of Carbon Dioxide with Epoxides

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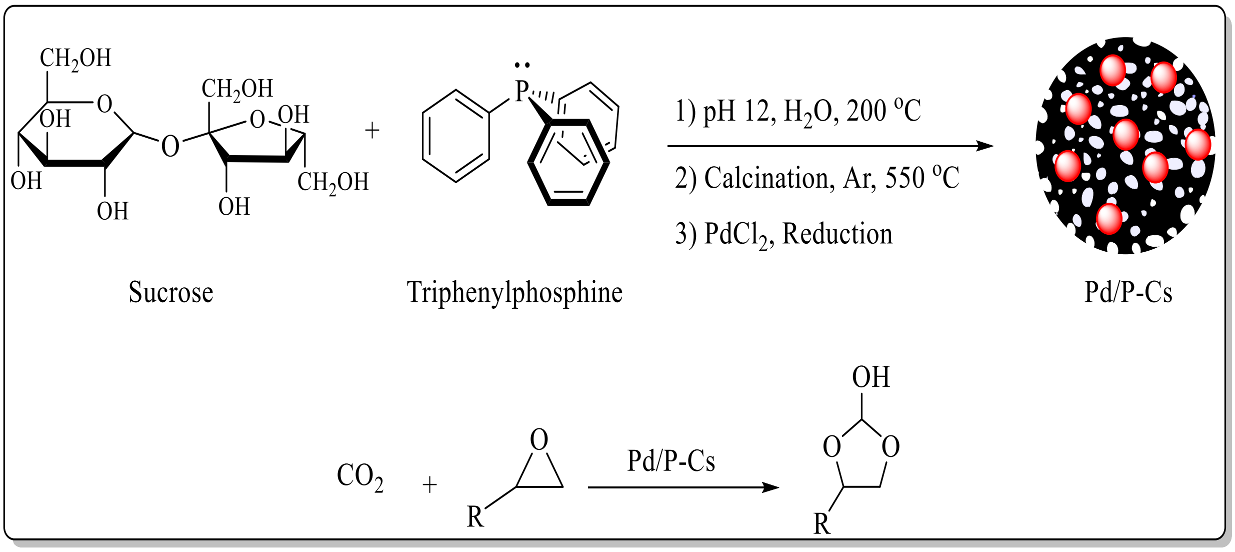
Since many environmental issues such as high consumption of fossil fuels and increasing air pollutions arise recently, we need to find a way to decrease the amount of green house gases like CO_2. Moreover various catalysis such as $CuO@SiO_2$ multi-yolk shell, SBA-15/N-Au NPs and etc, have been reported[1,2]. Herein mesoporous phosphorous–doped carbonspheres which supported palladium nanoparticles (Pd/P-CS) has been successfully utilized as an efficient, ecofriendly nanocatalyst that exhibits high activity in CO_2 fixation reactions with epoxides in solvent free condition.

Keywords: CO_2 Fixation, Carbon Spheres



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Effect of incorporating *Prunus amygdalus* extract in PCL-GEL nanofibers for bone tissue engineering

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The regeneration of bone and dental defects resulting from tumor resection, congenital abnormalities, trauma, fractures, surgery, or periodontitis in dentistry is a major health problem in our super-aging society [1]. Tissue engineering has advanced in recent years to meet this request for new therapeutics, with stem cells, appropriate scaffolds, and relevant growth factors. These techniques have enhanced graft incorporation and osteoconductivity [2]. The crude extracts derived from several parts of medicinal plants have been demonstrated to be a rich source of biologically active ingredients. Biologically active compounds, with antioxidant potency and other health-promoting effects, present in Prunus amygdalus extract are plant protein, dietary fiber, and lipids (mono- and polyunsaturated fatty acids), phenolic acids, falvonoids, tannins, and vitamin E. Because of structural similarities between polyphenols and hormones, capability to reduce oxidative stress, and ability to bind to certain proteins, they have considerable biocompatibility and can also participate in signal transduction pathways. Polyphenols can also be utilized as crosslinking agents for matrix materials, which improves the scaffold's mechanical characteristics and resistance [3]. PA extract was loaded onto poly(ε-caprolactone)-gelatin nanofibers were fabricated by electrospinning and their potential applications for bone tissue engineering were studied. The morphology and biochemical configuration of fabricated scaffolds were characterized using FESEM, FTIR, contact angle measurements and mechanical tests. The response of human cells to the PCL-GEL-PA nanofibers was evaluated using human dental pulp stem cells (hDPSCs). The hDPSCs had better adhesion and proliferation capacity on the PA loaded nanofibers than on the pristine PCL-GEL nanofibers. An alizarin red S assay and the alkaline phosphatase activity confirmed that the nanofibrous scaffolds induced osteoblastic performance in the hDPSCs. These results suggest that PCL-GEL-PA nanofibers might have potential applications for bone tissue engineering.

Keywords: Prunus amygdalus, Nanofiber, Electrospinning, Human dental pulp stem cell, Tissue engineering

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Preparation of Composite Nanohydrogels based on Graphene Oxide

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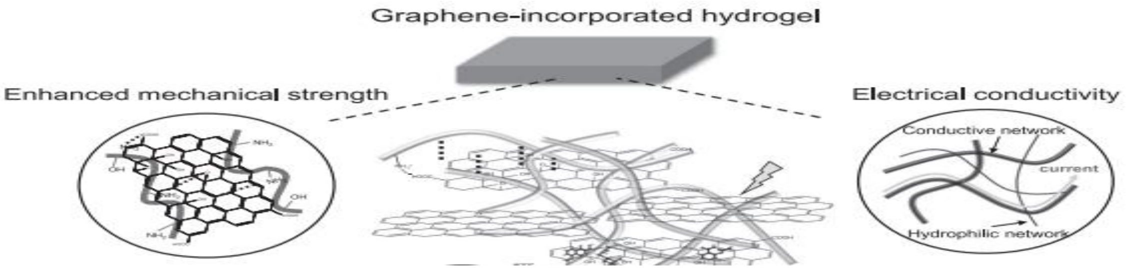
A hydrogel is a three-dimensional (3D) hydrophilic polymer network with several unique characteristics, including hydrophilicity, swelling, micro-nanosized pores, and softness. These characteristics of hydrogels make them very useful for various biomedical applications, such as tissue augmentation, drug delivery, and tissue engineering scaffolds [1]. The inclusion/incorporation of nanoparticles in three dimensional polymeric structures is an innovative means for obtaining multicomponent systems with diverse functionality within a hybrid hydrogel network. Nanoparticle-hydrogel combination adds synergistic benefits to the new 3D structures. Nanogels as carriers for cancer therapy and injectable gels with improved self-healing properties have also been described as new nanocomposite systems [2]. Among nanoparticles, nanoparticle graphene and its derivatives are the most important. The traditional hydrogel is composed of cross linked organic polymer, but its poor mechanical property and stability limit its wide application. Graphene-based hydrogels (including graphene oxide hydrogel and reduced graphene oxide hydrogel in this paper) can solve this application limits because of its excellent properties [3]. In this study, we synthesized hydrogels that are nanocomposite in nature and are loaded with graphene oxide nanoparticles that enhance the hydrogel in terms of thermal resistance and mechanical properties and increase and improve its absorption surface for drug delivery as well as medical applications and various industries.



Keywords: Hydrogels, Graphene Oxide, Nanocomposite hydrogehs

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Visible light induced photocatalytic degradation of rhodamine B and methylene blue over a novel nitrogen-doped carbon quantum dots

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Organic dyes discharged from printing, textile and leather industries have detrimental effects on the environment [1]. It should be noted that, most textile dyes are recalcitrant to biodegradation and are photolytically stable because of their complex structure. Additionally, studies have shown that, they are not only harmful to aquatic organisms, but also carcinogenic to humans and animals [2]. Therefore, the physic-chemical treatment of dye wastewater is a necessary way for controlling its pollution and has attracted many researchers in recent years [3].

A novel nitrogen-doped carbon quantum dots (N-CQDs) has been successfully synthesized. Then, it was completely characterized by various analytical techniques. The photocatalytic behaviour of the prepared N-CQDs was tested in dyes degradation, methylene blue (MB) and rhodamine B (RhB), in aqueous solution under Visible light irradiation. RhB (20 ppm) and MB (20 ppm) were almost completely decolorized in 60 min in given conditions. The effect of various parameters such as initial dye concentration, catalyst loading, *p*H of the medium and temperature of the dye solution, on the photo degradation of RhB and MB were investigated. To scrutinize the mechanistic details of the dye photo degradation, several critical analytical methods including UV−vis spectroscopy, HPLC and LC/MS were utilized to monitor the temporal course of the reaction. The degradation of RhB and MB was mainly attributed to the destruction of the conjugated structure, and then the intermediates transformed to acid molecules which were mineralized to water and carbon dioxide. Recovery of the N-CQDs also revealed slight decrease in photocatalytic performance after four cycles.

Keywords: Photocatalysis, Carbon Quantum Dots, Methylene blue, Rhodamine B

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Application of Graphene Oxide-based Nanocomposite Hydrogels for the Controlled Release of the Anti-Cancer Drug Methotrexate

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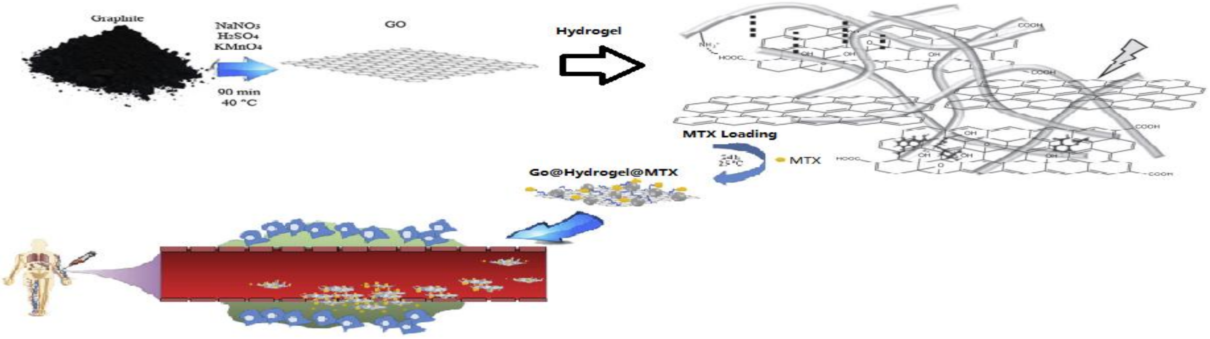
Cancer is considered as one of the most important reason of death in the world in these years. The different ranges of chemotherapy drugs are used as a significant way to treat various cancers. In spite of significant applications, anticancer drugs suffer from some limited effects on target cells due to lack of selectivity, low solubility, uniform tissue distribution, short half-life in the bloodstream and dose-related toxicity. Methotrexate (MTX), a chemotherapy drug, is a folic acid analog and uses for the treatment of many different kinds of cancers. MTX can mainly blocks the dihydrofolatereductase (DHFR) enzyme and subsequently prevents the production of thymidine [1]. For controlled release of this drug, the use of appropriate drug systems and carriers is very important. In this study, the application of graphene oxide nanocomposite hydrogels as carriers of this drug is described. When GO and hydrophilic polymers are composited, the GO components can increase the mechanical properties and stabilities of hydrogels compared with those of GO-free hydrogels. The incorporation of GO into hydrogels can also enhance the molecular adsorption and electrical conductivity of hydrogels. Numerous composite hydrogels containing various nanomaterials (e.g., metal nanoparticles and organic nanoparticles) have been fabricated to obtain hydrogens with improved properties. Compared with such conventional nanomaterials, GO presents an extremely high surface-to-volume ratio with a large lateral dimension, flexibility, electrical conductivity, biological activity, and multiple strong molecular interactions with various molecules [2].



Keywords: Hydrogel, Drug delivery, Controlled drug delivery, Nanocomposite hydrogels

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Design and synthesis of a new type dibenzosuberenone-dihydropyridazine based fluorescent dyes for heavy metal ion and multi-analyte sensing applications

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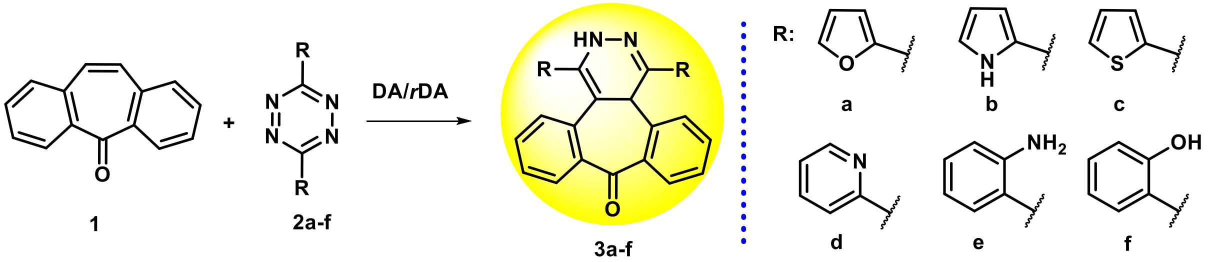
The widespread use of heavy metal ions in the industry results in serious environmental pollutions and human health problems, negatively affects agriculture, and destroys natural life [1]. Therefore, the development of fluorescence chemosensors for the determination of heavy and transition metal ions has attracted much attention in recent decades [2]. Dibenzosuberenone and polyconjugated derivatives exhibit photophysical properties such as photosensitizatione, fluorescence, and aggregation-indduced emission (AIE) [3]. Recently, our research group discovered a new class of dibenzosuberenone derived fluorescent dyes, and their photophysical and/or anion sensor properties were investigated [4,5]. In this study, various analogues of a new family of fluorophores based on derivatives dihydropyridazine-dibenzosuberenone were synthesized by inverse electron-demand Diels-Alder cycloaddition reactions between a dibenzosuberenone and tetrazines that bear various substituents (Scheme1). Then, the photophysical, heavy metal and multi-analyte sensor properties of these compounds will be investigated.



Schem 1. Derivatives dihydropyridazine-dibenzosuberenone.

Keywords: Fluorescence chemosensor, Heavy metal ion, Multi-analyte sensor, Dibenzosuberenone, pyridazine.

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Tandem intramolecular Pinner–Dimroth rearrangement assisted synthesis of fully-functionalized new selenopheno[3,2-*d*]pyrimidine heterocycles

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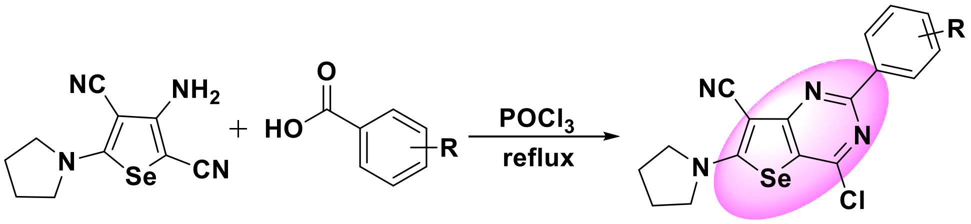
Heterocyclic condensed pyrimidines have attracted considerable attention due to their interesting biological properties. On the other hand, based on the variety of biological benefits associated to the presence of selenium, many protocols such as one-pot four-step sequential procedure [1], Cu-catalyzed cyclization [2], Se-metal exchange [3,4], microwave assisted seleno-clasien rearrangement and free radical condition [5] have been developed for the synthesis of selenophene scaffolds. Due to widespread biological activities of selenophenes and our interest for the synthesis of selenophenocondenced heterocyclic systems, we report an alternative procedure for the synthesis of various derivatives of selenopheno[3,2-*d*]pyrimidine via intramolecular Pinner–Dimroth rearrangement. These potential biologically active derivatives (3a-m) were synthesized through heterocyclization of synthetic 3-amino-5-(pyrrolidin-1-yl)selenophene-2,4-dicarbonitrile (1) with several commercially available benzoic acids (2a-m) in the presence of phosphoryl oxychloride in excellent yields. The products were characterized on the basis of spectral and microanalytical data.

Keywords: Selenophene, Selenopheno[3,2-*d*]pyrimidine, Pinner–Dimroth rearrangement, Heterocyclization



(1) **(2a-m)** **(3a-m)**

R: H, *o*-Cl, *m*-Cl, *p*-Cl, *o*-Br, *o*-I, *m*-OCH_3, *m*-CH_3, *p*-CH_3, *m*-NO_2, *p*-NO_2, *p*-CN, *o*-OH

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Synthesis of orthoaminocarbonitrile tetrahydronaphthalenes catalyzed by butyl-3-methylimidazolium hexafluorophosphate ionic liquid

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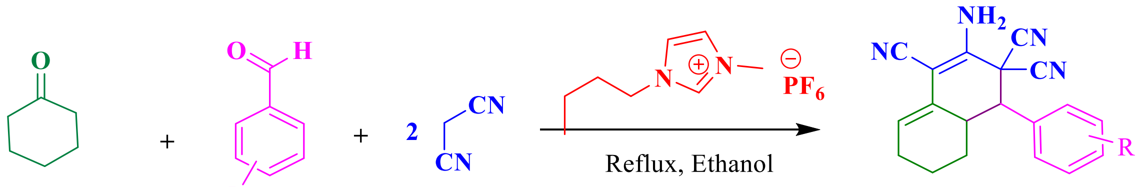
The important chemical compounds produced from benzaldehyde, cyclic ketones, and malononitrile are various derivatives of bicyclic ortho-aminocarbonitrile. Recently, these compounds were synthesized using the $CaMgFe_2O_4$ nanocatalyst in high yields and appropriate conditions [1]. Ionic liquids have a lot of potential for creating clean catalytic technologies because of their unique features. Ionic liquids can be employed as membrane systems in a variety of morphologies and topologies, such as supported liquid membranes, membrane contactors, and mixed matrix membranes [2]. Because the ionic liquid is non-volatile, the small vapor pressure can lead to a highly stable structure in each situation [3]. Ionic liquids with a variety of physical properties can be made in a variety of forms [4].

The combination of cyclohexanone malononitrile and aromatic aldehyde resulted in the effective synthesis of orthoaminocarbonitrile tetrahydronephthalene. In this research, we hope to report the synthesis of orthoaminocarbonitrile tetrahydro-naphthalene derivatives with high efficiency and short reaction time employing a butyl-3-methylimidazolium hexafluorophosphate as effective base catalyst under environmentally conscious conditions. All organic compounds were identified using the melting point, FT-IR, and ^1H NMR methods.



1 2a-l 3 4a-l

Keywords: Ionic liquids, BMIM-PF_6 , Orthoaminocarbonitrile tetrahydronaphthalenes.

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A convenient synthesis of novel fused chromene derivatives using nanocatalyst

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Benzopyran or chremene is a bicyclic organic compound that results from the fusion of a benzene ring to a pyran ring. This valuable heterocycle with various levels of saturation and oxidation is very common in nature. Chromene derivatives as an important class of organic compounds with diverse biological properties and therapeutic application have attracted many attentions. They are prominent natural products, widely distributed among many plants. Natural derivatives of chromene also exhibit a wide range of valuable physiological activities [1-5].

On the other hand, heterogeneous catalysts have been extensively used for acceleration of organic reactions. The efficiency of heterogeneous catalysis in organic synthesis can be improved by using nanocatalysts due to thier high specific surface area, facile workup and recyclability. At present study an efficient method was developed for the synthesis of indole substituted benzo[*f*]chromenes by the reaction of β–naphtol, arylaldehydes and 3-cyanoacetylindole in the presence of basic supported nanocatalyst. In this presentation the details of this novel method will be discussed.

Keywords: Benzo[*f*]chromene, Indole, Chromene, Nanocatalyst

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Synthesis and Evaluation of Biological and Antioxidant Activity of Some New Heterocyclic Compounds for Mefenamic Drug Derivatives

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In this study new heterocyclic derivatives were prepared. The most available Mefenamic acid (M) has been reacted with thionyl chloride to get (M1 compound) [1]. (M1) compound treated with hydrazinecarboxamide to get (M2) derivative then a ring closer reaction has been made to compound (M2) by NaOH solution to get the 1,2,4-triazole-3-ol ring compound (M3) [2].Compound (M)reaction with phenyl hydrazine hydrate to give (M4) compound then a ring closer reaction have been made using carbon disulfide and hydrazine hydrate in basic media to get (M5) . Compound (M1) treated with 3-aminopropanoic acid to get (M6) compound [3]. (M7) compound has been synthesis by reacting (M6) compound with benzaldehyde in the presence of acetic anhydride to get oxazin ring (M7 compound) [4].The synthesized compounds' antibacterial activity and antioxidant activity (M1-M7) were examined using the (DPPH) technique. The compounds show substantial antioxidant activity equivalent to the well-known (ascorbic acid) (IC50=31.95 g/mL) employed.

Keywords: Mefenamic acid , Hydrazinecarboxamide, Phenylhydrazine, Oxazin, Antioxidant activity

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Preparation of N-methyl-2-pyrrolidonium hydrogen sulfate ionic liquid and their application as an acidic catalyst for the synthesis of naphthopyranopyrimidines

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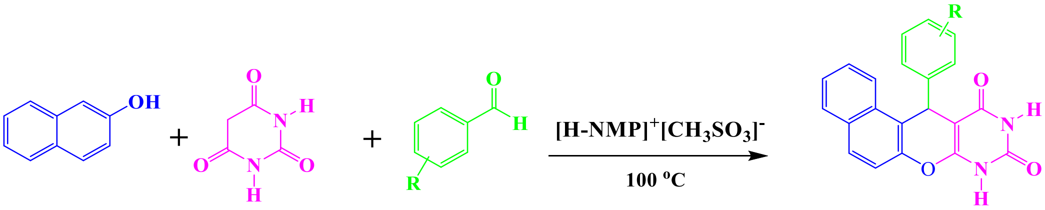
MCRs, which are one-pot reactions that lead to the products from more than two different starting chemicals, are suitable reaction systems for achieving significant structural diversity and molecular complexity in a single step. Multicomponent reactions can produce a wide range of products with better yields. MCRs have unique characteristics such as excellent atom economy, little waste output, and the utilization of widely available starting materials [1]. Ionic liquids with various physical properties can be created in many situations. Furthermore, physical and chemical qualities such as density, viscosity, hydrophobicity, and chemical affinity can be "tuned" for specific applications using this platform. The usage of ionic liquids in membrane systems is anticipated to rise [2]. The reactions were clean, so no chromatographic purification was required. In this research, we report the synthesis of naphthopyranopyrimidines through a three-component reaction involving 2-naphthol, aldehyde, and barbituric acid using *N*-methyl-2-pyrrolidonium hydrogen sulfate ($[H\text{-}NMP]^+[CH_3SO_3]^-$) as an acidic catalyst at 100 °C. The products were separated using a straightforward procedure and were of high purity and identified by melting point, FT-IR, and ^1H NMR analyses.

This methodology has various advantages, including reasonable conditions, operational simplicity, high yields, safety, the efficiency of workup and pure synthetic organic compounds, low catalyst loading, and economically prosses.

Keywords: $[H\text{-}NMP]^+[CH_3SO_3]^-$, Ionic liquids, Naphthopyranopyrimidine



Schem.1 . Synthesis of naphthopyranopyrimidine with $[H\text{-}NMP]^+[CH_3SO_3]^-$ ionic liquid

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Design and synthesis of Ti-MOF-UR using post-modification method of Ti-based MOF as novel hydrogen bond donor catalyst for the preparation of pyrazolo[3,4-*b*]quinoline derivatives

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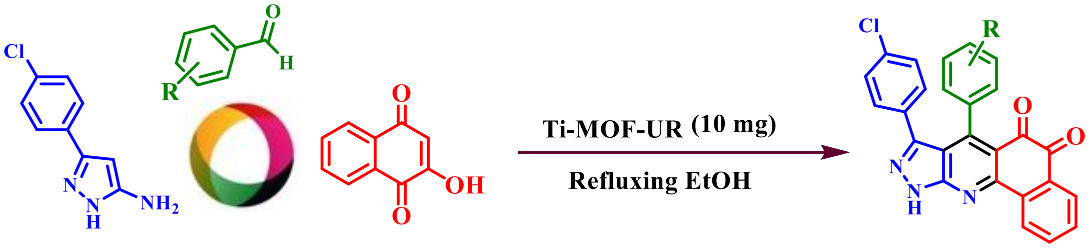
Metal-organic frameworks (MOFs) are a group of porous materials that are a new class of new generation nanoreactors consisting of metal and organic compounds as ligands. MOFs have distinctive features such as large surface area, adjustable pore size, very diverse structure, and adjustable chemistry due to their two-dimensional and three-dimensional porous structure [1-2]. This unique structure of MOFs has given them applications in various fields such as magnetic resonance imaging (MRI), catalyst, biotechnology, gas separation and storage, drug absorption, purification and drug delivery [3]. Hydrogen bond donor catalysis (HBD) is known as an effective method for the synthesis of highly valuable intermediates for the pharmaceutical and agricultural industries, as HBD catalysts are able to selectively bind and activate active substrates during the reaction process through hydrogen bonding [4]. The integration of metal-organic frameworks and compounds that play the role of HBD catalysts can be very attractive. In this research, a metal-organic frameworks (MOFs) was designed based on titanium. Then, using the post-modification method, we created the composition of urea in its structure. The Ti-MOF-UR was used as a as hydrogen bond catalyst in the synthesis of pyrazolo[3,4-*b*]quinoline (Scheme 1). The newly prepared catalyst showed a very good activity. The most important features of this work are the green and mild reaction conditions, short reaction time as well as high efficiency of products. Pyrazolo[3,4-*b*]quinoline have been used as a drug candidate for antimicrobial, cancer, malaria, anticonvulsant, antifungal, HIV, anti-tumor, antioxidant, antihypertension and urinary incontinence treatment [5].



Schem. 1: Preparation of pyrazolo[3,4-*b*]quinoline derivatives using Ti-MOF-UR as hydrogen bond catalyst.

Keywords: HBD catalysts, Metal-organic frameworks (MOFs), Pyrazolo[3,4-*b*]quinoline, Ti-based MOF, Ti-MOF-UR.

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Biocatalytic One-Pot C-C Bond Forming Reaction Using 4-Oxalocrotonate Tautomerase Homologue from *E. Coli*

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Biocatalysts recently have been used for performing non-native organic reactions known as promiscuous reactions. Exploiting biocatalyst in organic reactions has demonstrated many advantages including high stereoselectivity, mild condition and regulation as compared to chemical reactions. One of the major families of the isomerase is 4-oxalocrotonate tautomerase (4-OT). This enzyme has been shown to catalyze a number of promiscuous chemical reactions producing pharmaceutically active γ-aminobutyric acids[1]. The E. coli homolog of the 4-oxalocrotonate tautomerase has been suggested to contain tautomerase activity with 2-hydroxy-2,4-pentadienoate[2]. However, no other promiscuous (non-native) activity has been shown with this enzyme. To better characterize promiscuous reaction of E. Coli enzyme, using Polymerase Chain Reaction (PCR), the coding region of the enzyme was cloned in to an E. Coli expression vector and the corresponding recombinant protein was produced in high yield. To identify a proper non-native activity of E. Coli tautomerase enzyme, molecular docking was used for a number of organic small molecules as substrate. The purified recombinant tautomerase enzyme was examined for a number of promiscuous reactions. One such reaction was C-C bond forming between benzaldehyde (1) and nitromethane (2) in a mild condition. The products were analyzed using ^{1}H NMR and ^{13}C NMR. At the moment a number of different derivatives are being investigated by the action of the enzyme.

1 2 3

Schem.1.The enzyme catalyzed one pot C-C bond forming of 1 and 2[3].

Keywords:4-Oxalocrotonate tautomerase, C-C bond formation, Polymerase Chain Reaction.

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Surface modification of CdTe quantum dots with pH-responsive fluorescent dye-labeled metal-chelating polymer for controlled drug release

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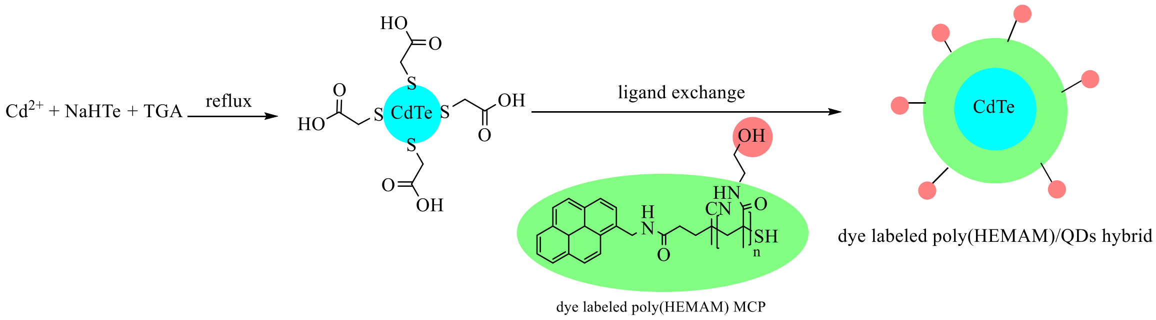
Among the various drug release systems, nanoparticles have received much interest. The colloidal fluorescent semiconductor nanocrystals in size range of 2−10 nm, called quantum dots (QDs) mainly used as powerful probes and critical diagnostic tool for fluorescence imaging.[1] the advancement of modern polymer/QDs materials with desirable biocompatibility without any cellular cytotoxicity has nowadays been a scientific challenge.[2] Among the variety of polymerization procedures, reversible addition fragmentation chain transfer (RAFT) polymerization is suitable to prepare polymer with controllable molecular weights and low polydispersity.[3] In this paper, we developed a novel strategy for surface modification of CdTe QDs by a dye labeled (HEMAM)-based MCP with hydroxyl pendant groups (Scheme 1). This end-labeled polymer has been papered by RAFT polymerization with a number average degree of polymerization (DP_n) of about 27. Labeling of polymers with dye provides a proper understanding of their interaction with QDs *via* successful ligand exchange. The hybrid was characterized by various experimental techniques such as optical absorption, fluorescence, and TEM. The poly(HEMAM) significantly increased the fluorescence intensity of QDs and made the aging of the CdTe QDs slower. The release rates of doxorubicin (DOX) anticancer drug conjugates were studied at pH 5.4 and pH 7.4.

Keywords: RAFT polymerization, Fluorescent dye, CdTe quantum dots, Drug release.



Schem 1. Synthesis of fluorescent dye-labeled poly(HEMAM)/QDs hybrid *via* ligand exchange.

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Phenacyl Thiocyanates, Potent Reagents for the Synthesis of Sulfur-containing Heterocycles

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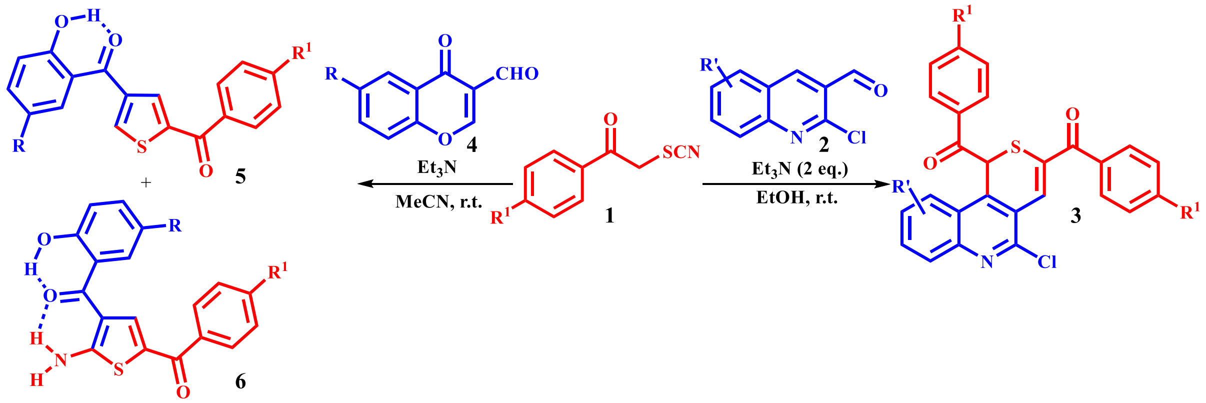
In the past few years, we have attempted to develop new, efficient protocols for the synthesis of sulfur-containing heterocycles with potential biological activity [1-2]. Thiophenes, 2-aminothiophenes, and thiopyrans are important classes of sulfur-containing heterocycles that have shown a wide range of biological and pharmacological activities such as anticancer, antifungal, anti-inflammatory, antibacterial, antiviral, and antimicrobial activities. In addition, the studies show that the presence of a thiopyran ring in a biologically active compound can improve its therapeutic profile. Also, thiophene derivatives have been found in the structure of several important drug molecules with lower side effects [1-3].

Recently, phenacyl thiocyanates have been considered potential reagents for the synthesis of sulfur-containing heterocycles [4-5]. Herein, we succeed to synthesize thiopyrano[4,3-*c*]quinolines 3, thiophenes 5, and 2-aminothiophenes 6 with *o*-acyl phenol substitution *via* the reaction between phenacyl thiocyanates 1 and quinoline-3-carbaldehydes 2 or 3-formylchromones 4, respectively (Scheme 1).



Schem. 1. The reaction between phenacyl thiocyanates **1** with quinolines **2** or chromones **4**

Keywords: Phenacyl thiocyanate, Thiophene, 2-Aminothiophene, Thiopyrane, Thiopyranoquinoline

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“Memory Effect” by Retaining Lysine Residue on Carbon Quantum Dot’s Surface for Catalyzing Organic Reactions

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“Memory effect” as a new term in carbon quantum dot characterization represents the retention of structural pattern of initial precursors used for synthesizing carbon quantum dots (CQDs) during and after the fabrication process. This fascinating behaviour of CQD has provided an efficient tool for exploring chemical biology phenomena in detail[1,2]. Folic acid-functionalized CQD, for example, demonstrated the response of folic acid receptor in vivo[3]. Impressed by “memory effect” of CQD we tried to retain lysine amino acid on the surface of CQD thereby reasoning its ubiquitous presence as well as catalytic function in the active site of different enzyme. Lysine-functionalized CQD was synthesized by a mild hydrothermal method using citric acid as carbon source and lysine residue. The “memory effect” of lysine on CQD surface was demonstrated by some analytical techniques such as IR and TEM. Of note, glycine- and arginine-functionalized CQDs were synthesized for control experiments and scrutinized in parallel with lysine functionalized-CQD for catalyzing some organic reactions such as carbonylation of aniline using urea as a renewable source of carbonyl moiety in nature. Comparing all designed CQDs as catalyst it was observeded that lysine functionalized CQD greatly exceeded the yield of the desired product via the same acid-catalyzed mechanism in comparison to other amino acid-functionalized CQDs. Here our results indicate a hypothesis about the common presence of lysine in the active site of enzymes in which the extended amino arm of lysine could provide more flexibility and accessibility to active site to easily meet the substrates thereby facilitating the catalytic operation.

Keywords: Bioinspired Catalysis, Carbon Quantum Dot, Memory Effect, Lysine Residue.

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Synthesis of 3-oxadiazole-substituted imidazo[1,2-*a*]pyridines by nickel immobilized on multifunctional amphiphilic porous polysulfonamide–melamine

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Recently, porous organic polymers (POPs) have been widelyused in basic and applied research such as adsorbents for gases, supports for catalysts and catalysts [1]. However, hydrophobic aromatic frameworks of POPs can be led to limited dispersion in aqueous media and poor catalytic activities [2]. Consequently, there is an urgent need in developing the amphiphilic POPs. Amphiphilic porous organic frameworks supported metal NPs have recently been announced, specifically when hydrophilic urea linkages (NHCO-NH) are introduced into the hydrophobic aromatic frameworks [3-5]. In this sense, a porous polysulfonamide–melamine amphiphile (PEMA–PSA), as a novel organic support system, has been successfully synthesized using the silica template method. The present research proposes the immobilization of Ni nanoparticles inside the polymer pores (PEMA–PSA@Ni) for better nanoparticle performance. PEMA–PSA@Ni was implemented as an inexpensive and reusable catalyst for the synthesis of a novel category of oxadiazoles (3-oxadiazole-substituted imidazo[1,2-*a*]pyridines). In this regard, benzhydrazide and 3-iodo-[1,2-*a*]pyridines *via* isocyanide insertion/cyclization were reacted in the presence of PEMA–PSA@Ni under mild conditions. It is worth mentioning that the catalyst had a very good performance due to the following features: greatly dispersed Ni, good surface area, unique amphiphilic structure and convenient recovery. The most significant advantages of this method include: simple operation, short reaction time, and wide substrate scope.

Keyword: Porous organic polymers, Oxadiazoles, Silica template

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Preparation and characterization of hexamethylenetetramine-functionalized magnetic nanoparticles and their application as novel catalyst for the synthesis of pyranopyrazole derivatives

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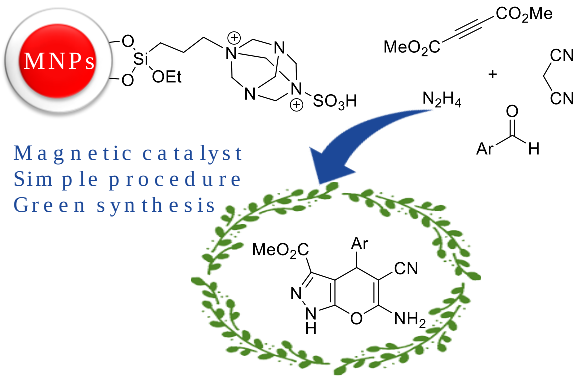
Pyranopyrazole compounds are oxygen- and nitrogen-rich fused heterocycles which show various biological activities such as molluscicidal activity,[1] inhibition of human Chk1 kinase,[2] and antioxidant,[3] antibacterial and anti-inflammatory properties [4,5]. In this regard, a new magnetic catalyst was prepared through the reaction of silanol groups, on the surface of silica-coated Fe_3O_4 magnetic nanoparticles, with (3- chloropropyl)triethoxysilane followed by hexamethylenetetramine and chlorosulfonic acid. The obtained magnetic catalyst was characterized using thermogravimetric analysis, vibrating sample magnetometry, scanning electron microscopy and energy-dispersive X-ray analysis. Its catalytic activity was investigated in the synthesis of pyranopyrazole compounds, and the results were excellent regarding high yield of the products and short reaction time.



Keyword: Green synthesis, Hexamethylenetetramine, Magnetic nanoparticles, Pyranopyrazole

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Catalytic application of Ti-based metal-organic frameworks for the preparation of novel tetrahydropyrido[2,3-*d*]pyrimidine derivatives

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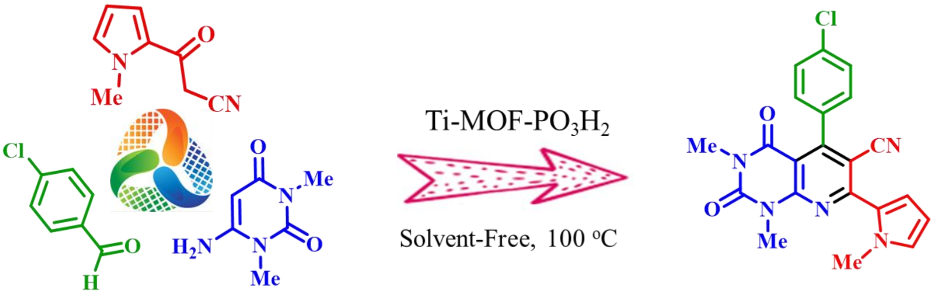
Nowadays, metal-organic frameworks (MOFs) have known as a unique type of porous solid materials, because they have been utilized in different fields such as drug delivery, catalyst, battery, super capacitor, sensor, gas storage, separation and adsorption of molecules [1]. These materials consist of multifunctional organic materials bind to metal or metal clusters through coordinated components such as carboxylates to form crystalline materials with high surface area and high thermal stability [2]. Heterocyclic compounds containing N and/or O heteroatoms show biological properties [3]. Therefore, the attention of many scientists has been attracted to the synthesis of these compounds. Also, tetrahydropyrido[2,3-*d*]pyrimidines are a well-known group of these compounds that show great importance biological properties like adenosine kinase inhibitors, anti-tumor, antifungal, antibacterial, anti-proliferative CDK2 inhibitor, antipyretic, anticonvulsant agents, analgesic and also used in CNS depressant activity [4]. In this work, we have synthesized novel tetrahydropyrido[2,3-*d*]pyrimidines *via* vinylogous anomeric based oxidation mechanism (Schem1).



Schem. 1. Preparation of tetrahydropyrido[2,3-*d*]pyrimidines using Ti-MOF-PO_3H_2 as catalyst.

Keywords: Anomeric effect, Metal-organic frameworks (MOFs), Ti-MOF-PO_3H_2, Tetrahydropyrido[2,3-*d*] pyrimidine.

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Synthesis of (dimethyl-tert-butyl-silyloxy) and (triethyl- silyloxy) piroxicam, investigation of their lipophilic property and comparison with the original drug.

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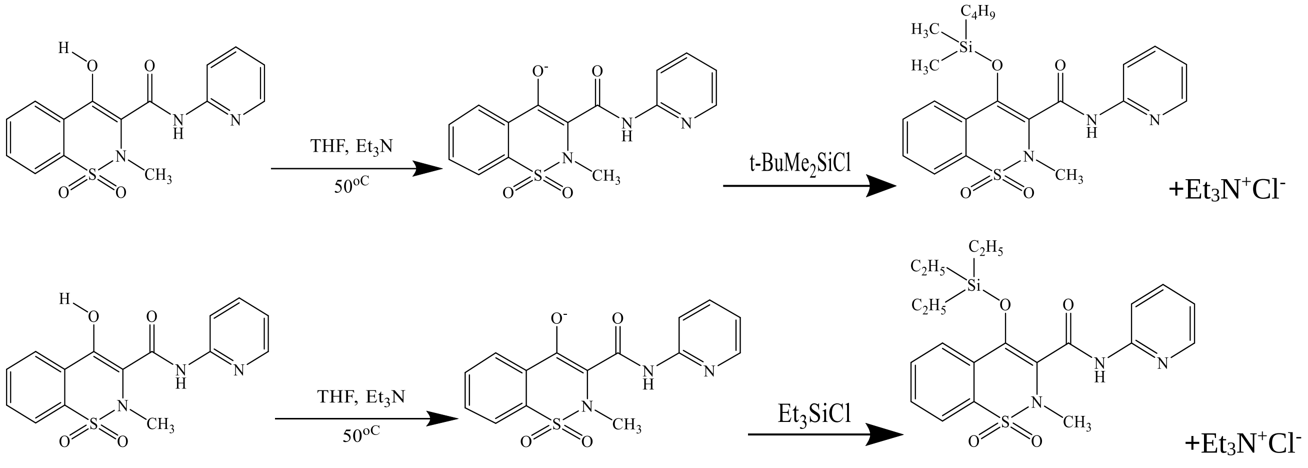
Piroxicam is a painkiller and its main use is to reduce or stop pain. In osteoarthritis, this drug has anti-inflammatory effects. This drug is used to treat many diseases such as headache and toothache, leg pain and piroxicam reduces the production of prostaglandins by controlling cyclooxygenase, thus showing its effectiveness in reducing and eliminating pain. Piroxicam is a phenolic drug. These drugs are difficult to pass through the lipid barrier, and the presence of lipophilic groups, such as organosilicon, will increase this property, that is, increase the property of the drug, so the introduction of these groups will modify the property of the drug. For this reason, we did this work with various silyl groups [1]. Herein, derivatives of a) dimethyl-tert-butyl-silyloxy b) Triethyl-silyloxy of piroxicam were synthesized. The Thin-Layer Chromatography (TLC) technique with different solvent ratios was used to separate piroxicam precursor from piroxicam raw material. The investigation of products by FT-IR and 1HNMR techniques was showed that the derivatives were synthesized with acceptable efficiencies. These compounds were showed high thermal stability. Then, in the final step, the lipophilicity properties of silyl derivatives were investigated by Reversed-phase High-performance Liquid Chromatography (RP-HPLC) [2]. The obtained results show an enhancement in the lipophilicity of silyl derivatives compared to piroxicam. Piroxicam can be used as tablets and also ointments. That is, it can be viewed from the stand point of both prodrug and lipophilic properties of ointment.

Keywords: Piroxicam, Prodrug, Silyl derivative, Lipophilicity



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Synthesis of novel halogenated bicyclo[4.2.0]inositols from *syn*-bisepoxide

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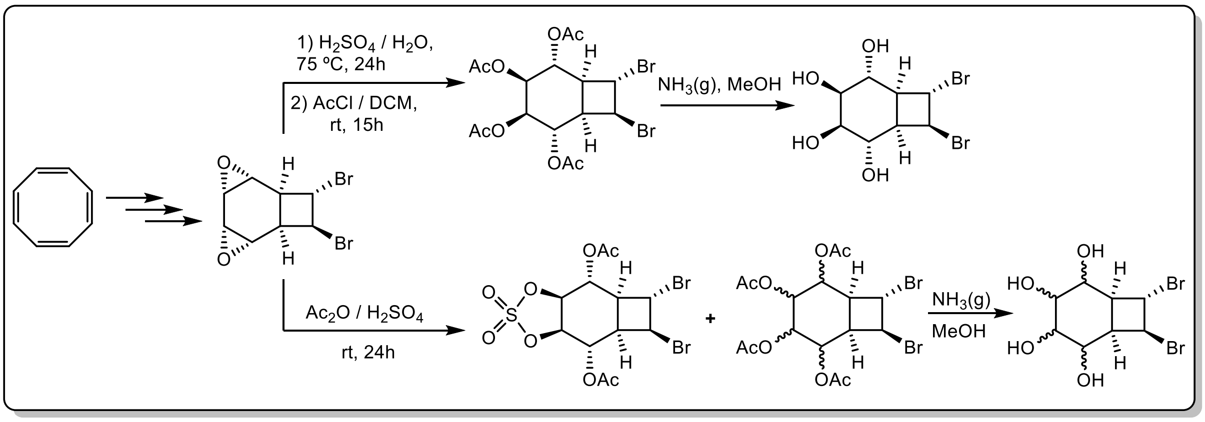
Poly hydroxylated carbon cycles namely cyclitols have numerous subclasses such as inositols and conduritols with their import roles in living organism and miscellaneous biological activities. For example scyllo-Inositol which is one of the inositol isomer has been shown to have promising potential as a therapeutic for Alzheimer's disease [1]. On the other hand a number of conduritol derivatives have been found to possess antifeedant, antibiotic, antileukemic, and growth-regulating activity [2]. Introduction of a small ring in polyhydroxylated carbocycles in stereoselective fashion may lead a locked specific conformation wherefore interesting biological profile [3]. Moreover, a substituent on the new ring like bromine could be used to introduce additional functionalities properly designed and tailored to fit specific biological targets.

Due to the aforementioned properties synthesis of bicyclo cyclitol skeletons gain interests. Herein, we describe the synthesis of novel halogenated bicyclo inisitols which have the same configuration as dihydroconduritol-A, -B, and -F structures. Syn-bisepoxide functionalized bicyclo[4.2.0]octane skeleton was synthesized starting from the cyclooctatetraene. Acid-catalyzed ring opening reactions of the bisepoxide gave the tetrols after ammonolysis [4].



Keywords: Cyclitol, Halogenated cyclitol, Ring-opening of syn-bisepoxide

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Stereoselective Synthesis of a Conduritol-A Derivative Including Halogene

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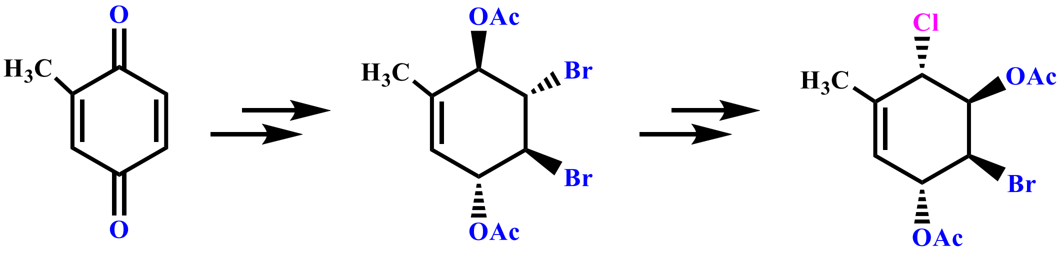
Conduritols and carbasugars are a class of polyhydroxylated cyclohexanoids that have continued to attract the attention of chemists and biologists due to their involvement in various biological processes [1]. Conduritols which are precursors for the synthesis of cyclitols and their derivatives have interesting biological activities. Their biological activities, particularly glycosidase inhibition, have extensively been evaluated [2]. Bromoconduritol (6-bromo-3,4,5-trihydroxycyclohex-1-ene) is an active-site-directed irreversible inhibitor of glucosidases [3]. Thus, halo-conduritols have attracted researchers' attention and they have been found to possess enzyme-specific inhibition against α-glycosidase.

The stereoselective synthesis of 2-bromo-6-chloro-5-methylcyclohex-4-ene-1,3-diyl diacetate, methyl-substituted dihaloconduritol-A is reported. Bromination of 2-methylbenzo-1,4-quinone followed by the reduction in the carbonyl groups with $NaBH_4$ to give a dioldibromo compound. The diol was converted to diacetates by acetylation with Ac_2O-pyridine. Reaction of methyl-dioldibromodiacetate with LiOH gave stereoselectively the monoepoxide compound. Controlled reaction of the epoxide with AcCl in methylene chloride furnished the desired new dihaloconduritol-A derivative [4]. All the synthesized compounds were characterized by FT-IR, ^{1}H-NMR, ^{13}C-NMR, COSY (2DNMR), and HRMS analyses.



Keywords: Conduritol, Cyclitol, Halogenated cocduritol, Conduritol-A derivative

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High performance magnetic nanocatalyst in Heck reaction in green conditions

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The conditions for coupling reactions in organic chemistry depend on the type of bond between the two carbon atoms and the carbon, so that for each there is a different name given to the name of the scientist who first discovered it. In this project, the main purpose is to investigate the carbon-carbon bond coupling reaction in two dual bands of two different aryl compounds. For this purpose, a new nanocatalyst has been used to perform this reaction, which is a new magnetic nanocatalyst with silicate coating with isopropyl triethoxy chloride, morpholine and copper metal linkers that have been fixed on the nanocomposite surface. The amount of stabilized copper is about 12%, which is adsorbed on the substrate of magnetic nanoparticles at 75° C and isopropyl alcohol solvent (ie green conditions). The products obtained from the hacking reaction by this nanocatalyst are above 98%, which is due to its magnetic controllability and inhomogeneous surface. This catalyst can also have many applications in the medical industry [1], and is also very effective in other types of carbon-carbon coupling reactions like the work of other researchers [2-4].

Keywords*:* Magnetic nanoparticles, Copper nanoparticles, Heck reaction

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The best way to perform a Suzuki reaction under standard conditions is with a magnetic nanocatalyst

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From 2010 until today, carbon-carbon coupling reactions have been very widespread and have attracted the attention of many interested researchers. To this end, new catalysts are synthesized and designed each year to be used for the reaction and evaluated with other researchers' catalysts. Therefore, in this project, we have tried to examine one of the most interesting and unique catalysts that we have recently synthesized and used for the Suzuki reaction. The Suzuki reaction, named after Akira Suzuki (winner of the 2010 Nobel Prize in Chemistry), is a very interesting reaction that results from the bonding of two different carbons (one aryl boronic acid and the other an aryl halide). Synthetic catalyst is a magnetic nanocatalyst with capabilities such as external field control, creating a wide substrate surface for reaction, high catalytic speed, creating a connection between two aqueous and organic phases and easy separation from the reaction medium, with organic ligands And copper metal (ie copper metal loaded on the catalyst bed) is very suitable for this reaction. The reasons for using this metal instead of Pd are cheap and available, creating suitable spaces between the two reactors, helping the catalyst to accelerate the Suzuki reaction. Finally, the obtained products have an efficiency of over 98%, which has been widely used in the medical industry [1], and many reports have been published by chemical researchers to perform the Suzuki carbon-carbon coupling reaction [2-4].

Keywords*:* Magnetic nanoparticles, Copper nanoparticles, Suzuki reaction

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Optimal Synthesis Conditions of Products from Carbon-Nitrogen Coupling Reaction Using Suitable Substrate Magnetic Nanocatalyst

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Carbon-nitrogen coupling reactions have been named in honor of Mr. Buchwald, which are very important in the medical industry for the production of biological products [1]. Every year, many articles are published and published on this subject, each of which has its own important and special features. In this project, the main purpose is to investigate the efficiency of nanocatalysts containing morpholine linkers and silica coatings with copper metal loaded on its surface in order to perform the Buchwald reaction in a completely optimal way and in very cost-effective conditions. For this purpose, the reaction temperature was reduced from 100 to 80 and potassium carbonate salt was used to create ionic bonds between the reactants. The composition of the percentage of products obtained by this method is very high and is about 97%, which according to recent research [2-4] in this field, has a much higher efficiency. So that in the first half hour, the desired product is synthesized and with more time, the raw materials are completely consumed and converted into a product. The power of the nanocatalyst is so high that, in several re-uses, it is reduced by less than 10% of its power, which is a very good figure for more reactions and clearly shows the high efficiency of this nanocatalyst.

Keywords*:* Magnetic nanoparticles, Copper nanoparticles, Buchwald reaction

References

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Synthesis of 1,4-Dihydropyridine derivatives Incorporating the Adamantane Motif

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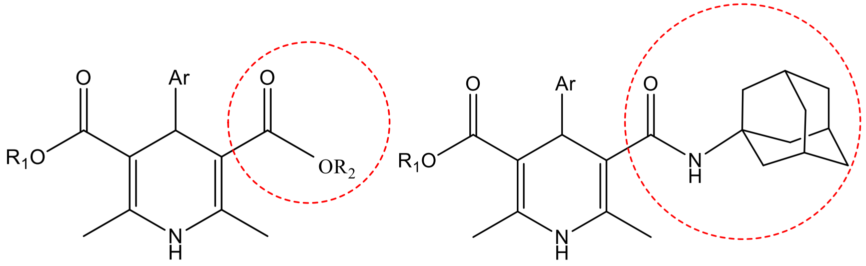
Hypertension is a common medical and social problem leading to cardiovascular diseases worldwide.[1] The five major classes of antihypertensive drugs- diuretics, β-blockers, angiotensin-converting enzyme (ACE) inhibitors, angiotensin receptor blockers (ARBs), and calcium channel blockers (CCBs), including dihydropyridines (DHPs) and non-dihydropyridines- are clinically applied to decrease the morbidity and mortality induced by hypertension itself and its complications.[2] 1,4-Dihydropyridine drugs are nowadays the most used drugs in the treatment of hypertension. As of now, there are four generations of DHPs clinically available.[3] The first-generation nicardipine and nifedipine have proven efficacy against hypertension, but due to their short half-life time and rapid onset of vasodilator action, these drugs were more likely to be associated with adverse effects. The second generation benidipine, and efonidipine with slow-release and short-acting preparations allowed better control of the therapeutic effect and a reduction in some adverse effects. The third-generation amlodipine and azelnidipine are more lipophilic with stable pharmacokinetics and long-term actions, and less cardio-selective and well tolerated in patients with heart failure. The fourth-generation lercanidipine and lacidipine (L/N-type CCB) are highly lipophilic with a real degree of therapeutic comfort in terms of stable activity, a reduction in adverse effects and a broad therapeutic spectrum, especially in myocardial ischemia and potentially in congestive heart failure. As can be seen, the higher generations of DHPs with more lipophilicity are much more potent drugs. Adamantne, the smallest diamondoid, is often viewed as providing just the critical lipophilicity, and it is used as a "lipophilic bullet" for modification of known drugs.[4,5] In this study, we wish to combine the remarkable structure and chemical properties of bulky and lipophilic adamantane with privileged 1,4-DHP scaffold and synthesis of novel more potent DHP CCBs.



Keywords: 1,4-Dihydropyridine, Adamantane, Lipophilic bullet, Diamondoid, Nanodiamond

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Catalytic application of UiO-66-NH_2/TCT/$_2$-Py@Cu for the synthesis of pyrazolo[3,4-*b*]pyridine derivatives *via* cooperative vinylogous anomeric-based oxidation

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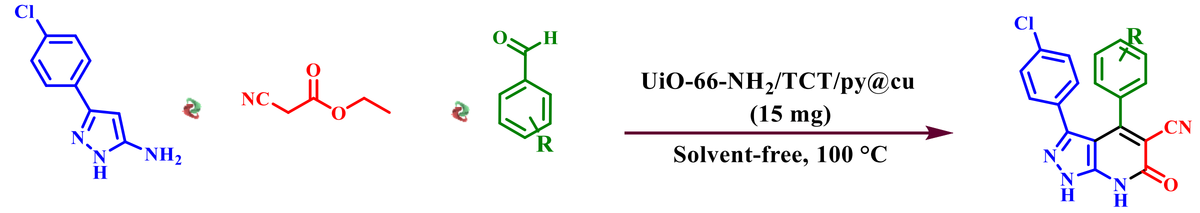
Metal-organic frameworks consists of organic compound as ligand and metal that make large surface area, high flexibility and pore size planning namely metal-organic frameworks (MOFs). These porous materials was applied as gas storage and separation, drug delivery, sensors, batteries, supercapacitors as well as catalyst [1]. Historically, anomeric effect (AE) was introduced by J. T. Edward on the development of organic chemistry. This hypothesis, which is propagated through double bonds, has been termed as a vinylogous anomeric effect (VAE) [2]. Anomeric based oxidation (ABO) concept has been known for the final step of oxidation/reduction mechanism in the preparation of biological compounds [3]. The development of cooperative vinylogous anomeric-based oxidation (CVABO) is at the forefront of organic chemistry due to the importance of this concept in promoting the synthesis of organic compounds with biological properties [4]. Also, fused *N*-heterocycle compounds such as pyrazolo[3,4-*b*]pyridines may be suitable candidates for biological and pharmacological activity [5]. According to the above-mentioned idea, we have designed and synthesized of novel heterogeneous and porous complex based on Zr-MOFs. This porous complex was applied for the synthesis of pyrazolo[3,4-*b*]pyridine derivatives by condensation reaction of various aromatic aldehydes (bearing electron-donating and electron-withdrawing groups), ethyl cyanoacetate and 3-(4-chlorophenyl)-1*H*-pyrazol-5-amine *via* cooperative vinylogous anomeric-based oxidation under solvent-free condirion at 100 °C (**Scheme1**).



Scheme1: Preparation of pyrazolo[3,4-b]pyridine derivatives by UiO-66-NH_2/TCT/$_2$-Py@Cu

Keywords: Anomeric based oxidation, Copper complex, UiO-66-NH_2, Zr-MOFs.

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Post-modification of metal-organic frameworks (MOFs) as catalyst

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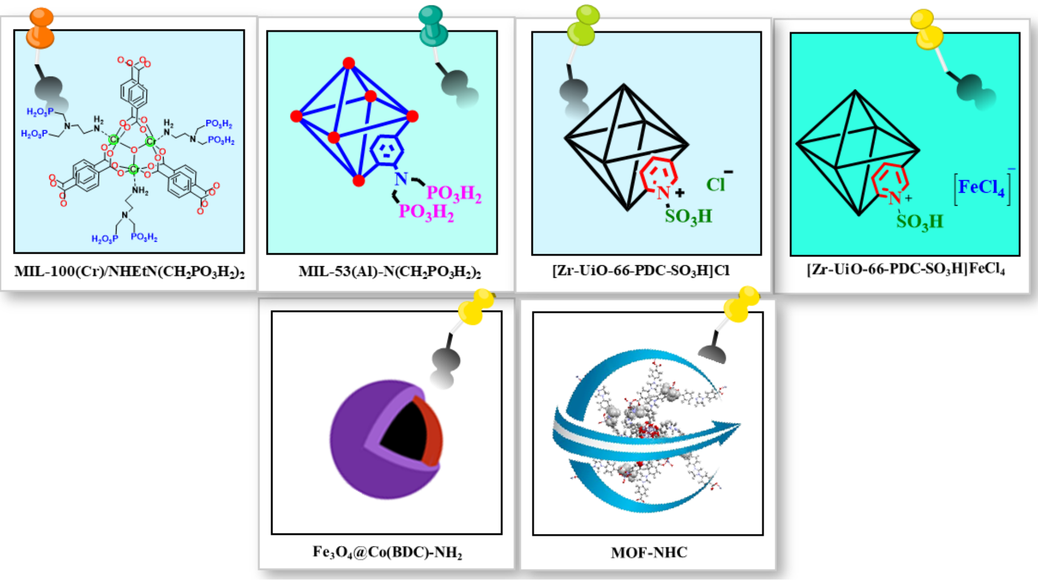
Nowadays, post-modification method is a versatile strategy for the preparation of catalyst, storage, absorbent, sensor. Among the recent application in metal-organic frameworks (MOFs) are created due to modular structure and adjustable porous crystal [1]. The structure of MOFs structure is composed of metal or metallic cluster coordinated by polyhedral organic ligands [2]. Increasing or increased in quantity of level area, pore volume and flexibility of architecture of metal-organic frameworks has revealed a new field in research that is mainly aimed at preparing a new framework of materials and research their applications in catalytic processes, gas separation, adsorption and drug delivery [3]. For this purpose, post-modification method is known new architecture for preparation of heterogeneous catalyst. Therefore, this method is a general discussion of the potential benefits of metal-organic frameworks (MOFs) as a heterogeneous catalyst [4]. However, post-modification of metal-organic frameworks show improved catalytic efficiency [5]. In this work, we overview the recent developments of catalysis at single metal sites in MOF-based materials with emphasis on their structures and applications for the synthesis of organic compounds with biological activates (**Scheme 1**).



Scheme 1: Post-modification of metal-organic frameworks (MOFs) as catalyst.

Keywords: Metal-organic frameworks (MOFs), Organic compounds, Post-modification.

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A new approach for the synthesis of bis(3-indolyl)pyridines via a cooperative vinylogous anomeric based oxidation using ammonium acetate as a dual rule reagent-catalyst under mild and green condition

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Nowadays, research and development (R&D) based on the presentation of new strategy is essential for the synthesis of organic compounds without the use of catalysts, hazardous solvents, toxic chemical materials, easy reaction conditions and etc [1]. On the other hand, extension the principles of green chemistry are one of the main goals of organic chemistry. For this purpose, ammonium acetate (NH_4OAc) is known as a green, non-toxic and safe compound, which has been applied as a source of nitrogen for the synthesis of *N*-heterocycle compounds. Also, NH_4OAc can also applied as efficiently and eco-friendly catalyst in the synthesis of organic compounds [2]. Indole compounds are an important group of heterocycle compounds that have received much attention due to their unique properties. This compounds and especially their bis structures have important inhibitory effects on leukemia, ovarian cancer, non-small cell lung cancer, breast cancer, colon cancer and kidney cancer [3-4]. Due to the attractive strategy of using ammonium acetate as a dual rule reagent-catalyst in the synthesis of biological active organic molecules, catalytic application of ammonium acetate was investigated for the synthesis of bis(3-indolyl) pyridine derivatives via cooperative vinylogous anomeric based oxidation (CVABO) concept. Herein the synthesis of biological derivatives without the use of toxic and expensive materials was occurred (Scheme 1).

Scheme 4: Preparation of bis(3-indolyl) pyridine derivatives using ammonium acetate as a dual rule reagent-catalyst.

Keywords: Ammonium acetate, Anomeric effect, Bis(3-indolyl)pyridine, Dual rule reagent-catalyst.

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Incorporation of phosphorous acid tags into UiO-66-NH₂ as porous and heterogeneous catalyst for the preparation of novel spiro-oxindoles

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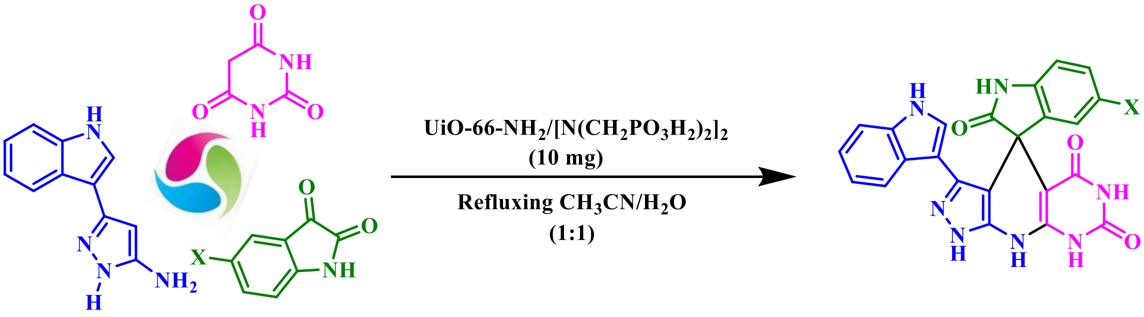
In recent years, metal-organic frameworks (MOFs) are known as a new group of porous materials that have high design ability due to the variety of ligands and metals [1]. These frameworks have properties such as ultra-high surface area, adjustable pore size, adjustable inner surface and charge conduction [2]. Recently, metal zirconium(IV) cuboctahedral secondary building unit -organic frameworks (MOFs) based on the (SBU), $Zr_6O_4(OH)_4(CO_2)_{12}$ and related expanded analogues with ditopic organic struts have been reported [3]. All of these MOFs have a face-centered-cubic (fcu) topology and high thermal and chemical stability. Thus far, no other topologies have been reported for this important class of zirconium-based MOFs [4]. Also, *N*-heterocycle compounds such as spiro-oxindoles have attracted much attention due to their application in solar cells and their medicinal properties such as human NK-1 receptor inhibitors, antitumor agents, antibiotics, anticancer and antibacterial [5]. Due to the biological structure and post-modification of metal organic frameworks (MOFs) with phosphorous acid tags, we found a strategy for the preparation of UiO-66-NH_2/$[N(CH_2PO_3H_2)_2]_2$ as a heterogeneous and porous catalyst by the condensation reaction of UiO-66-NH_2 and phosphorous acid under EtOH reflux. This efficient and reusable catalyst was tested in the preparation of novel spiro-oxindole derivatives under refluxing CH_3CN/H_2O condition (**Scheme1**).



Scheme1: Preparation of spiro-oxindoles using UiO-66-NH_2/$[N(CH_2PO_3H_2)_2]_2$

Keywords: Metal-organic frameworks (MOFs), Spiro-oxindoles, UiO-66-NH_2.

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Catalytic application of Fe/Zr-MOF-N($CH_2PO_3H_2$) for the synthesis of fused pyridine structure with indole moieties *via* a cooperative vinylogous anomeric-based oxidation

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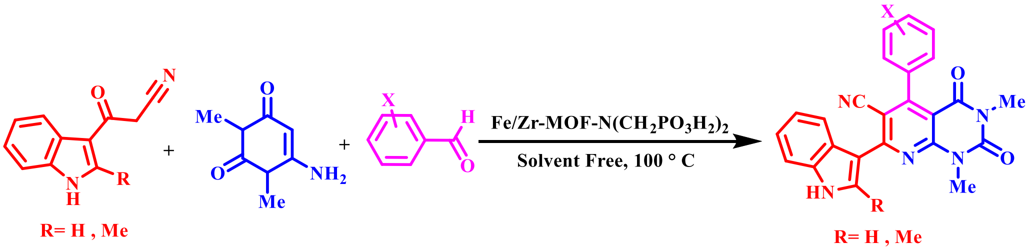
Nowadays, metal-organic frameworks (MOFs) are hybrid compounds where metal nodes are linked into infinite arrays through multitopic ligands. These crystalline solids with accessible open spaces have rapidly grown into a major area of chemical research attracting interest and enthusiasm from a wide community over the past two decades [1-2]. Advances have been made in synthesis, crystal engineering, functionality and applicability of MOFs [3]. Even so, achieving desired MOF structures with targeted properties and functions still present a significant challenge, which sets the foundation for major improvement for future industrial application of these promising materials. The cyclization reaction between amines and carbonyl compounds was the most common method for preparing pyridine like frameworks [4]. The pyridine ring structures are biological activity like as inhibiting HIV protease, antidepressant, anti-inflammatory, inhibiting acetylcholinesterase, treating hypotension or hypertension [5]. Among of them, pyrido[2,3-*d*]pyrimidine is a structure with biological potency such as a drug resistant to malaria and tuberculosis, anti-inflammatory, antiviral, antibacterial, insecticidal, antifolate, and antitumor activities [6]. In continuation of our investigations on development of preparation of metal-organic frameworks (MOFs) *via* PSM strategy. Herein, we decide to synthesis of novel Fe/Zr-MOF-N($CH_2PO_3H_2$) as an efficient catalyst for the preparation of pyrimid[2,3,*d*] pyrimidine derivtives with indole moieties (Scheme 1).



Scheme 1: Preparation of pyridine compound with indole moieties using Fe/Zr–MOF-N($CH_2PO_3H_2$)$_2$.

Keywords: Fe/Zr–MOF-N($CH_2PO_3H_2$)$_2$, Indoles, Metal-organic frameworks, Pyrimido[2,3,*d*] pyrimidine.

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Synthesis of one-component polyurethane adhesive for rubber granules bonding

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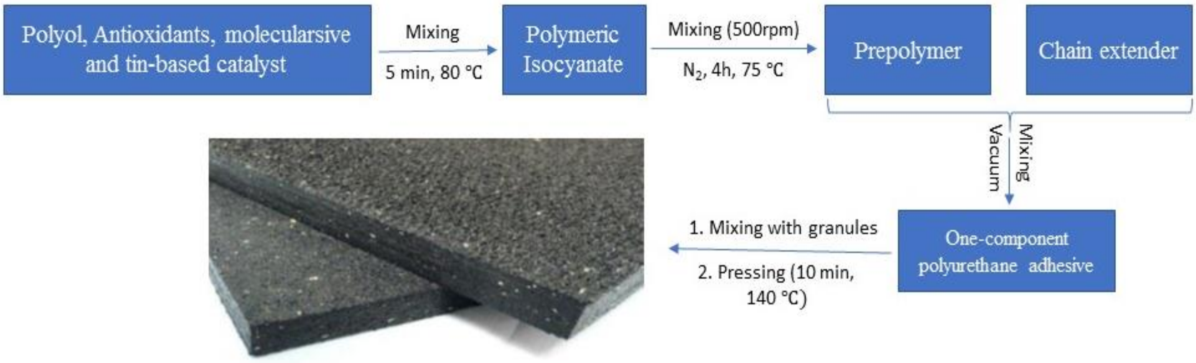
For floors of vehicles and building, rubber flooring is generally used because of its abrasion-resistance, resistance to chemicals, resistance to thermal deformation and etc. [1, 2]. This work explores the synthesizing one-component thermal-curable polyurethane adhesive in order to bonding the rubber granules. A schematic model of synthesizing and utilization of the adhesive is depicted in Figure 1. The NCO-terminated polyurethane prepolymer was prepared by polymerization reaction based on polyether polyol and polymeric isocyanate under an inert atmosphere. Antioxidants, molecularsive, chain extender and tin-based catalyst were utilized as additives in the formulation of adhesive. The prepolymers were synthesized with NCO/OH ratios of 2.5, 3 and 3.5. The results revealed that the viscosity of the prepolymer decreased with increase in NCO/OH molar ratio. By increasing NCO/OH molar ratio, the curing time of the polyurethane adhesive is increased. The obtained results showed that the resistance to separation of granules increased with increasing NCO/OH molar ratio.



Schem 1. Schematic of manufacturing process of the rubber flooring

Keywords: Rubber bonding, One-component polyurethane adhesive, Polyether polyol

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Large-scale preparation and characterization of semi-rigid polyurethane foam

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Semi-rigid polyurethane foam is widely used as heat insulating building materials in the automotive interiors. This type of foam has a lower apparent density and higher thermal conductivity in comparison to the closed cell foam [1]. Flexible foam shows high recovery properties, while rigid foam displays high load-bearing and absence of recovery. The semi-rigid foam shows a blend of these characteristics [3].

The semi-rigid polyurethane foam was produced by reaction of formulated polyether-based polyol and polymeric isocyanate. Chain extenders (glycerin and sorbitol), blowing agent (water), surfactant (silicone oil), catalysts (tin and amine based) and nano-fumed silica were used in the formulation of polyol. Results indicate that the addition of nano-silica contributes to preparing foams with higher compressive strength, and increases the density of the foams due to the decrease in cell size. By addition of nano-silica (0.2 %Wt.) in the formulation of polyol, the sound absorption coefficient of the foam is increased by %18.6 (Figure 1). Scanning electron microscopy (SEM) has been used in order to investigate cellular morphology of the prepared foams (Figure 2).

Figure 1. sound absorbing responses of the synthesized foams with nano-silica (solid line) and without nano-silica (dotted line).

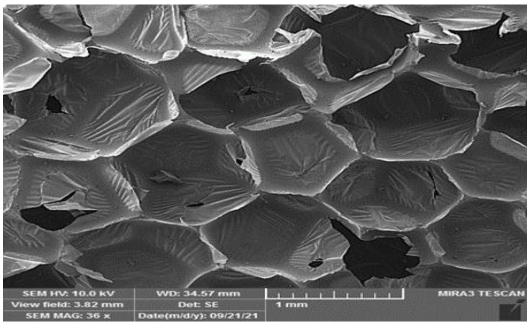

Figure 2. SEM micrograph of the prepared polyurethane foam with nano-silica.

Keywords: Semi-rigid polyurethane foam, Nano-silica, Polyol formulation

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Phosphonic acid tagged carbon quantum dots encapsulated in SBA-15 as a novel catalyst for the preparation of *N*-heterocycles with pyrazolo, barbituric acid and indole moieties

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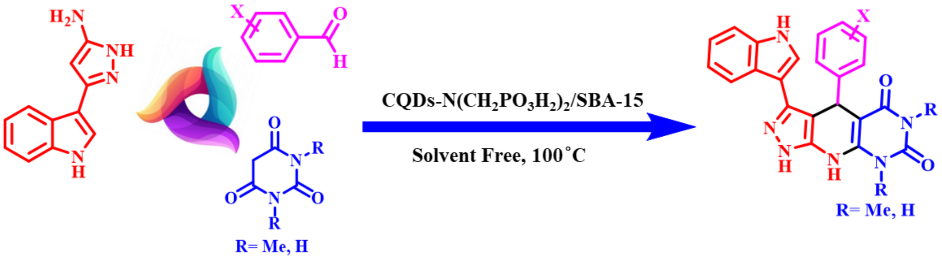
In recent years, composite materials have become well-known as catalyst, absorbent and sensor in modern science [1]. Quantum dots based on carbon, nitrogen and graphene as nano-materials with small size 10 nm have exhibited great potential uses in photocatalysis, biosensing, heavy metal elements sensing and biomolecule/drug delivery [2]. Despite the success of existing materials and technologies, the stability of CDs especially in harsh chemical and physical conditions and weak thermal stability is still highly desirable. Also, mesoporous silica catalysts are very much more functional due to their easy and fast separation from reaction media, which is high surface area, pore volume and tunable pore size. CQDs integrated with SBA-15 particles have been widely used as catalysts in chemical reactions due to their high porosity and increased chemical and thermal stability [3]. Compounds containing indole and barbituric acid have properties such as analgesic, antibacterial, anti-inflammatory, etc. Due to these properties, these compounds are widely used in various chemical reactions [4]. In this strategy, we have synthesized novel pyrazolo[4',3':5,6] pyrido[2,3-*d*]pyrimidine derivatives by one-pot condensation of benzaldehydes, pyrimidine-2,4,6(1*H*,3*H*,5*H*)-trione derivatives and as-synthesized 5-(1*H*-indol-3-yl)-1*H*-pyrazol-3-amine using CQDs-N($CH_2PO_3H_2$)$_2$/SBA-15 as an excellent mesoporous heterogeneous catalyst (Scheme 1).



Scheme 1: Preparation of pyrazolo[4',3':5,6]pyrido[2,3-*d*]pyrimidine derivatives using CQDs-*N*($CH_2PO_3H_2$)$_2$/SBA-15.

Keywords: Composite, CQDs-N($CH_2PO_3H_2$)$_2$/SBA-15, 1,4-Dihydropyridine, Indole.

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Synthesis of 1,4-dihydropyridine derivatives with indole section using bimetal-organic frameworks with phosphorous acid tags

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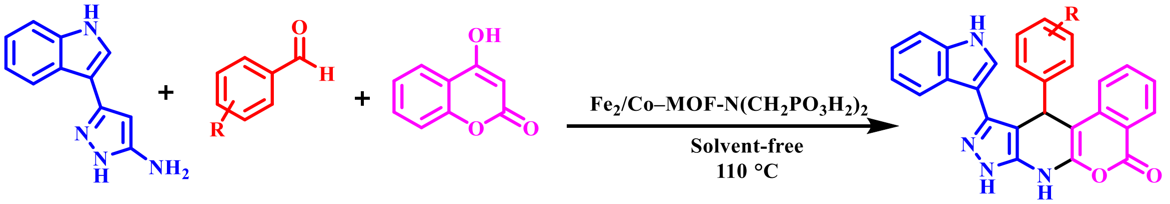
Chemical transformations via catalysis are known as key processes in organic synthesis and energy storage/conversion, in which metals usually serve as central roles in catalysts, such as, metal nanoparticles (NPs) and metal complexes [1]. As a type of classical heterogeneous catalysts, metal NPs present significant promise in a wide range of catalytic fields, where the active metal sites are often located at crystal corners, edges, and facets, bearing different catalytic properties. To normalize the catalytic behaviors and maximize the utilization efficiency of metals, downsizing the metal NPs is considered as an effective method to greatly boost the catalytic performances with enhanced activities and selectivity [2]. Metal-organic frameworks (MOFs) (also called porous coordination polymers, PCPs), as constructed by both inorganic nodes (metal ions/clusters) and organic ligands via coordination bonds, have gained considerable attention, achieving overall and breakthrough progress since the 1990s [3]. The structural diversity, ultrahigh surface area, and easy tailorability as well as the crystalline nature allow the MOFs to be widely applied in various fields including the early discovered catalysis [4]. Also, 1,4-dihydropyridine with indole and coumarin structures have significant biological properties such as analgesic, anticoagulant, antibacterial and etc. [5]. On the basis of above-mentioned facts, synthesis of biological structure with indole moieties in the presence of reusable solid acid is our main research interest. With this aim, bimetal-organic frameworks with phosphorous acid tags as a porous-catalyst structure was synthesized, characterized and used in synthesis chromeno[3,4-b]pyrazolo[4,3-e]pyridin with indole moieties under mild and green condition (Scheme 1).



Scheme 1: Preparation of 1,4-dihydropyridine with indole derivatives using $Fe_2/Co–MOF-N(CH_2PO_3H_2)_2$.

Keywords: Bimetal-organic frameworks, 1,4-Dihydropyridine, Indole, Phosphorous acid.

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Development of a new magnetic and biocompatible covalent organic framework; Synthesis and characterization

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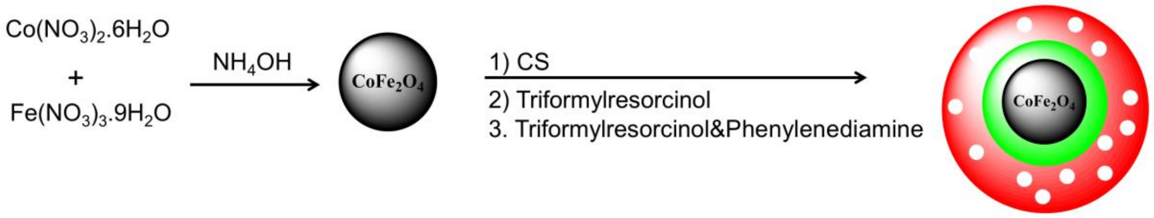
In recent years the development of the new multifunctional biocompatible platforms with both magnetic properties and porous structure has drawn considerable attention. Cobalt ferrite nanoparticles ($CoFe_2O_4$ NPs) are one the well-known nanomaterials with moderate magnetization, special chemical stability, and high coercivity. These positive features can be further combined with higher biocompatibility as a result of modification with chitosan (CS) biopolymer. This deacetylation product of chitin can obtain the biocompatible and biodegradable amine functional groups containing nanoparticles after capping the $CoFe_2O_4$ NPs [1-2]. It has been recently revealed that the systems having terminal amine functionalized systems like the CS-based systems can be an excellent substrate for the fabrication of porous covalent organic frameworks (COFs) [3-4]. Considering this the aim of the present research work was to develop a novel biocompatible, magnetic, and porous structure. Hence, initially, the $CoFe_2O_4$ NPs were prepared via the co-precipitation technique. Then it was modified with CS biopolymer via a facile sonochemical technique ($CoFe_2O_4$@CS). Finally, the imine-based COFs were in situ grown on the $CoFe_2O_4$@CS hybrid ($CoFe_2O_4$@CS/COFs). A schematic view of the $CoFe_2O_4$@CS/COFs fabrication procedure is presented in Scheme 1. Several characterization techniques approved the success in $CoFe_2O_4$@CS/COFs fabrication. $CoFe_2O_4$@CS/COFs displayed porous structure in Brunauer-Emmett-Teller (BET) analysis. Also, the presented enhanced height profile compared to $CoFe_2O_4$ NPs in atomic force microscopy (AFM) analysis.



Scheme 1. Schematic view of the $CoFe_2O_4$@CS/COFs fabrication procedure.

Keywords: Cobalt ferrite nanoparticles, Chitosan, Covalent organic frameworks.

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Synthesis of a magnetic metal organic framework (Fe_3O_4@Co-MOF) as a novel and recyclable catalyst for the synthesis of quinazolin-4(3*H*)-ones under mild aerobic condition

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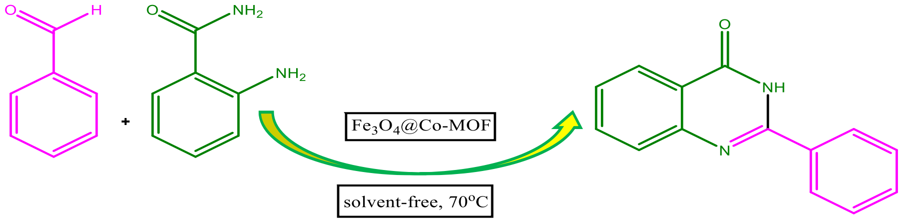
This work reports an eco-friendly and inexpensive route to the synthesis of magnetic metal organic framework (MOF) catalyst *via* a step-wise manner. The chemical structure of the synthesized nanocatalyst was characterized by various methods, including FT-IR, XRD, BET, TEM, FE-SEM, EDX, EDX-mapping, VSM, and ICP-OES. The combination of Fe_3O_4 NPs with a metal organic framework leads to achieve a Fe_3O_4@Co-MOF nanocatalyst with a relatively high specific surface area, an average pore size 15.6 nm and microporous structure. The catalytic performance of Fe_3O_4@Co-MOF nanocatalyst was evaluated in the synthesis of quinazolin-4(3*H*)-ones derivatives and the obtained results demonstrated that the as-prepared nanocatalyst could be an efficient catalyst to produce the desired products with good to excellent yields under solvent free conditions. More importantly, due to the super paramagnetic behaviour of Fe_3O_4@Co-MOF, this nanocatalyst showed the high stability under the reaction conditions and could be easily reused by means of an external magnetic field [1,2].



Keywords: Metal organic framework, Quinazolinones, Heterogeneous catalyst

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Photoluminescent and biocompatible starch coated biobased-derived carbon dots as a promising platform for methotrexate delivery

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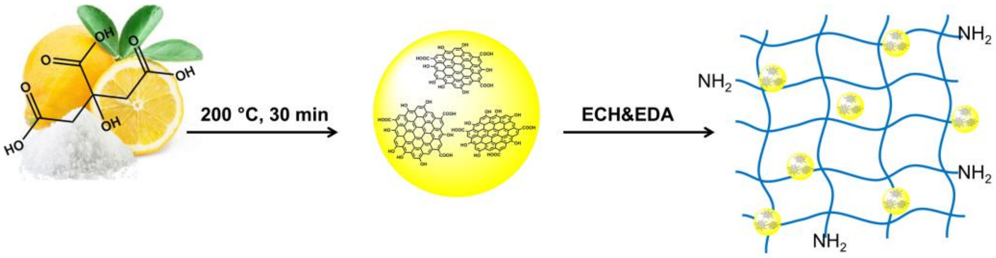
Photoluminescent materials like carbon dots (CDs) have received considerable attention because of their potential applications in a variety of fields, for example, optoelectronic devices, bioimaging, and sensing. Up to now, the various reagents have been evaluated as the precursors for CDs synthesis [1]. Herein we report a green synthetic for CDs from garlic by a one-step hydrothermal synthesis. CDs could be combined with polysaccharides in order to avoid their aggregation, as well as increase their biocompatibility, biodegradability economic efficiency which are good characteristics of drug delivery. Starch is considered a high-potential resource for the development of applicable bio-nano composites in medicine because it is abundant, low in cost, renewable, and biodegradable features [2-3]. By considering these in this work at first carbon dots (CDs) were green synthesized from low-cost and more available garlic. Then the synthesized CDs were mixed with starch and then crosslinked with epichlorohydrin in the presence of ethylenediamine (CDs/starch). The schematic of CDs/starch crosslinking is shown in Scheme 1. All used implemented physicochemical characterization methods, for instance, FT-IR, EDX, and XRD confirmed the CDs/starch fabrication route. Then the methotrexate load capability and its release profile were evaluated for CDs/starch.



Scheme 1. Schematic view of the CDs/starch fabrication pathway.

Keywords: Carbon dots, Starch, Drug delivery.

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Design, synthesis, and characterization of bio-MOF(Zn)@carboxymethyl starch/graphene quantum dots nanoplatform

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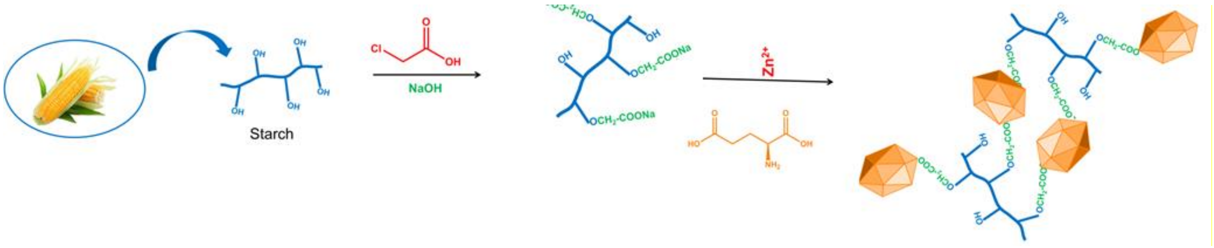
Emerging new drug delivery systems that can eliminate the drug-resistant turmeric cells and obtain higher efficiency is essential in chemotherapy [1]. In between, carbon-based nanomaterials, especially graphene quantum dots (GQDs), are in the prime position of the nanomaterial list as compared to others due to their special characteristics. Nowadays, bio-nanocomposites are known to offer many improved features owing to the incorporation of nanomaterials. Polysaccharides like carboxymethyl starch (CMS) have gained significant attention in the prepared nanocomposites for use in drug delivery. The association of MOFs with biocompatible polymers could be a versatile strategy to make the new hybrid porous materials in a synergistic combination of their respective features [2-4]. Therefore, thanks to the complementary features between photoluminescent GQDs, biocompatible nature of CMS, and porous structure of MOFs, initially new photoluminescent zinc crosslinked system was prepared by a physical crosslinking technique. Then the Bio-MOF(Zn) was in-situ synthesized in the presence of Zn-CMS/GQDs by an eco-friendly and economic route at room temperature in which zinc centers are connected by L-glutamic acid units. The formation of zinc-glutamate Bio-MOF in the presence of Zn-CMS/GQDs was elucidated by the common characterization techniques. BET analysis obtained the pore diameter of Bio-MOF(Zn)@CMS/GQDs at about 4.5 nm



Scheme 1. Schematic view of the Bio-MOF(Zn)@CMS/GQDs fabrication pathway.

Keywords: Graphene quantum dots, Carboxymethyl starch, Bio-MOF(Zn).

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Synthesis of 1H-isochromene derivatives using triethylamine as a homogeneous metal-free base catalyst

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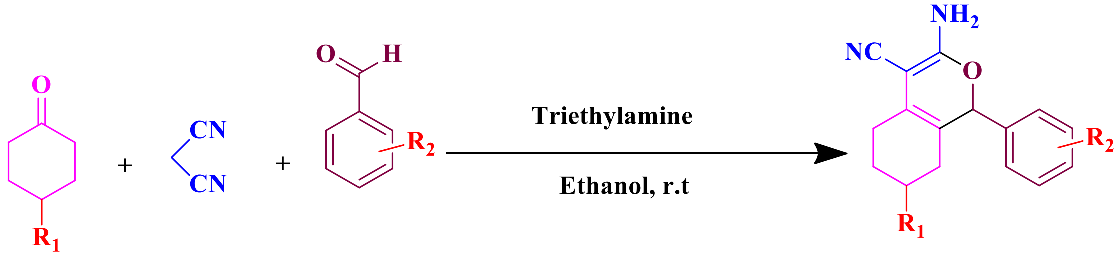
Isochromene derivatives are a class of chemical compounds found in various natural, biologically active, and medicinal compounds. These chemicals treat stomach cancer because they contain anti-tumor effects [1]. The enormous value of these compounds has inspired much effort to advance a vast number of practical and dependable procedures for their synthesis [2]. Multicomponent reactions (MCR's) are an excellent idea for synthesizing a complicated organic product. These reactions have three or more reactants to form a new significant and applied product [3].

This research hopes to report the synthesis of 1H-isochromenes from cyclohexanone, malononitrile, and benzaldehyde through the Michael addition and aldol condensation reactions using triethylamine as a homogeneous base catalyst. This reaction was performed at room temperature in ethanol solvent under mild conditions. The obtained compounds were identified by the melting points, FT-IR, and ^{1}H NMR analyses. In this protocol, all the reactions had excellent yields of products with short reaction times.

Keywords: Isochromene**,** Nanocatalyst**,** Triethylamine**,** Anti-tumor



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Novel design and synthesis of Zr-MOF-UR as hydrogen bond donor catalyst: Its application for the preparation of pyrrolo[2,3-*b*]pyridines

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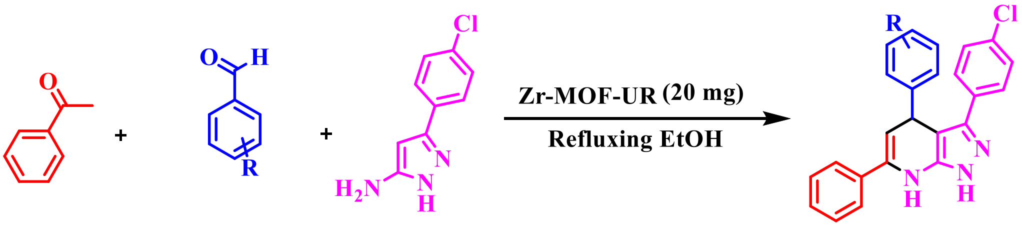
Metal-organic frameworks (MOFs) have been employed in various fields such as catalysts, electrocatalysts, supercapacitors, drug delivery, sensors, batteries, membranes, and absorbents due to the eye-catching features such as various synthesis methods, structural diversity, high surface area, and attractive architectures [1]. Among the large family of metal-organic frameworks (MOFs), Zr-based MOFs much research has been invested to directly construct MOFs with inherent stability in structure and composition [2]. Hydrogen-bonded organic frameworks (HOFs) are novel type of porous crystalline solids assembled by organic or metal-organic building blocks through hydrogen-bonding interactions. The concept for the construction of porous HOF materials using hydrogen bonding interactions was proposed in the early 1990s, almost the same period as that of MOFs. Most of H-bonding interactions are essentially weak, flexible and of low directionality, as compared with covalent and coordinate bonds in terms of bonding energies and angles. Many HOFs thus possess different isomers depending on their synthesis solvents or conditions, which significantly increases the structural diversity of HOFs [3]. The pyrrolo[2,3-*b*]pyridine core structure, a bioisostere of quinolones, is found in several molecules as biological activity [4]. Herein, we have synthesized new pyrrolo[2,3-*b*]pyridines in percent of Zr-MOF-UR as hydrogen bond donor catalyst under reflux condition (Scheme 1).



Scheme 1: Preparation of pyrazolo[3,4-*b*] pyridines using Zr-MOF-UR as hydrogen bond donor catalyst.

Keywords: Hydrogen-bond donor catalyst, Zr-MOF-UR, Metal-Organic Frameworks, Zr-MOFs, Pyrrolo[2,3-*b*]pyridines.

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Biocompatible UV protective cotton fabric modified with chitosan/carbon quantum dots nanocomposite

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Production of protective cotton fabrics to UV radiation is necessary to increase the longevity and durability of the clothes prepared from these fabrics. This study mainly aims to produce protective cotton fabric against UV modified by biocompatible chitosan/carbon quantum dots (CS/CQDs) nanocomposite. CQDs have drawn lots of attention in production of fluorescent and UV absorbent materials [1-3]. Chitosan is considered as a biopolymer and suitable for various industrial applications owing to having nontoxic features, compatibility with environment, and thermal and chemical stability [4].

To achieve this goal, first, CQDs were prepared from pyrolysis of starch in water blending and then, preparation method and characterization of the CS/CQDs nanocomposite were performed in accordance with a previous published work [5]. Next, 10 g cotton fabric was set in two separate beakers. One of the beakers was regarded as blank sample and the other was charged with 0.5 g CS/CQDs and 100 mL water. The two beakers were exposed to UV radiation and results of UV-vis spectroscopy proved following the modification of cotton fabric (CF) by CS/CQDs 5 wt% nanocomposite, CF/CS/CQDs absorbed about 98% of UV rays while the blank sample offered inconsiderable UV absorption. Additionally, by use of photoluminescence spectroscopy one could conclude that CF/CS/CQDs possess a strong fluorescence property whereas this is not true for the blank sample. As these findings approve, usage of CS/CQDs nanocomposite for chemical modification of the cotton textiles is a biocompatible method and results in production of fluorescence textiles with UV absorbance ability for use in chemical and textile industries.

Keywords: Biocompatible, Cotton fabric, Chitosan, Carbon quantum dots, UV protective

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Developing melamine-rich COF modified magnetic chitosan bio-adsorbent for diclofenac sodium removal

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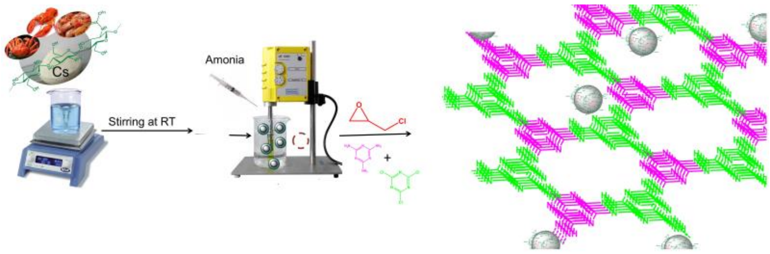
Water contamination is a collective problem all over the world that might be geological or anthropogenic, therefore, the pollutants removal from water is of great importance to human survival [1]. Polysaccharide-based adsorbents like chitosan (CS) is the only polycation endowed for the anionic pollutants removal. There are too plenty of reactive hydroxyl and primary amine functional groups in the structure of CS that can be protonated in acid media and afford strong electrostatic attractions for the adsorption of the anionic molecules [2-3]. Another interesting approach that is growing up in water treatment is focused on the development of novel nanoporous systems like covalent organic frameworks (COFs) as promising candidates for the further enhancement of the performance [4]. Inspired by these given facts in the current study, for the first time, a novel hybrid bio-adsorbent was fabricated from a combination of Fe_3O_4, CS, and COFs. Typically, in the beginning, the CS/Fe_3O_4 was prepared via a convenient and green sonochemical technique. Then the synthesized CS/Fe_3O_4 was used as a platform for the growth of nitrogen-rich melamine-based mesoporous COFs. The CS/Fe_3O_4@TCOFs product was characterized and the optimum conditions of the main affecting parameters to remove DS were identified. Moreover, the achieved experimental data were fitted to the adsorption isotherm and kinetic model respectively to obtain the adsorption mechanism and maximum adsorption capacity.



Scheme 1. Schematic view of the CS/Fe_3O_4@TCOFs fabrication pathway.

Keywords: Magnetite, Chitosan, COFs.

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Synthesis of Benzopyrano[2,3-*d*]pyrimidines in the Presence of Sodium Carbonate Silica Catalyst

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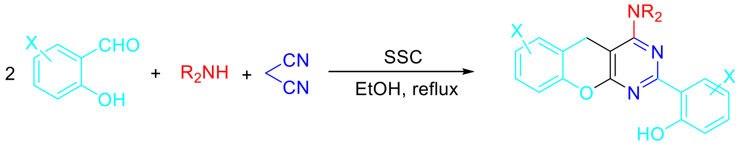
These benzopyrano[2,3-*d*]pyrimidines are attractive class of heterocyclic compounds with biological activities, including in vivo antitumor, antibacterial, antioxidant, antiangiogenic, analgesic, in vitro anti-aggregating, and antigenotoxic [1]. Due to the widespread applications of benzopyrano[2,3-*d*]pyrimidines, the development of new methods aimed at the synthesis of these valuable heterocycles is an striking topic of current research in many laboratories [2]. In this contribution, sodium carbonate silica (SSC) was synthesized and its catalytic activity was studied for the synthesis of derivatives of benzopyrano[2,3-*d*]pyrimidines (Scheme 1).



Scheme 1 Green synthesis of benzopyrano[2,3-*d*]pyrimidines

The approach began with the development of the optimal conditions using salicylaldehyde, malonitrile, and piperidine as the model in various conditions. A screening of various amounts of catalyst showed the optimal amount of 0.05 g of catalyst led to 80 % of product in 70 min in ethanolic conditions. The condensation of malonitrile with different salicylaldehydes and various secondary amines under these optimized conditions led to a variety of benzopyrano[2,3-*d*]pyrimidines. Salicylaldehydes bearing either electron-withdrawing or electron-donating groups reacted successfully with malonitrile and 2° amines under green conditions in the presence of 0.05 g of catalyst refluxing ethanol to give the corresponding benzopyrano[2,3-*d*]pyrimidines in good to excellent yields. In addition, SSC catalyst was shown to be recyclable without significant loss of efficiency after fourth use.

Keywords: Benzopyrano[2,3-*d*]pyrimidines, Green synthesis, Sodium carbonate silica

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Preparation and application of a Deep Eutectic Solvent-based on one of the triphenylphosphonium derivatives as a capable and new catalyst for the one pot synthesis of The piperidine derivatives

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Deep eutectic solvents (DESs) are solvents that moreover to having the properties of g reen solvents due to properties such as easy synthesis, low melting point, stability towards moisture and air, low vapor pressure, and high thermal stability can be used as an alternative to ionic liquids (IL)[1]. DESes are be made of mixture a hydrogen-bond acceptors (HBA) and hydrogen-bond donors (HBD). Generally, a DES is a type of solvent composed of a mixing two or more components under simple operation of that forms an eutectic with a much lower melting point than either of the individual components[2].

The piperidine ring system is one of the most found in numerous natural products such as alkaloids, drug candidates and drugs[3]. The piperidine derivatives are abundant in synthetic bioactive molecules as well as in various natural products which exhibit a plethora of biological properties such as analgesic, anticonvulsant, antimalarial, nicotinic and antiinfluenza[4-5].

In this study, a novel, efficient and recoverable DES was designed, made and fully investigated by using Fourier transform infrared (FT-IR) spectroscopy, thermogravimetric analysis/ differential thermal analysis (TGA/DTA), differential scanning calorimetry (DSC), density, eutectic point and 1HNMR. The DES was made of mixture one of the triphenylphosphonium derivatives as HBA and a acidic compound as HBD and used for synthesis derivatives of the piperidine derivatives.

Keywords: Deep eutectic solvent, Four-component, Piperidine ring

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Preparation and application of a Deep Eutectic Solvent based on triphenylphosphonium as a capable and new catalyst for the synthesis of benzopyranophenazine

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At the beginning of our century, Abbott's group published a few papers that triggered research in the area we call today Deep Eutectic Solvents (DES) [1]. An alternative family of ionic liquids (IL), DES, is rapidly emerging. DES is a fluid generally composed of ionic compounds hydrogen-bond acceptors (HBA) and hydrogen-bond donors (HBD) (often cheap and derived from safe components) that are capable of self-association to form a eutectic mixture. Two salts with high melting points are mixed and form at eutectic with a melting point lower than that of each component [2].

Lawsone, 2-hydroxy-1,4- naphthoquinone, is the primary coloring agent found in the henna plant (Lawsonia inermis L.). Lawsone has been reported to have biological activities such as antibacterial, antifungal, and antitumor, and is often used as a hair dye and as a sunscreen in ultra-violet (UV) filters [3].

Phenazines are a large class of well-known natural and synthetic nitrogen-containing heterocyclic compounds [4]. Henna-based compounds such as benzo [a]pyrano[2,3-c] phenazines and their derivatives are of substantial interest as they possess a broad range of biological properties [5]. such as anti-cancer, spasmolytic, diuretic, anti-coagulant,anti-tumor, anti-parasitic, anti-malarial, anti-tuberculosis, and anti-anaphylactic activity.

In this project, a cheap, simple, and non-toxic method was considered for the synthesis of benzo [a]pyrano[2,3-c] phenazines derivatives. the structure and properties of the DES catalyst were investigated by FT-IR, TGA/DTA, DSC, Density, eutectic point, and ^{1}HNMR. Advantages provided by this study include reaction in solvent-free conditions (reduction of contamination), short reaction time, high productivity, easy recycling and separation of the catalyst, as well as high selectivity.

Keywords: Deep eutectic solvent, Synthesis, benzo[a]pyrano[2,3-c] phenazines, Henna-based compounds

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Catalytic synthesis of 1,4-dihydropyridine derivatives using $CoNiFe_2O_4$ hollow nanospheres and optimization by Box-Behnken design

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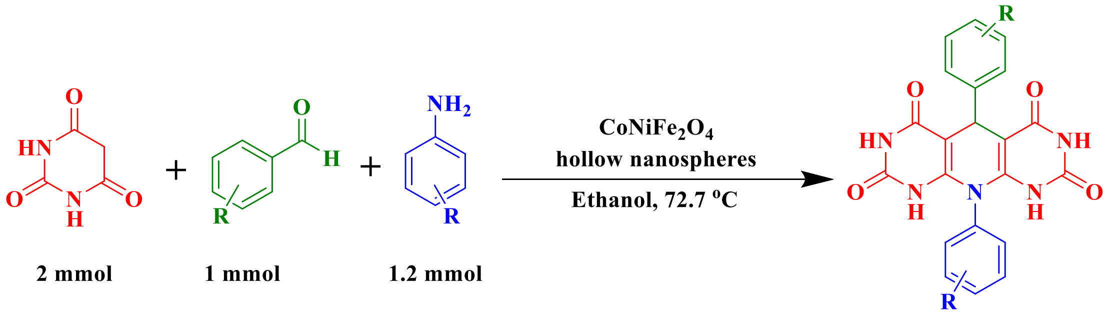
Hollow nanostructures serve as catalysts because of their properties of low density, high surface area, and controlled hollow spaces [1]. These hollow nanostructures could be used for diverse catalytic reactions depending on the arrangement of the hollow shell or the contents inside the hollow shell [2]. The unique structure of 1,4-dihydropyridine derivatives makes them a group of heterocycles with interesting medicinal properties. Because of their properties and biological activities, these compounds have been used widely in therapeutics such as antihypertensive, hypnotic, anti-inflammatory, and anti-ischemic agents [3]. For the synthesis of 1,4-dihydropyridine, several methods have been described [4].

In this study, barbituric acid, various aniline and aldehyde derivatives in the presence of $CoNiFe_2O_4$ hollow nanospheres as a catalyst in ethanol as a solvent were employed to synthesize 1,4-dihydropyridine derivatives. Also, the Box-Behnken design improved the reaction conditions. As a result, the efficiency of the products was increased, and the reaction time was dramatically decreased. Finally, the obtained organic compounds were identified by utilizing melting point, FT-IR and ^{1}H NMR analyses.

Keywords: Hollow nanostructures, 1,4-Dihydropyridine, Box-Behnken design



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Sodium Carbonate Silica: an Efficient Catalyst for Three-Component Synthesis of Arylmethylidene-isoxazole-5(4*H*)-ones in Green Medium

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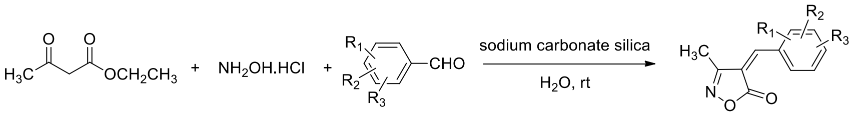
Heterocycles are obtaining more importance in recent years due to their pharmacological activities. The isoxazole core is a significant synthetic line of attack in drug discovery, and plays a significant role in arena of natural products, agrochemicals, and medicinal chemistry [1]. Compounds containing this scaffold exhibit versatile biological properties such as antibacterial, anti-obesity, anti-inflammatory, antifungal, analgesic, and fungicidal activities [2]. Conventional methods for the synthesis of arylmethylidene-isoxazole-5(4*H*)-ones are the cyclization of *O*-propioloyl oximes, the reaction of ethyl acetoacetate and hydroxylamine hydrochloride followed condensation with aromatic aldehydes, and condensation of 1,3-dicarbonyls with benzaldoximes. Significant development has been made in reviewing different routes for the construction of an arylmethylidene-isoxazole-5(4*H*)-one skeleton [2-3]. A highly yielding approach for the synthesis of arylmethylidene-isoxazole-5(4*H*)-ones has been established using sodium carbonate silica as the efficient catalyst. The three-component reaction of ethyl acetoacetate, various aromatic aldehydes, and hydroxylamine hydrochloride, under aqueous conditions at room temperature is described. This procedure has expectant features, including shorter reaction times, easy of separation of pure products with high yields, simplicity experimental procedure, and eco-friendly.



Schem. 1 Three-component synthesis of arylmethylidene-isoxazole-5(4*H*)-ones in green solvent

Keywords: Isoxazole-5(4*H*)-one, Sodium carbonate silica

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Synthesis of 2,2,2-trifluoro-*N*-aryl-1-(2-(1-aryl-2-(trifluoromethyl)-1,8a-dihydroimidazo- [1,2-*a*]pyridin-3-yl)-1*H*-benzo[*d*]imidazol-6-yl)ethan-1-imine derivatives

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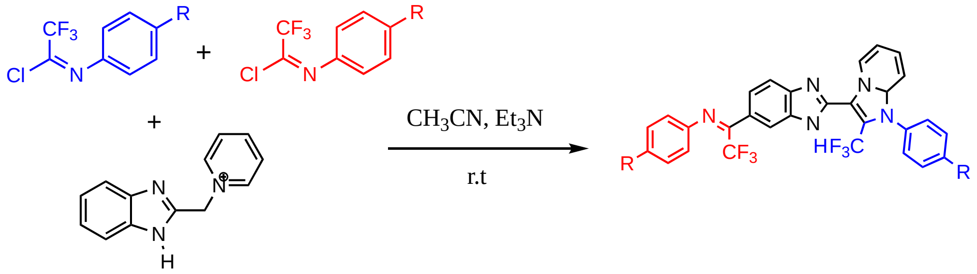
Today, trifluoromethyl heterocyclic compounds have important role in chemistry, design of new drugs and agricultural [1]. Also, imidazole derivatives play an important role in the synthesis of biological active compounds. In this research, in order to synthesis and development of new trifluoromethylated heterocyclic compounds base on the benzimidazole nucleus, reaction between N-aryl-2,2,2-trifluoroacetimidoyl chloride derivative and 1-((1*H*-benzo[*d*]imidazol-2-yl)methyl)pyridin-1-ium has been investigated. Combination of trifluoromethylated heterocycles and benzimidazole moiety, can be greatly improve and enhance the biological properties of these compounds [3,4]. The structures of products confirmed by IR, ^{1}H-NMR, ^{13}C-NMR, ^{19}F-NMR.



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Keywords: N-aryl-2,2,2-trifluoroacetimidoyl chlorides, Imidazole.

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$ZnFe_2O_4$@SiO_2@APTES@DHBS-Cu NPs: as a novel, green, and efficient heterogeneous magnetic nanocatalyst for the synthesis of bis (pyrazolyl)methanes and chemoselective oxidation of sulfides

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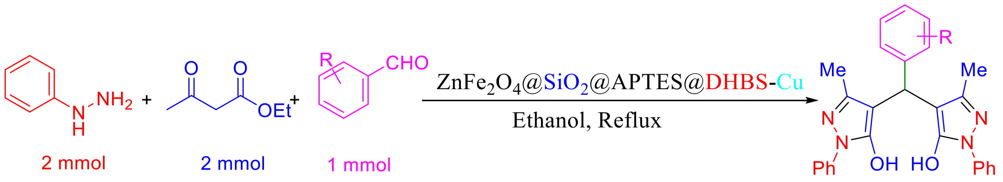
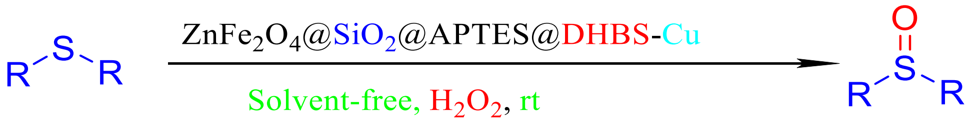
In this paper, we report the synthesis of $ZnFe_2O_4$@SiO_2@APTES@DHBS-Cu as a novel magnetic nanocatalyst, in a mild and green environment. The structure of the described magnetic compound was characterized by different physicochemical techniques including XRD, EDS, SEM, FT-IR, X-ray elemental mapping, TGA, and VSM analyses. The prepared magnetic nanoparticles exhibit excellent catalytic activity in synthesizing bis (pyrazolyl)methanes and oxidation of sulfide derivatives under green conditions (Scheme 1 and 2). The heterogeneous nature of the catalyst was confirmed via the hot filtration experiment. Further, $ZnFe_2O_4$@SiO_2@APTES@DHBS-Cu showed high efficiency and reusability that could be reused for at least five consecutive runs[1,2].

Keywords: Bis (pyrazolyl) methanes; Oxidation of sulfides; $ZnFe_2O_4$@SiO_2@APTES@DHBS-Cu; Zinc ferrite; Cupper.



Scheme 1. preparation of bis (pyrazolyl)methanes model reaction



Scheme 2 Oxidation of sulfides to sulfoxides catalyzed by $ZnFe_2O_4$@SiO_2@APTES@DHBS-Cu.

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FDU@l-Histidin-Zr: green, novel and efficient catalysts for the one-pot synthesis of 5-substituted tetrazole and polyhydroquinoline derivatives

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The development of a highly efficient and green catalyst for the one-pot synthesis of 5-substituted tetrazole and poly hydro quinoline derivatives is an extremely important and ground challenging area in organic chemistry. In this study, the catalyst was prepared by the immobilization of Zr on ordered mesoporous silica (FDU) coated with l-Histidine. The proposed catalysts were characterized by FT-IR, XRD, BET, TGA, EDX, and ICP-OES studies and were successfully applied in the synthesis of 5-substituted tetrazoles and poly hydro quinoline derivatives. This designed protocol offers several advantages including the use of commercially available and inexpensive materials, simple procedure, short reaction times, high yield, and easily separable and reusable catalyst [1–3].

Keywords: 1H-tetrazole; FDU, l-Histidin, Green, Novel, Tetrazole.

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$ZnFe_2O_4@SiO_2@n$-pr@xantin-pr: A novel, green, recyclable, and highly versatile catalyst for the synthesis of 1H-tetrazoles and oxidation of sulfides to the sulfoxides

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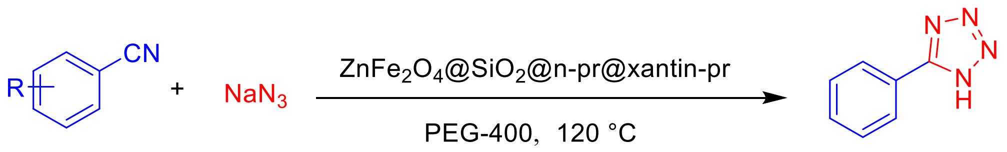
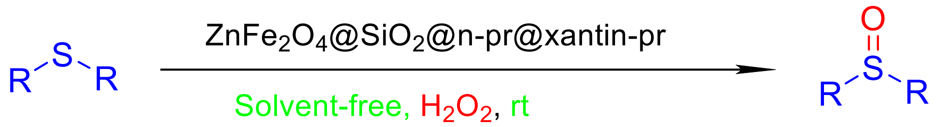
In this work, we report the synthesis of $ZnFe_2O_4@SiO_2@n$-pr@xantin-pr as a novel and green nanomagnetic catalyst, which is containing the $SiO_2@n$-pr@xantin-pr catalytic sites on the surface of $ZnFe_2O_4$ as the catalytic support. The as-synthesized $ZnFe_2O_4@SiO_2@n$-pr@xantin-pr MNPs were characterized with accuracy by different physicochemical methods; including, ICP-MS, XRD, EDS, SEM, FT-IR, X-ray elemental mapping, TGA, and VSM analyses. The prepared magnetic nanoparticles exhibit excellent catalytic activity in synthesizing 1H-tetrazole derivatives and oxidation of sulfides to the sulfoxide under green conditions (Scheme 1 and 2). The heterogeneous nature of the catalyst was confirmed via the hot filtration experiment. Furthermore, the activity of the recycled nanocatalyst was examined for at least five cycles with a negligible loss of its activity[1,2].

Keywords: 1H-tetrazole; Sulfide; $ZnFe_2O_4@SiO_2@n$-pr@xantin-pr; Zinc ferrite; L-Arginine.



Scheme 1 Synthesis of tetrazole catalyzed by $ZnFe_2O_4@SiO_2@n$-pr@xantin-pr.



Scheme 2 Synthesis of Oxidation of sulfides to sulfoxides catalyzed by $ZnFe_2O_4@SiO_2@n$-pr@xantin-pr.

References

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Green synthesis of Cu nanoparticles using *Cyperus rotundus* aqueous extract and its catalytic activity in the Biginelli Reaction

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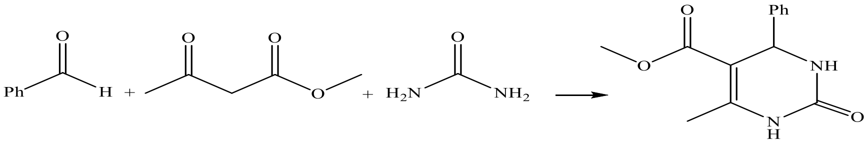
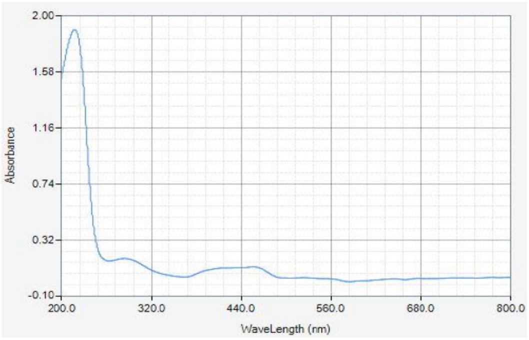
Cyperus rotundus belongs to Cyperaceae (sedge family). The plant is a perennial weed with slender, scaly creeping rhizomes, arising singly from the rhizomes which are about 1-3 cm. its rhizomes are externally blackish in color and white inside with a characteristic odor [1]. C. rotundus has several medicinal uses in traditional medicine around the world.

3,4-dihydropyrimidine-2(1H)-one (DHPM) Biginelli product is a preferable compound widely used in the organic and pharmaceutical industries ,which exhibits vital pharmacological properties namely calcium channel blockers, antihypertensive, hepatitis B virus replication inhibitors, antiviral, antimalarial and different countless activities . [2]

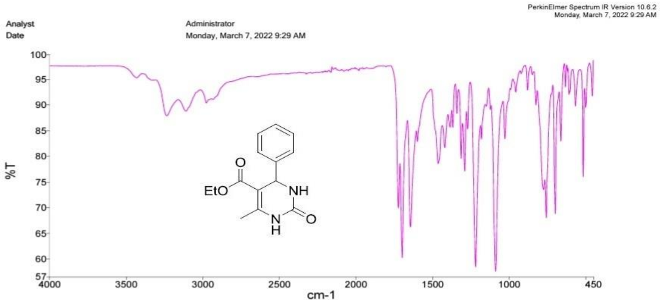
In this research, we green synthesized copper nanoparticles using the aqueous extract of C. rotundus as the reducing agent and $CuNO_3.3H_2O$. The green synthesized CuNPs were used as the catalyst in Biginelli-type reaction. For this proposal, benzaldehyde, urea, ethyl acetoacetate (b-dicarbonyl,) and catalyst were refluxed for 1 h at 90 °C. The progress of the reaction was monitored by TLC. (Schem A) Schem B approves the synthesis of CuNPs by the band at 310 nm. The presence of the bands at 3100 -3300 (N-H),1720(C=O), 1495-1620(C=C), and 1100-1200(C-O) in the FT-IR spectrum. Schem C confirm the synthesis of 3,4-dihydropyrimidin-2(1H)- one.



Schem. A . Biginelli reaction



Schem. B.The UV-Vis spectrum of CuNPs



Schem. C . The FT-IR spectrum of 3,4-dihydropyrimidin- 2(1*H*)-one

Keywords*:* Biginelli reaction, Cu nanoparticles, Cyperus rotundus

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Cyperus rotundus aqueous extract mediates for green synthesis of Ag nanoparticles

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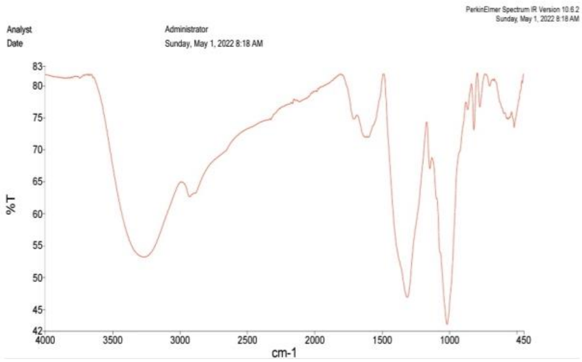
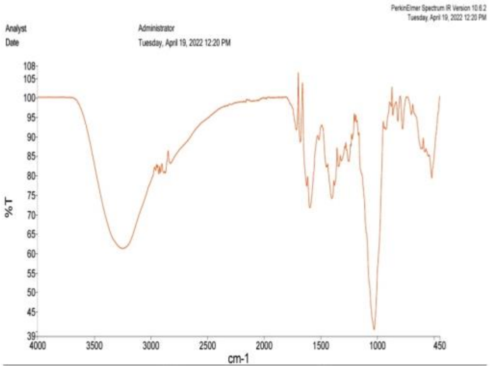
Cyperus rotundus belongs to Cyperaceae (sedge family). The plant rhizomes are known as the most important part with a variety of medicinal uses . The extract of C. rotundus rhizomes showed significant effects against gram-negative, gram-positive bacteria, and fungi. On the other hand, aqueous extract of C. rotundus as activity against parasitic worms. The rhizomes have anticancer effects [1].

The major methods for the synthesis of AgNPs are physical and chemical pathways. However, in recent years the green synthesis of the AgNPs using plant extracts have considered by researchers due to many advantages compared to chemical and physical In this method, the synthesis is carried out without any dangerous chemicals, and also wasteful purifications [2].

In the present study, The aqueous extract of C. rotundus was mixed with a solution of $AgNO_3$ and stirred at 50 ^{0C} for 1 hour. During the reaction time, the dark brown of AgNPs was formed. The synthesis of AgNPs was confirmed by FT-IR spectroscopy. A similarity in FT-IR spectra of C. rotundus and AgNPs (Schem A and Schem B respectively) is observed.



Schem A. FTIR spectra of *Cyperus rotundus* extract



Schem B .FTIR spectra of AgNPs

The bands at (O-H), (C-H), (C=O,C=C), (C-O) belong to the functional groups of the secondary metabolites in the plant extract such as phenolic, flavonoids, and terpenoids. (Schem A) .The band belongs to the Ag-O bond.(Schem B)

Keywords: Ag nanoparticles , Cyperus rotundus , Green Synthesis

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Synthesis of Polyhydroquinoline Derivatives Using Fe_3O_4@polyethylene glycol (PEG) Core/Shell

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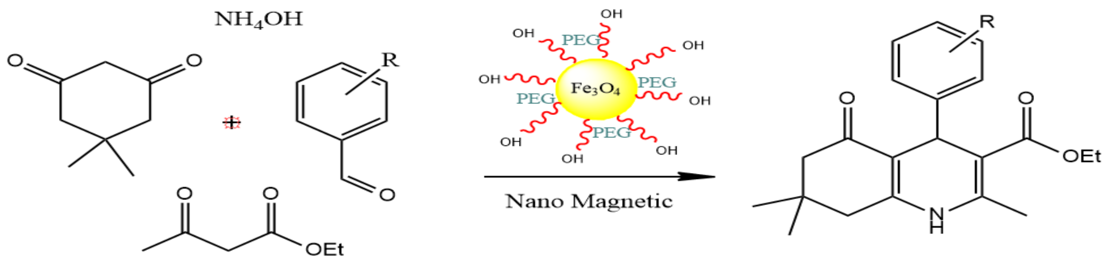
1,4-Dihydropyridines as analogues of nicotinamide adenine dinucleotide (NADH) coenzymes exhibit a wide range of biological activities, such as calcium channel blocking, and today they are widely used in pharmacology [1]. Some of the representative compounds of this class possess antimicrobial, antitubercular, insecticidal, and neuroprotectant [2] activities. Recently, 1,4-DHPs have been used as organocatalysts for asymmetric reactions. Most of the methods reported previously usually require long reaction times, afford 1,4-dihydropyridines in relatively low yield, and suffer from utilizing harmful organic solvents in most cases [3]. In recent years, core/shell nanoparticles have received considerable attention because of their unique properties [4]. The magnetic core/shell Fe_3O_4 nanoparticles have been utilized as a suitable catalyst in many reactions. Therefore, the development of surface modification of magnetic nanoparticles (MNPs) as important candidates in the search for supporting of catalysts is currently an issue of increasing interest in chemical reactions. The surface of MNPs can be functionalized easily through appropriate surface modifications to enable the loading of a variety of desirable functionalities [5]. In the present paper, Fe_3O_4/ polyethylene glycol (PEG) magnetic composite nanoparticles with a core–shell structure were prepared. Then, we disclosed a novel methodology for the synthesis of polyhydroquinoline derivatives by a one-pot, four-component unsymmetrical Hantzsch condensation of dimedone, aldehydes, ethyl acetoacetate, and ammonium acetate catalyzed by core/shell Fe_3O_4/PEG nanoparticle as a magnetic catalyst under reflux conditions in ethanol.

Keywords: Polyethylene glycol, 1,4-Dihydropyridines, Magnetic nanoparticles, Core/shell



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Synthesis of Molybdenum-graphene Nanocomposites as an Efficient Catalyst of Nitroarenes Reduction

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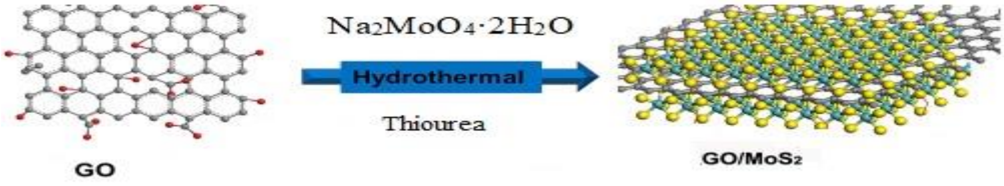
Nitro compounds derived from industrial and agricultural wastewater due to their solubility and stability in water, are classified as toxic and environmental pollutants. One of the strategies of chemists in combating environmental pollution, is eliminating or reducing pollutants or using wastes as starting materials for preparation of useful chemicals [1]. The reduction of nitro compounds to the corresponding amines which are valuable chemicals in synthetic organic chemistry, is one way to solve this problem [2]. Various nanostructured materials especially nanocomposites have been used as catalysts for the reduction of nitro compounds under mild reaction conditions. Graphene-based nanocomposites due to their high surface area, their extended π-system, and variable functionalities demonstrate optimal features in the field of intended application. On the other hand, 2-D-layered transition metal dichalcogenides like MoS_2 is used as one of the most suitable substitutes for rare metals in the catalytic field [3]. So, we designed and synthesized molybdenum-graphene nanocomposites and investigated their catalytic properties on the reduction of some nitro compounds (Schem 1).



Schem.1. Synthesis of Molybdenum-graphene Nanocomposite.

Keywords: Graphene, Catalyst, Reduction, Nitro compounds and Molybdenum disulfide

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Design and synthesis of efficient and reusable Biochar phosphoric acid nanocatalyst for 1-amido alkyl-2-naphthols synthesis

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Multicomponent reaction (MCR) condensations involve three or more simple substrates is considered that approach close to the "ideal synthesis" due to atomic economy, and high bond forming efficiency. Compounds containing 1,3-amino oxygenated functional groups such as 1-amidoalkyl-2-naphthol derivatives frequently found in variety biologically active natural products and potent drugs such as a number of nucleoside antibiotics and HIV protease inhibitors [1]. Recently, nanoparticles were emerged in various fields including science, industry, pharmacy, medicine, and green chemistry [2]. Biochar is one of the novel nanoparticles, which is a stable carbon solid and used in various fields in past few years for science and engineering. Biochar is made *via* pyrolysis of biological source such as woody materials, agricultural wastes, green waste, animal manures and other waste products [3], therefore it is inexpensive and environmentally friendly. In this work Phosphoric acid-activated walnut shell biochar efficiently catalysis one-pot multi-component condensation of 2-naphthol with aromatic aldehydes and amide derivatives under solvent-free conditions to afford 1-amidoalkyl-2-naphthols in excellent yields and in very short reaction times

Keywords: Biochar, Nanocatalysts, Multicomponent Reaction , 1-Amidoalkyl-2-naphthols

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The Application of Vilsmeier Reagent in the Synthesis of Pyrazolobisindoles

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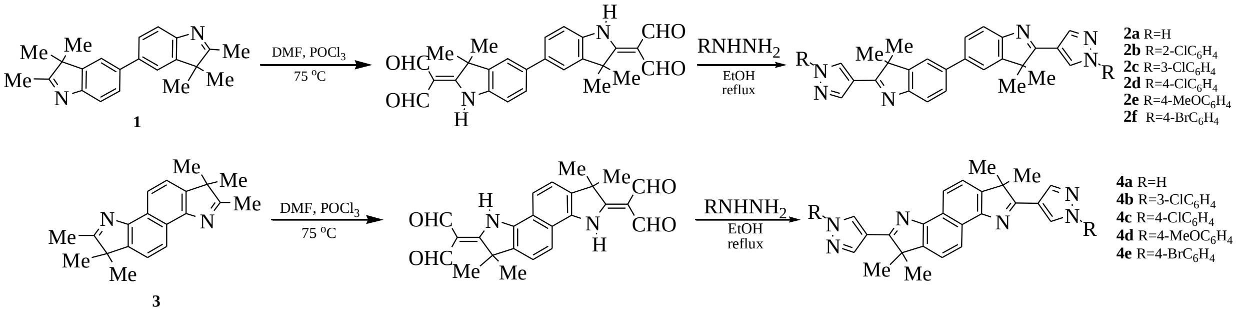
We have shown previously that the reaction of 2,3,3-trimethyl-3*H*-indoles (indolenines) with the Vilsmeier reagent formed from *N*,*N*-dimethylformamide and phosphorus oxychloride (phosphoric trichloride), producing aminomethylene malondialdehydes, is a general process, by demonstrating the transformation using variously substituted 2,3,3-trimethyl-3*H*-indoles. Additionally, we have described a simple and straightforward preparation of 4-(2,3,3-trimethyl-3*H*-indol-2-yl)-substituted pyrazoles.[1-3]



In this research, we have been able to show that the principles embodied in transformations of simple indolenines *via* Vilsmeier formylations can be incorporated into more complex bisindolenine systems **1**,**3** and thus have prepared several pyrazoles **2a-f**, **4a-e** in excellent yields (Scheme).

Keywords: Indolenine, Aminomethylene Malondialdehydes, Vilsmeier reagent, Pyrazol

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The Synthesis of 6-Substituted Pyrido[2,3-*d*]pyrimidine-2,4(1*H*,3*H*)-diones Using Aminomethylene Malondialdehydes and 6-Aminouracils

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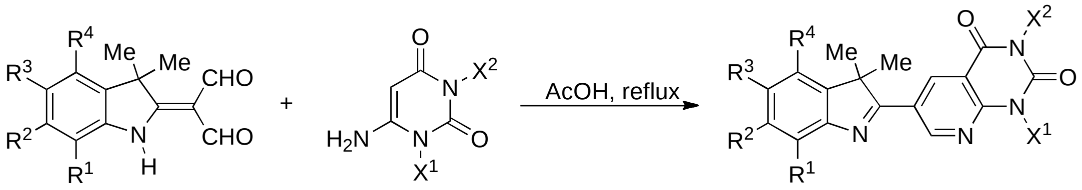
In recent years, our research group has been developing a project centered on the synthesis of novel indolenines and bisindolenines, and reactions of them with the Vilsmeier reagent to produce aminomethylene malondialdehydes.[1-4] These malondialdehydes, as 1,3-dicarbonyl compounds, can be used to produce new heterocyclic systems.[1,3,4]



1a R^1, R^2, R^3, R^4=H
1b R^1=Cl, R^2, R^3, R^4=H
1c R^1=Me, R^2, R^3, R^4=H
1d R^1, R^2, R^4=H, R^3=OMe
1e R^1, R^3=H, R^2, R^4=Cl

2a X^1, X^2=H
2b X^1=Me, X^2=H
2c X^1=Me, X^2=Me

3a-k

In this reaserch, we have extended our studies of aminomethylene malondialdehydes 1a-e and demonstrated the synthesis of pyrido[2,3-*d*]pyrimidine-2,4-diones 3 by condensations with various 6-aminouracils 2a-c (Scheme). After some preliminary experiments, it was found that a mixture of aminomethylene malondialdehyde 1a and 6-aminouracil 2a afforded 6-(3,3-dimethyl-3*H*-indol-2-yl) pyrido[2,3-*d*]pyrimidine-2,4(1*H*,3*H*)-dione 3a in 79% yield in refluxing acetic acid for 12 h. Encouraged by this success, we extended this reaction to various aminomethylene malondialdehydes 1b–e and 6-aminouracils 2b–c under similar conditions (acetic acid at reflux), furnishing the respective compounds 3b–k in good yields.

Keywords: Pyridopyrimidines, Aminouracil, Indolenine, Aminomethylene Malondialdehydes

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Synthesis of Molybdenum disulfide-based Nanocomposites as Lubricant Additives

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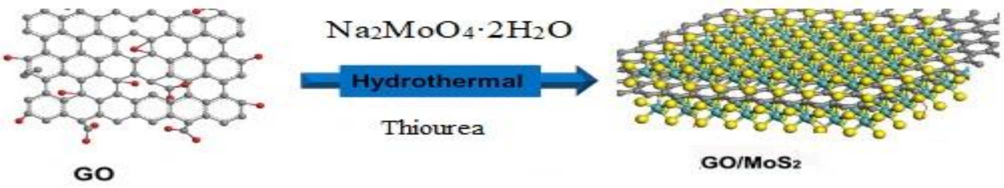
Friction is the most important phenomenon that emerges in everywhere two surfaces in close proximity to each other moves. The resulting wear and release of thermal energy causes failures of engines. Wear and friction lead to a decrease in the performance of the mechanical system and most importantly lead to energy loss [1]. The most effective ways to control friction and wear, is lubrication which plays an important role in conserving energy. In recent years, nanoparticles such as pure metals, metal oxides, metal sulfides and carbon allotrops due to their potential in emission reduction and improving fuel economy are widely used as lubricant additives [2,3]. Among nanoadditives, molybdenum disulfide (MoS_2) with lamellar individual atomically-thin planes that can easily slide against each other, holds special importance [4]. We have synthesized molybdenum-graphene nanocomposites and have investigated the synergistic effect of carbon allotropes and MoS_2 on tribology properties of them (Schem 1).



Schem. Synthesis of Molybdenum-graphene Nanocomposite.

Keywords: Friction, Nanocomposite, Lubricants additive, Molybdenum disulfide

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Synthesis of magnetic β-cyclodextrin core modified with folic acid as a pH-responsive system for targeted delivery of doxorubicin

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One of the most important applications of nanotechnology in cancer treatment involves the design of magnetic nanocomposites for the targeted delivery of anticancer drugs to cancer cells [1, 2]. This study aims to develop a novel, appropriate, and efficient magnetic carrier having antioxidant properties for the controlled release of anticancer drug, hydrophilic doxorubicin (DOX), to cancer cells using folic acid conjugated with magnetic β-CD (Fe_3O_4-β-CD-FA). The synthesized carrier was characterized using EDX, XRD, BET, FT-IR, Zeta potential, VSM, and SEM analysis. The encapsulation efficiency (EE) and loading capacity of Fe_3O_4-β-CD-FA was found to be 91.06% and 9.1 % for DOX. The release studies of DOX from Fe_3O_4-β-CD-FA showed that maximum release occurs at pH 5 which means it has a controlled pH-responsive behavior. *In vitro* cytotoxicity of the as-synthesized Fe_3O_4-β-CD-FA in MDA-MB-231 cells clearly showed that the prepared carrier had no significant cytotoxicity and could easily enter the cell. Furthermore, the in vitro antioxidant capacity of Fe_3O_4-β-CD-FA was evaluated by DPPH assay and the results exhibited that the synthesized carrier has excellent antioxidant activity (73.05%). Therefore, the obtained nanocarrier in this study due to their target ability under a magnetic field, excellent biocompatibility, good colloidal stability, simple preparing method, and good antioxidant activity could be used as a promising targeted drug delivery system for cancer therapy.

Keywords: β-Cyclodextrin, Folic acid, Doxorubicin, Cancer treatment.

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Chitosan-coated layered double Hydroxides for the co-delivery of vitamin D3 and amoxicillin

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Layered double hydroxide (LDH) nanoparticles have potential applications for the loading and controlled release of drugs [1, 2]. This study investigated the synthesis of Zn/Al-LDH using the co-precipitation methods, coating with chitosan and precise control of the release of vitamin D3 and amoxicillin (AM). The surface of the D3-AM-loaded LDH NPs was coated with chitosan. The structure, surface morphology, and drug loading were characterized and the drug release profile and release kinetics of the intercalated LDHs were studied. The encapsulation efficiency and loading capacity of this system were obtained approximately 91% and 9.1%, respectively. The release study of vitamin D3 and amoxicillin was performed in the simulated gastric fluid (SGF) (pH 1.2) and simulated intestinal fluid (SIF) (pH 6.8) and (pH 7.4) at 37 °C. The drug release assay showed that the amount of the vitamin D3 and amoxicillin release from prepared nanocarrier was noticeably pH depended. The encapsulation of hydrophobic vitamin D3 and amoxicillin in LDH with an external chitosan coating approach enhances their controlled and sustained release property at the target site. MTT assay was performed on at varying concentrations on kidney (HEK) and liver (Hep G2) cell lines after 48 h exposure to ensure its biocompatibility. In-vitro cytotoxicity test results confirmed that the non-toxic LDH has excellent biocompatibility on n the HEK and Hep G2 cell lines. Meanwhile, colloidal stability and enzymatic degradation studies showed that nanocarrier has good stability and biodegradability. According to the obtained results, the as-prepared system can be proposed for use as a new safe and efficient vehicle for targeted delivery and controlled release of drugs for biomedical applications.

Keywords: Layered double hydroxide, Chitosan, Vitamin D3, Amoxicillin, Controlled release.

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Preparation of magnetic cellulose-metal-organic framework capped PEG for targeted anticancer drug delivery

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Recently, metal organic frameworks (MOFs) have been demonstrated as a promising carrier for drug delivery, as they possess many advantages like large surface area, high porosity and tunable functionality [1]. However, there are no reports about the functionalization of MOFs, which combines cancer-targeted drug delivery/imaging, magnetic property, high drug loading content and pH-sensitive drug release into one system. Existing formulations for integrating target molecules into MOF are based on multi-step synthetic process [2]. However in this study, we report an approach that combines MIL-100(Fe) MOF synthesis and target molecule (PEG) encapsulation on the surface of cellulose modified magnetic nanoparticles. The MIL-100-coated magnetic regenerated cellulose-coated nanoparticles (MIL-100(Fe)@cellu@Fe_3O_4) were successfully prepared and characterized. The result showed that MIL-100(Fe) was successfully composited on to the surface of the cellulose-coated Fe_3O_4 nanoparticles. Moreover, the poly(ethylene glycol) (PEG) was efficiently immobilized by the MIL-100(Fe)@Cellu@Fe_3O_4 nanocarrier. Finally, The anti-cancer drug doxorubicin (DOX) was effectively loaded on PEG MIL-100(Fe)@Cellu@Fe_3O_4 nanocomposite with the drug loading capacity up to 85.3 mg/g. The release properties of the developed nonocarriers in phosphate buffer saline (PBS) were studied in two certain pHs: pH=7.4 (the human blood pH) and pH=5.5 (pH of cancer cells). When the pH of the release medium (PBS) was changed from 7.4 to 5.5, the drug release increased significantly from 20% of the adsorbed drug to about 80%. In a cytotoxicity assay using HeLa cells, an immortal human cervical cancer cells, the doxorubicin-loaded PEG MIL-100(Fe)@Cellu@Fe_3O_4 exhibited better antitumor activity than that shown by doxorubicin. Overall, this study demonstrated that prepared PEG MIL-100(Fe)@Cellu@Fe_3O_4 are promising candidates as carriers for sustained targeted antitumor drug delivery system.

Keywords: Cellulose, Drug delivery, Cytotoxicity assay, Metal organic frameworks.

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Metal-organic frameworks modified magnetic mesoporous silica nanoparticles capped with hydroxyapatite for doxorubicin delivery to cancer cells

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Mesoporous silica nanoparticles (MSN) are one of those compounds which have recently drawn attention in biomedical applications. But premature cargo leakage and uncontrolled release from bare MSN makes them unsuitable for drug delivery applications [1, 2]. Herein we report a new approach to modifying bare MSN to inhibit burst cargo release. The primary goal of this work was to combine metal organic framework (MOF) and MSN to form a nanocomposite to build a hybrid drug delivery system to prevent premature drug release from bare-MSN. In this paper, we report novel multifunctional nanocomposite composed of a magnetite nanocrystal core and a mesoporous silica shell (Fe_3O_4@mSiO_2) modified metal organic frameworks (MIL-53), end-capped with pH-stimuli-responsive hydroxyapatite (HAp) nanovalves for pH-responsive drug release. The as-prepared nanocomposites were characterized by XRD, FT-IR, SEM, EDS, and VSM technique. The pH-responsive release of the model drug Doxorubicin (DOX) showed that the Fe_3O_4@mSiO_2@MIL-53-HAp nanocomposites possessed pH-responsive drug-release functionality. The dissolution of hydroxyapatite in an acidic environment triggers the release of the loaded drugs in Fe_3O_4@mSiO_2@MIL-53-HAp nanoparticles. Therefore, the HAp gate with favorable bio-compatibility and pH response characteristics could be used to control the release of loaded DOX from Fe_3O_4@mSiO_2@MIL-53-HAp-DOX nanocomposite in the simulated acidic tumor cell environment, which could effectively kill tumor cells and reduce the toxic side effects on normal tissue. This study provides a smart design on the tunable shell and gate-controlled architectures for the sensitive release of drugs and efficient antitumor.

Keywords: Mesoporous silica nanoparticles, Hydroxyapatite, Metal organic frameworks, Drug delivery, Cytotoxicity assay.

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Preparation of layered double hydroxide (Ca-Al) encapsulated with pectin-chitosan as a targeted drug delivery system for cancer therapy

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Achieving a new drug delivery system with controlled drug release behavior is valuable in cancer therapy [1, 2]. Therefore, for the first time, doxorubicin (DOX) and methotrexate (MTX) were simultaneously co-loaded on the as-synthesized layered double hydroxides (LDH (Ca-Al)). The resulted system was encapsulated with pectin-chitosan (PC) to improve its efficiency for breast cancer therapy. Several characterization techniques were used to evaluate the successful synthesis of the LDH (Ca-Al)-DOX-MTX-PC microspheres. The in vitro release studies of DOX and MTX from LDH (Ca-Al)-DOX-MTX-PC were performed at various pH values and found that the release process was noticeably controlled pH-responsive behavior. In vitro cytotoxicity studies of the as-synthesized LDH (Ca-Al)-DOX-MTX- PC against breast cancer cell line (MCF-7) confirmed that the sustained drug release pattern from LDH (Ca-Al)-DOX-MTX- PC against MCF-7 cell line. Therefore, the obtained results in this work suggesting that LDH (Ca-Al)-DOX-MTX-PC is a promising nanocarrier for targeted delivery and controlled release of anticancer drugs for biomedical applications.

Keywords: Drug delivery system, Layered double hydroxide, Cancer therapy, Pectin, Chitosan

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Uremic toxins removal by newly synthesized coupled mesoporous silica nanoparticles- molecular imprinted polymer

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Urea is the main toxin that accumulates in the blood of people with kidney failure and uremia. Current hemodialysis systems still cannot effectively remove uremic toxins, especially urea [1]. The combination of extracorporeal hemodialysis and blood adsorption provides a potential and promising method for urea removal [2]. Mesoporous silica nanoparticles (MSN) is a possible candidate materials for urea adsorption. The pore size of mesoporous silica could be varied on a larger scale compared to other poeous materials [3]. Additionally, various surface functional groups could be introduced on mesoporous silica, an advantage which zeolite does not possess. The fact that functional groups, such as amine, could easily be introduced on the surface of mesoporous silica is worth investigating [4]. Beside MSNs, moleculary imprinted polymers (MIP) are an other porous materials which can be used to remove urea. MIP with high selectivity and good stability can be used as the preferred adsorbent for removing urea, and they are particularly suitable for the regeneration of dialysate in hemodialysis systems [5]. In this work we have suceeded in couoling MSN with MIP to increase the adsorption capacity of urea. Therefore after synthesizing MSN, it was functionlized through a linker, and then the MIP part was growed on it. The adsorption tests were done with 150 mg of adsorbent mixed with 15 ml 38000 μM urea solution. The results wfrom UV spectroscopy showed complete removal of urea from the analyte.

Keywords: Mesoporous silica, Moleculary imprinted polymer, Urea, Adsorption

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Recent advances in nitration reaction

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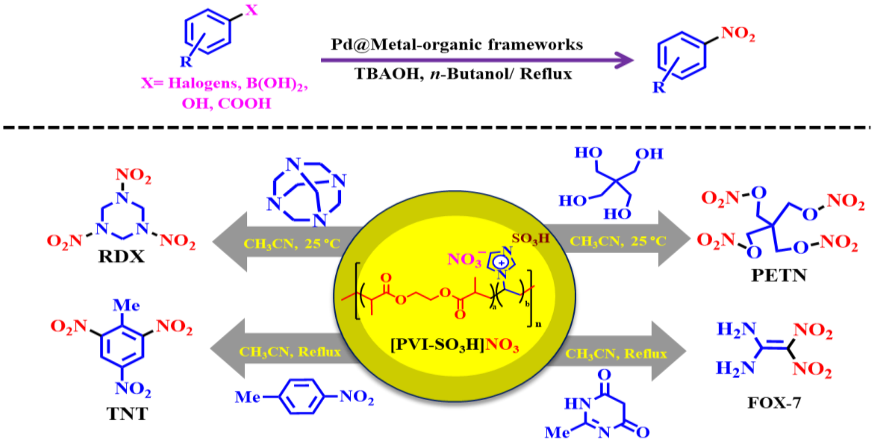
Nitro compounds are important due to their applications on the preparation of chemical intermediates for the synthesis of dyes, plastics, perfumes, energetic materials and pharmaceuticals. They have been used as intermediates in various important functional group transformations.[1] Nitroolefins as another group of nitro compounds, are widely used in cycloaddition reaction, Diels-Alder reaction and Michael reaction to prepare various organic intermediates. Also, nitroalkanes could be prepared by reduction of nitroolefins.[2] Architecture of novel renewable and sustainable nitrating reagent in the organic transformation has attracted much attention in the science and industry because of their unique properties, such as efficiency, reusability, reactivity, stability, selectivity, generality and easy separation of the catalyst.[3] These methods of preparation of nitro materials were previously reported in the presence of some various nitrating agents, cocatalysts, and solvents, mixed acid of concentrated nitric acid and sulfuric acid, high temperature, long reaction times, and low yields.[4] In this overview, we disclose novel nitrating agents such as poly (vinyl imidazole) sulfonic acid nitrate [PVI-SO_3H]NO_3 and palladium-catalyzed based on metal-organic frameworks (MOFs) for synthesis of high-value nitro compounds and explosive materials in high yields (Scheme 1).



Scheme 1: Recent advances in nitration reaction.

Keywords: Coupling based nitration reaction**,** High-energetic materials, Ipso nitration, Metal-organic frameworks (MOFs), Nitro compound.

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$CoFe_2O_4@SiO_2$@n-Pr@Schiff base-Pr: green, magnetic, and versatile catalyst for the synthesis of chromeno[2,3-d] pyrimidine-8-amine and tetrazole derivatives

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In this research project, silica-modified $ZnFe_2O_4$ magnetic nanoparticles were prepared in a simple, short, and straightforward way. Subsequently, an efficient catalyst through immobilization of Schiff base-Pr on the surface of silica-coated $ZnFe_2O_4$ nanoparticles has been produced. The physical and chemical properties of $CoFe_2O_4@SiO_2$@n-Pr@schiff base-Pr acid were considered by XRD, FT-IR, TGA, SEM, EDS, and vibrating sample magnetometer (VSM) analyses. The catalytic activity of described magnetic nanocatalyst was checked out for the synthesis of chromeno[2,3-d] pyrimidine-8-amine and tetrazole derivatives. The described catalyst was recovered and reused for five continuous cycles without considerable change in its catalytic activity[1].

Keywords: Cobalt ferrite ($CoFe_2O_4$); Nanoparticles; Pyrimidine-8-amine; Tetrazole.

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Effective removal of ibuprofen drug from aqueous solutions by activated carbon derived from green tea leaves functionalized with hydroxyapatite

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Wastewaters are generally polluted with various inorganic and organic contaminants which require effective multipurpose purification technology [1]. Amongst, the presence of the drugs in water bodies is worrisome due to their high toxicity, which makes crucial their monitoring and removal, especially by means of advanced technologies [2]. For this purpose, in this study a new adsorbent material was synthesized through the activated carbon derived from green tea leaves functionalized with hydroxyapatite (GAC-HA). The prepared nanocomposite was used for adsorption of ibuprofen drug from an aqueous solution by batch adsorption processes. Isotherm, kinetic and thermodynamic parameters were determined for predicting the ibuprofen adsorption on synthesized nanocomposite. The equilibrium data obtained from adsorption were well represented by the Langmuir model and kinetics data were well fitted by the pseudo-second-order model. The maximum adsorption capacity obtained for ibuprofen was 203.893 mg g^{-1}. The thermodynamic analysis showed that the adsorption process for this drug was spontaneous and endothermic. Therefore, the synthesized nanocomposite can be a suitable new absorbent for ibuprofen removal from aqueous solutions due to its high adsorbing capacity.

Keywords: Activated carbon, Green tea leaves, Ibuprofen, Removal

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A novel Zirconium complex of PYAPD immobilized on the surface of $CrFe_2O_4$ MNPs: as a novel, green, and efficient heterogeneous magnetic nano catalyst for the synthesis of tetrazoles and oxidation of sulfides

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In this paper, we report the synthesis of $CrFe_2O_4$@SiO_2@n-pr@PYAPD-Zr as a novel magnetic nanocatalyst, in a mild and green environment. The structure of the described magnetic compound was characterized by different physicochemical techniques including XRD, EDS, SEM, FT-IR, X-ray elemental mapping, TGA, and VSM analyses. The prepared magnetic nanoparticles exhibit excellent catalytic activity in synthesizing tetrazole and oxidation of sulfide derivatives under green conditions. The heterogeneous nature of the catalyst was confirmed via the hot filtration experiment. Further, $CrFe_2O_4$@SiO_2@n-pr@PYAPD-Zr showed high efficiency and reusability that could be reused for at least five consecutive runs[1,2].

Keywords: Tetrazole; Oxidation of sulfides; $CrFe_2O_4$@SiO_2@n-pr@PYAPD-Zr; Zirconium.

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$ZnFe_2O_3@SiO_2@$L-Methionine-Zr: A novel, green, recyclable, and highly versatile catalyst for the synthesis of 1H-tetrazoles and polyhydroquinolines

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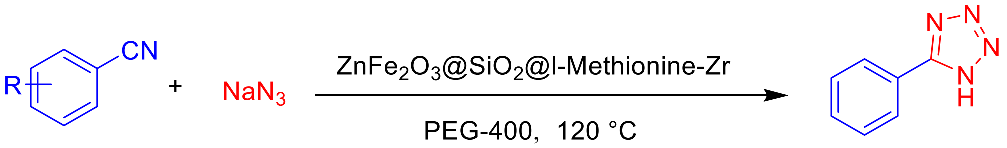
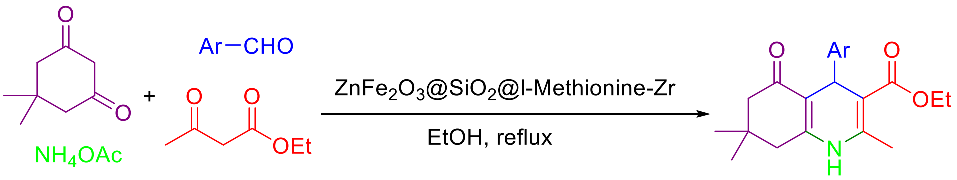
In this research project, silica-modified $ZnFe_2O_4$ magnetic nanoparticles were prepared in a simple, short, and straightforward way. Subsequently, an efficient catalyst through immobilization of l-Methionine-Zr on the surface of silica-coated $ZnFe_2O_4$ nanoparticles has been produced. The physical and chemical properties of $ZnFe_2O_3@SiO_2@$l-Methionine-Zr were considered by XRD, FT-IR, TGA, SEM, EDS, and vibrating sample magnetometer (VSM) analyses. The catalytic activity of described magnetic nanocatalyst was checked out for the synthesis of 1H-tetrazole and poly hydro quinoline derivatives (Scheme 1 and 2). The described catalyst was recovered and reused for five continuous cycles without considerable change in its catalytic activity[1,2].

Keywords: Zinc ferrite ($ZnFe_2O_4$); Nanoparticles; Catalyst, Poly hydroquinoline, Tetrazole



Scheme 1 Synthesis of tetrazole catalyzed by $ZnFe_2O_3@SiO_2@$l-Methionine-Zr.



Scheme 2 Synthesis of poly hydro quinoline catalyzed by $ZnFe_2O_3@SiO_2@$l-Methionine-Zr

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$ZnFe_2O_4$@SiO_2@L-Histidine-La MNPs: a novel, green, and efficient heterogeneous magnetic nanocatalyst for the synthesis of tetrazole and tetrahydrobenzo[b]pyran derivatives

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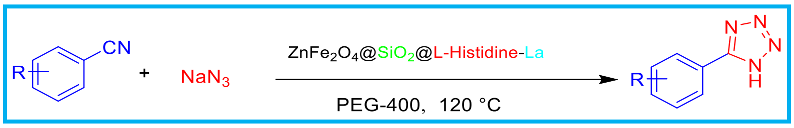
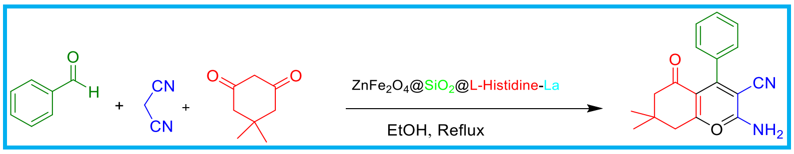
In this work, a novel and efficient catalyst through immobilization of L-Histidine-La on the surface of $ZnFe_2O_4$ nanoparticles was successfully synthesized by a simple procedure. The physical and chemical properties of raw and modified samples ($ZnFe_2O_4$, $ZnFe_2O_4$@SiO_2@L-Histidine-La) were characterized by XRD, FT-IR, EDX, Map, TGA, SEM, and vibrating sample magnetometer (VSM) analyses. The catalytic activity of described magnetic nanocatalyst was checked out for the synthesis of tetrazole and tetrahydrobenzo[b]pyran derivatives (Scheme 1 and 2). The described catalyst was recovered and reused in five continuous cycles without considerable change in its catalytic activity[1,2].

Keywords: $ZnFe_2O_4$@SiO_2@L-Histidine-La; Nanoparticles; Lanthanum; Zinc ferrite ($ZnFe_2O_4$); L-Histidine.



Scheme 1 Synthesis of tetrazole catalyzed by $ZnFe_2O_4$@SiO_2@L-Histidine-La.



Scheme 2 Synthesis of tetrahydrobenzo[b]pyran catalyzed by $ZnFe_2O_4$@SiO_2@L-Histidine-La.

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$BiFe_2O_4$@SiO_2@n-pr@amido sulfuric acid MNPs: a novel, green, and efficient heterogeneous magnetic nanocatalyst for the synthesis of f bis-coumarins and tetrahydrobenzo[b]pyran derivatives

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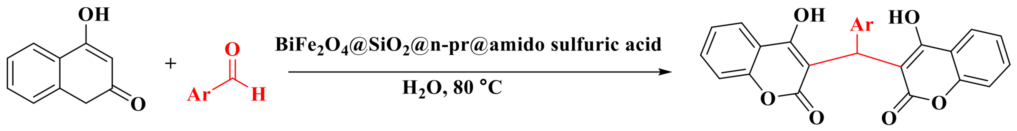
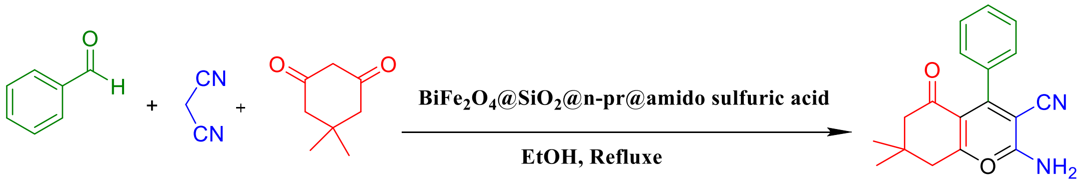
In this work, we report the synthesis and identification of $BiFe_2O_4$@SiO_2@n-pr@amido sulfuric acid as a novel and green nanomagnetic solid acid catalyst, which is containing the sulfuric acid catalytic sites on the surface of $BiFe_2O_4$ magnetic nanoparticles as the catalytic support. The as-synthesized $BiFe_2O_4$@SiO_2@n-pr@amido sulfuric acid MNPs were characterized with accuracy by different physicochemical methods; including, XRD, EDS, SEM, FT-IR, X-ray elemental mapping, TGA, and Value Stream Mapping (VSM) analyses. The catalytic activity of this nanomagnetic material is considered for the synthesis of the diversely substituted tetrahydrobenzo[b]pyran and f bis-coumarins, which affords excellent yields (Scheme 1 and 2). The heterogeneous nature of the catalyst was confirmed via the hot filtration experiment. Furthermore, the activity of the recycled nanocatalyst was examined for at least five cycles with a negligible loss of its activity[1,2].

Keywords: $BiFe_2O_4$@SiO_2, Sulfuric Acid; Nanoparticles; Amido Sulfuric Acid; Tetrahydrobenzo[b]pyran, Tetrazole.



Scheme 1 Synthesis of f bis-coumarins catalyzed by $BiFe_2O_4$@SiO_2@n-pr@amido sulfuric acid.



Scheme 2. Synthesis of tetrahydrobenzo[b]pyran catalyzed by $BiFe_2O_4$@SiO_2@n-pr@amido sulfuric acid.

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Synthesis of 1,2-Disubstituted Benzimidazoles in Water by a novel Magnetic Zeolitic Imidazolate Framework

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The benzimidazole core is classified by medicinal chemists as one of the ‘privileged substructures’ for drug design [1]. Interest in benzimidazole containing structures stems from their widespread occurrence in molecules that exhibit significant activity against several viruses such as HIV, herpes (HSV-1), RNA, influenza, and human cytomegalovirus (HCMV) [2, 3]. In view of the tremendous biological activities of substituted benzimidazoles, their preparation has gained considerable attention in recent years. The traditional synthesis of benzimidazoles involves the reaction between an *o*-phenylendiamine and a carboxylic acid or its derivatives (nitriles, amides, orthoesters) under harsh dehydrating conditions [4]. In the this study, we present the synthesis of magnetic ZIF-8 as an efficient acid catalyst for the selective synthesis of 1,2-disubstituted benzimidazoles. Magnetic zeolitic imidazolate frameworks [ZIF-8] with excellent stability have been synthesized at room temperature by simple mixing of 2-methylimidazole and zinc nitrate hexahydrate in methanol. The properties of the catalyst were investigated by various techniques such as FT-IR, FESEM, and EDX. The magnetic ZIF-8 performs as a novel and recyclable acid catalyst for the selective synthesis of 1,2-disubstituted benzimidazoles from a wide range of substituted *o*-phenylenediamines and aldehydes in moderate to excellent isolated yields using water as solvent at ambient temperature.

Keywords: Benzimidazole; Acid catalyst; ZIF-8; Recyclability

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Preparation and Flocculation Properties of Novel Acrylamide-Based Copolymer

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One of the main problems of the oil well drilling industry in the world is the swelling and absorption of water by clay particles in the ground during drilling operations by water-based fluids, which causes a very high cost and sometimes it is the loss of all oil wells [1-3]. Therefore, there are various methods in the oil industry to prevent this from happening, and the use of polymers with high thermal stability is one of the most important methods [4,5]. In this design, we will increase the thermal stability of new polymers by introducing chemical groups that are useful for thermal stability based on the initial design of the existing industrial molecule. We study the effects of changing the type and intensity of electric charge on how the clay plates interact with the copolymer chain with placing amorphous, cationic and anionic groups in each of the acrylamide-based copolymer chains, and finally propose a model and mechanism with the highest clay plate interaction with the copolymer.

Keywords: Acrylamide, Copolymer, Flocculant.

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Study of enantioselective synthesis of dihydropyrimidinones in the presence of chiral polymer

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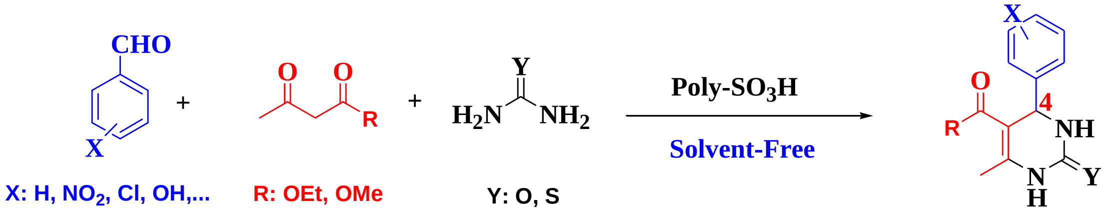
The synthesis of 3,4-dihydropyrimidin- 2(1H)-ones via the Biginelli reaction “a three-component condensation reaction between an aldehyde, urea and an easily enolizable carbonyl compound” was originally described by the Italian chemist Pietro Biginelli in 1893 [1]. In recent times, dihydropyrimidinone derivatives have attracted considerable attention owing to their high activity as antihypertensive, antiviral, antitumor and anti inflammatory agents. Pharmacological activity various dihydropyrimidinones depends on the absolute configuration in C(4). For this reason, the control of the stereochemistry of the substituent at C(4) has essential importance [2]. Many catalytic strategies have been proposed to asymmetric synthesis the Biginelli reaction. Some examples include organocatalytic,[3] chiral ligands and transition metal source,[4] Chiral auxiliaries polymer supported [5] and many other catalytic systems. A chiral polymer was produced and then chlorosulfonic acid was supported on the polymer in dichloromethan at room temperatur. Poly-SO_3H was indenticated by FTIR, ^{1}HNMR spectrometer. A mixture of aromatic aldehyde (1 mmol), carbonyl compound (1 mmol), and urea or thiourea (1 mmol) in the presence of Poly-SO_3H(0.03 g) at 90 ° C was heated under solvent free condition. Completion of the reaction was monitored by TLC. The reaction mixture was cooled to ambient temperature, then were dissolved in hot ethanol, the catalyst was filtered off and the products were obtained with high yields. The catalyst was completely washed with ethanol and reused. Products were identified by FT-IR compared to the reported samples in the literature. The samples showed optical activity in the polarimeter.

Keywords: Biginelli Reaction, Chiral Polymer, DHPM



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Synthesis, characterization, and application of $SrFe_2O_4@SiO_2@n$-pr@Tromethamine-Zr as a novel, green, nanomagnetic and reusable catalyst for the efficient synthesis of bis (pyrazolyl)methanes and polyhydroquinoline derivatives

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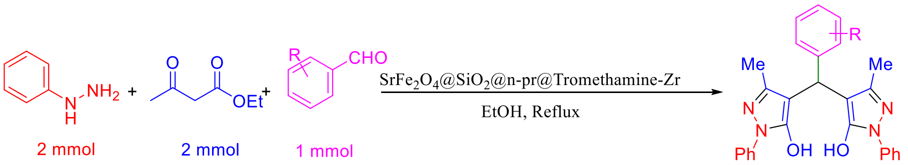
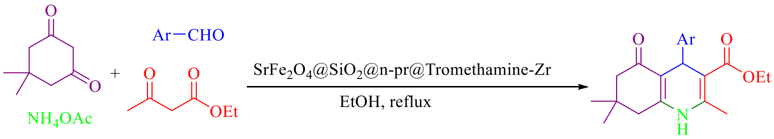
In this paper, we report the synthesis of $SrFe_2O_4@SiO_2@n$-pr@Tromethamine-Zr as a novel magnetic nanocatalyst, in a mild and green environment. The structure of the described magnetic compound was characterized by different physicochemical techniques including XRD, EDS, SEM, FT-IR, X-ray elemental mapping, TGA, and VSM analyses. The prepared magnetic nanoparticles exhibit excellent catalytic activity in synthesizing bis (pyrazolyl)methanes and poly hydroquinolinederivatives under green conditions (Scheme 1 and 2). The heterogeneous nature of the catalyst was confirmed via the hot filtration experiment. Further, $SrFe_2O_4@SiO_2@n$-pr@Tromethamine-Zr showed high efficiency and reusability that could be reused for at least five consecutive runs[1,2].

Keywords: Bis (pyrazolyl)methanes, Polyhydroquinoline, Tromethamine, $SrFe_2O_4$.



Scheme 1 A general method for the synthesis of bis (pyrazolyl)methanes catalyzed by $SrFe_2O_4@SiO_2@n$-pr@Tromethamine-Zr.



Scheme 2 A general method for the synthesis of polyhydroquinolines catalyzed by $SrFe_2O_4@SiO_2@n$-pr@Tromethamine-Zr.

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Application of new magnetic graphene oxide-porphyrin nanoparticles for synthesis of pyridines and pyrimidines via anomeric-based oxidation

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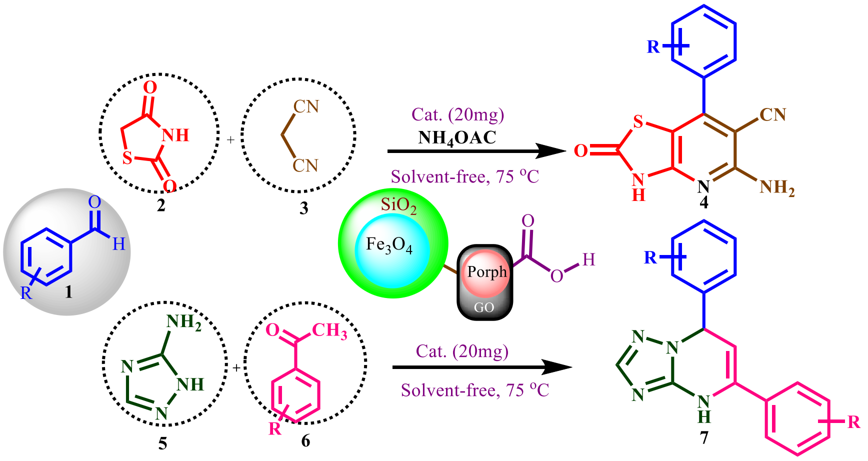
Herein joining of poly graphene oxide-porphyrin to magnetic nanoparticles {poly $Fe_3O_4@SiO_2@(CH_2)_3$-GO-[PTTA-NH-Ni] MNPs} occurred. The synthesized catalyst was characterized by several techniques such as FT-IR, CHN elemental analysis, EDX, WDX elemental maps, TGA, DTG, DTA, XRD, FE-SEM, TEM, BET, BJH, VSM, and ICP-AES. The described magnetic nanoparticles were employed as a benign catalyst for the expedient synthesis of 5-amino-7-aryl-2-oxo-2,3-dihydrothiazolo[4,5-*b*] pyridine-6-carbonitriles via anomeric-based oxidation mechanistic pathway. Target molecules were prepared through a four-component reaction of 2,4-thiazolidinedione, aldehydes, malononitrile, and ammonium acetate under solvent-free conditions at 75 °C (Scheme 1). Also, the application of the presented catalyst was investigated under the same reaction conditions for the synthesis of 5,7-diaryl-4,7-dihydro-[1,2,4]triazolo[1,5-*a*]pyrimidines through the three-component reaction of aldehydes, acetophenones, and 3-amino-1,2,4-triazole [1-3].



Scheme 1. Synthesis of pyridines and pyrimidines via anomeric-based oxidation catalyzed by poly $Fe_3O_4@SiO_2@$ $(CH_2)_3$-GO-[PTTA-NH-Ni] MNPs.

Keywords: Anomeric effect, Anomeric-based oxidation (ABO), Magnetic nanoparticles

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Nano Oxovanadium (V)-[5, 10, 15, 20-tetrakis (pyridinium)-porphyrinato]-tetra (tricyanomethanide) as a benign and expedient catalyst for the synthesis of pyrimidine-6-carbonitrile, pyrimidine-5-one, and tetrahydroquinoline-3-carbonitrile compounds *via* a cooperative geminal-vinylogous anomeric based oxidation

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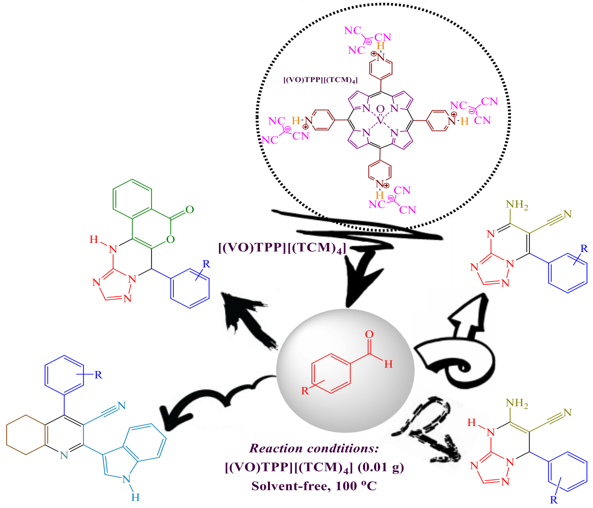
Nano oxovanadium(V)-[tetrakis(pyridinium)-porphyrinato]-tetra(tricyanomethanide) [(VO)TPP][(TCM)$_4$] was designed, synthesized, and characterized by various techniques. Then, 0.01 g of [(VO)TPP][(TCM)4] was used as a benign and expedient catalyst for the synthesis of numerous heterocyclic compounds such as 5-amino-7-(aryl)-4,7-dihydro-[1,2,4]triazolo[1,5-*a*]pyrimidine-6-carbonitriles, 5-amino-7-(aryl)-[1,2,4]triazolo[1,5-a]pyrimidine-6-carbonitriles, 7-(aryl)-7,12-dihydro-5H-isochromeno[4,3-d][1,2,4]triazolo[1,5-*a*]pyrimidin-5-ones, and 4-(aryl)-2-(1*H*-indol-3-yl)-5,6,7,8-tetrahydroquinoline-3-carbonitriles under solvent-free conditions at 100 °C via a cooperative geminal-vinylogous anomeric based oxidation (scheme 1) [1-2].



Scheme 1. Synthesis of triazolopyrimidines and tetrahydroquinolines by using [(VO)TPP][(TCM)$_4$] as a catalyst.

Keywords: Anomeric based oxidation; Polycyclic compounds; Solvent-free conditions.

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Effect of nitrogen-doped graphene quantum dots on the thermal stability of papain

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The unique structural properties of graphene quantum dots (GQDs), such as high availability surface area, chemical structure, fluorescence properties, good water solubility, high thermal stability, and low cytotoxicity, have attracted intense research interest. Doping of heterogeneous atoms in GQDs, such as nitrogen-doped graphene quantum dots (NGQDs), is a successful approach to enhancing and controlling the optical and electrical properties [1]. In recent years enzymes had many applications in different industries. Papain is a natural plant cysteine protease and one of the essential enzymes with many industrial applications [2]. Due to the complex industrial processes, free enzymes are unstable in these circumstances. Therefore, stabilization of papain increases its application [3]. According to the high thermal stability, NGQDs can be used as a suitable support for the immobilization of enzymes [4]. Therefore, immobilization of Papain on NGQDs significantly improves the enzyme thermal stability. The results showed that, by incubating the enzymes at 90 °C, immobilized papain maintained 53% of its activity after 60 minutes, while the free enzyme lost all activity only after 10 minutes.

Keywords: Papain, Immobilization, Graphene quantume dot

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Synthesis and characterization of $ZnFe_2O_4$@SiO_2@L-lysine@SO_3H and its catalytic applications in the oxidation of sulfides to the sulfoxides

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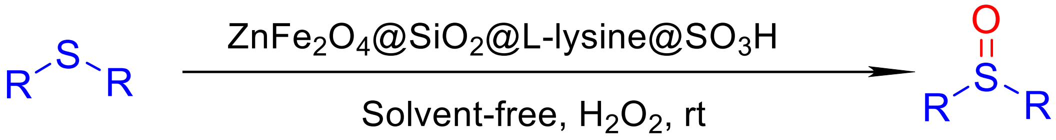
Herein, we report the synthesis of $ZnFe_2O_4$@SiO_2@L-lysine@SO_3H as a novel nanomagnetic solid acid catalyst, containing the sulfuric acid catalytic sites on the surface of $ZnFe_2O_4$MNPs as the catalytic support. The as-synthesized nanocomposite was meticulously characterized using a wide range of physicochemical techniques; including, FT-IR, XRD, EDX, X-ray-mapping, SEM, and VSM analysis. The prepared magnetic nanoparticles exhibit excellent catalytic activity in synthesizing the oxidation of sulfides to the sulfoxide under green conditions (Scheme 1). Moreover, it is worth mentioning that the heterogeneity of the catalyst was measured through its excellent reusability and hot-filtration test[1,2].



Scheme 1 Oxidation of sulfides to sulfoxides catalyzed by $ZnFe_2O_4$@SiO_2@L-lysine@SO_3H.

Keywords: $ZnFe_2O_4$@SiO_2@L-lysine@SO_3H, $ZnFe_2O_4$, L-lysine, SO_3H, Sulfoxide.

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Preparation of antimony supported on bio based catalyst and its use in the synthesis of 1,2,4,5-tetrasubstituted imidazoles under thermal conditions

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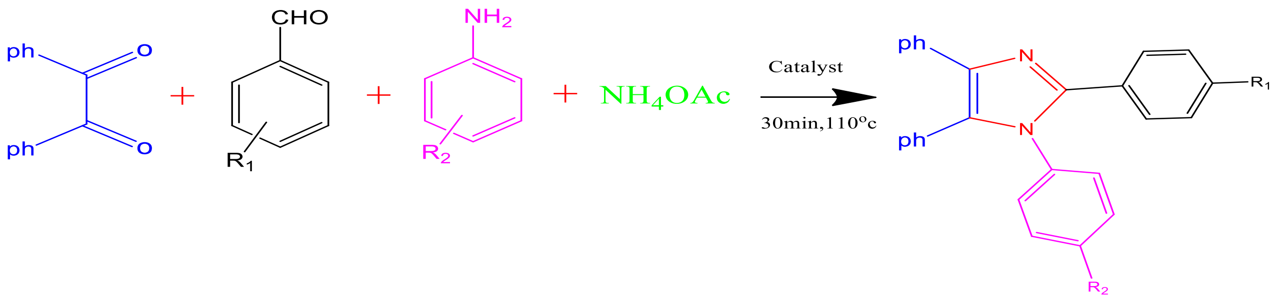
The naturally occurring five-member imidazole derivatives have shown interesting biological as well as physiochemical properties. Consequently they have found several chemicals, optical, pharmaceutical, and other useful biological applications [1].For instance, in medicine, they are extremely used for targeted drug delivery, in which the desired medication is delivered to the target tissue with high selectivity [2,3]. Multicomponent reactions (MCR's) are an excellent idea for synthesis of a complicated organic product. These reactions have three or more reactants to form a new significant and applied product.[4]

An antimony supported bio based catalyst was used to synthesis of 1,2,4,5-tetrasubstituted imidazole derivatives utilizing aromatic aldehydes, aromatic amines, benzyl and ammonium acetate, in thermal condition (schem1). The obtained compounds were identified by the melting points, FT-IR, and ^{1}H NMR analyses. FT-IR, XRD, EDX, FESEM, TGA, BET and TEM studies were used to find catalyst structure. Heterogeneously catalyzed approaches have useful rule in generalization of the procedure, easy separation, shrinking of waste production and recycling of the catalysts.

Keywords: Bio based catalyst, One-pot synthesis, Solvent free, Imidazole



Schem.1: synthesis of tetrasubstituted imidazoles

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Synthesis of Tetrahydrobenzo[a]xanthen-11-one Derivatives in the Presence of Biochar/Zinc Oxide Composite as an Efficient Nanocatalyst

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Biochar is a highly porous, carbon-based material produced from a range of different feedstock biomass, usually either vegetal or animal waste, under low-oxygen conditions that has significant aromatiztion and anti-decomposition capabilities. Biochar is reported to have a high specific surface area and contain a wide variety of negative surface functional groups (e.g., hydroxyl, carboxyl, amino), and therefore it has gained the interest of the scientific community in a multifunctional fields such as support for catalysis sythesis [1].

Novel catalyst based on zinc oxide on biochar is prepared through a simple route and is proposed for the synthesis of tetrahydrobenzo[a]xanthen-11-one derivatives. Highly effective ZnO/biochar catalyzed solvent-free synthesis of some tetrahydrobenzo[a]xanthen-11-one derivatives via one-pot multi-component reaction of aldehydes, 2-naphthol and dimedone. The salient features of this nanocomposite as catalyst are: easy preparation, cost-effective, high stability and reusability of the catalyst [2].

Keywords: Zinc oxide , Biochar, Nanocatalyst, Multicomponent reaction, Tetrahydrobenzo[a]xanthen-11-one

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Synthesis of Tryptanthrin Schiff Bases *via* One Pot and Catalyst Free Reaction

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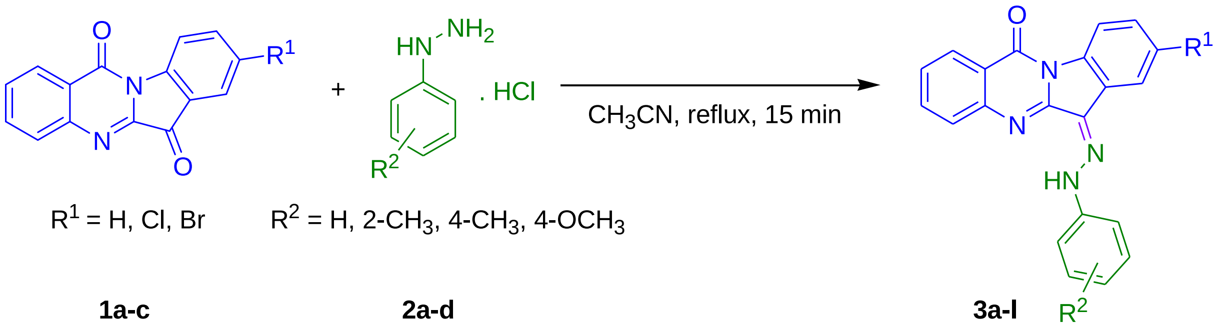
Schiff bases (SBs) are a group of organic compounds containing the azomethine or imine functionality. These compounds show significant biological activities and possess wide applications [1-2].

There are many reports about SBs of isatin in the literature. For example, arylhydrazones were prepared from isatins or N-methylisatins with corresponding arylhydrazins in methanol at room temperature by Catto et al. in 2020. In 2019, Hacini and coworkers studied the synthesis of isatin aldazines through a reaction of isatins, hydrazine monohydrate, and various aromatic aldehydes [3-4].

Considering the importance of Schiff base structures, using tryptanthrin instead of isatin would be more attractive and bring new interesting features for these structures. On the other hand, there is not any report around tryptanthrin SBs.

In this work, we are interested in investigation of tryptanthrin SBs through a reaction of tryptanthrins and different arylhydrazin hydrochlorides in CH_3CN, under reflux condition, in 72% - 92% yields (Scheme 1).



Scheme 1. Synthesis of aryl-hydrazono-6*H*-indolo[2,1-*b*]quinazolin-12-ones

Keywords: Tryptanthrin, Schiff base, Arylhydrazin Hydrochloride.

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Preparation, characterization and theoretically investigation of NLO properties of cellulose nanowhisker citrate as green organicTitle

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Nowadays, Materials with none linear optical properties due to their wide range of applications such as molecular switches, sensors, optoelectronic devices etc[2]. have attracted the attention of many researchers. Although, many reports addressed design and application of inorganic compounds with remarkable NLO properties, recently organic compounds have received much attention due to their properties such as their low cost, low toxicity and excellent processability . Moreover, their optoelectronic properties could modulated by adapting their molecular structure easily. In this context, cellulose citrate [1,2] prepared through one step acid hydrolysis processes and characterized using conventional spectroscopic methods including FT-IR spectroscopy, UV-vis spectroscopy and filed emission SEM microscopy. Finally, the NLO properties of the Glucose Citrate (GC) as its building block investigated theoretically[3]. The DFT and calculations was performed using B3LYP hybrid functional theory and 6-311G(d,p) basis set in the Gaussian 09 package. The molecular polarizability α(187), first-order hyperpolarizabilities β(1037), dipole μ(2.15), and quadrupole (Q) moments were 1, 2 and 3, respectively. The results showed that the nanocellulose citrate cold be promising organic material for NLO application.

Keywords: Nano Cellulose , Cellulose Nanowhiskera , Citric Acid hydrolysis , DFT , B3LYP

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Comparison and evaluation of CO_2 adsorption of activated carbon and $TiO(OH)_2$ particles

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Climate changing and global warming due to the increasing of greenhouse gases emission; especially CO_2, is one of the most important environmental issues in the last decades. Since CO_2 emissions affected by industrial developments and human activities, its reducing is the main challenge in the 21st century [1]. Over the past decades, using amine solutions to reduce CO_2 levels has been the most common method worldwide. The main drawbacks of this method are the high corrosion rate of equipment, high volatility of amines, releasing of toxic vapors as well as high energy and cost demands to recover the solvent. According to above mentioned disadvantageous, the adsorption method by solid adsorbents could be a more suitable alternative for carbon dioxide adsorption from the gas mixtures. Activated carbon is a known adsorbent due to its high porosity, high CO_2 selectivity, and high adsorption capacity and can be prepared by various sources which are easily available worldwide. Also, $TiO(OH)_2$ as a nanostructured material accelerate the CO_2 desorption process as well as adsorption kinetics [2,3]. In this study, date seeds as a biomass source and titanium isopropoxide were used for the preparation of activated carbon and $TiO(OH)_2$, respectively. In this regard, activated carbon was prepared by using KOH as an activating agent at 600 °C where the biomass/ KOH ratio was 1:1. After performing SEM, FTIR, XRD and EDS analyzes to confirm the successful synthesis of these adsorbents, their adsorption behavior at 25 and 50 °C under 10 and 90% of CO_2 in the feed, were evaluated by TGA analysis. According to the results, the synthesized activated carbon showed the highest CO_2 uptake at 25 °C and 90% CO_2, which was 2.659 $mmol.gr^{-1}$.

Keywords: Activated carbon, $TiO(OH)_2$, Adsorption, Carbon dioxide

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Mn-Schiff-base complex supported onto the silica coted $FeAl_2O_4$ MNPs: A novel nanomagnetic catalytic system for Annulation Reactions

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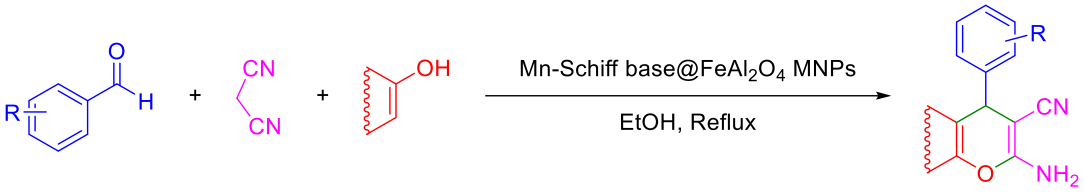
Green chemistry in the recent years has many interest in the world. One important aspect of this field is due to the use of low-cost and eco-friendly materials and methods in the synthesis process [1]. Ferrous nanomagnetic particles, also known as spinel ferrite compounds, have attracted attention, which has led to a variety of applications [2, 3]. In this study spinel normal $FeAl_2O_4$ MNPs was produced with the coprecipitation method. Then, $FeAl_2O_4$ samples were functionalized with a novel Mn-Schiff-base complex via the post-synthesis method in green medium. The obtained nanomagnetic Mn-complex has been characterized by different instrumental analysis and successfully applied as a magnetically recyclable heterogeneous catalyst for the efficient one-pot, multicomponent synthesis of anulated chromene and pyran derivatives. The catalyst can be recovered by magnetic separation and recycled several times without significant loss of catalytic activity (Schem 1).



Schem 1. Synthesis of anulated chromene and pyran derivatives catalyzed by Mn-Schiff base@$FeAl_2O_4$ MNPs.

Keywords: $FeAl_2O_4$, Mn-complex, Schiff base, Chromene derivatives, Pyran derivatives**.**

References

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Synthesis and characterization of a siloxane-based crosslink agent.

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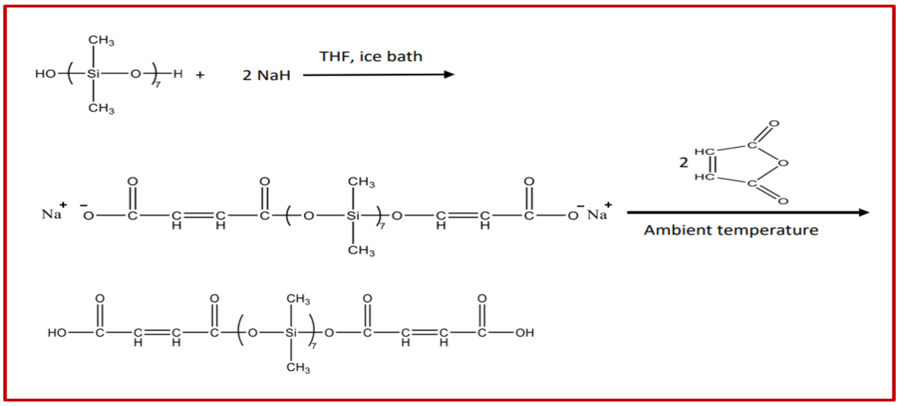
Polydimethyl siloxane (PDMS) derivatives are widely used material to improve the mechanical and hydrophobic properties of other components, especially emulsion polymerization products [1,2]. An oligomeric PDMS hydroxy terminated was used to synthesize a novel crosslinker. The synthesis was performed in tetrahydrofuran (THF) as a solvent in two consecutive reactions under an inert atmosphere. At first, PDMS was reacted to sodium hydride in an ice bath and then maleic anhydride was added to the reaction mixture, temperature increased to ambient temperature and condition was kept about 2 hours [3]. Reaction progress monitored by thick layer chromatography (TLC). Product washed several times by THF and dried at room temperature. The product chemical can have a multi-functional role in the emulsion polymerization processes, for instance as crosslinker and even improve the stability of latex by its ended functional groups. The synthesis is characterized using FT-IR and H-NMR methods.



Keywords: Polydimethyl siloxane, Crosslink agent, Emulsion polymerization

References

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Silica-based nanospheres supported Pd nanoparticles as a recyclable catalyst for the synthesis of primary amide

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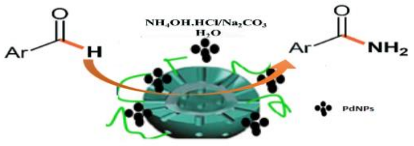
Amide bond formation is one of the most important organic chemistry reactions and is essential for the synthesis of drugs, natural products, and polymers such as peptides [1]. In fact, more than 25% of drugs contain at least one amide group [2]. In the search for cost-effective atomic protocols for the synthesis of amides, metal transformations have been considered attractive alternatives for developing pathways other than carboxylic acids and their derivatives [3]. Herein, we synthesized a new hollow inorganic polymer nanosphere (PANI-Si-HNS) for stabilizing Pd nanoparticles as a green and stable catalyst for the synthesis of primary amide (Scheme 1). The catalytic system was investigated for a wide range of aldehyde in the presence of 5 mol% of catalyst at 80 °C. Pd_{NPs}/HSN demonstrated excellent performance with high yields (Up to 95%) for the synthesis of corresponding amides. This catalyst was recovered and reused ٧ consecutive times without loss of activity.

Keywords: Silica, nanospheres, Palladium nanoparticles, primary amide



Scheme 1 Schematic view of synthsis of primary amide by Pd_{NPs}/HSN catalyzed green.

References

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A Narrative and Proficient Zeolite Catalyst of Palladium Nanoparticles-Decorated ATPS@ (2-Aminopyridine/Terephtalaldehyde) Functionalized ZSM-5, Towards The Suzuki, Miyaura and Heck Coupling Reactions

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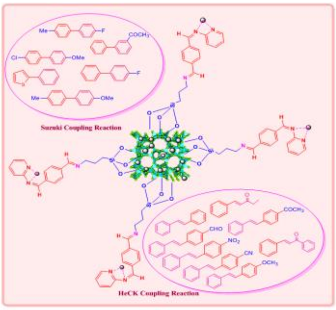
This study is motivated by very good and excellent results, attempts to evaluate and the ability to fully measure and identify newly synthesized catalyst ZSM-5@APTS@ (2-Aminopyridine / terephtalaldehyde) @$PdCl_2$ using ZSM-5 functionalized APTS@ (2-Aminopyridine / terephtalaldehyde) and stabilization of Palladium Nanoparticles. On the above substrate to form a highly efficient and new green catalyst ZSM-5@APTS@ (2-Aminopyridine / terephtaldehyde) @ $Pd(Cl)_2$ as a heterogeneous catalyst for use in Suzuki and Heck coupling reactions have been investigated. Zeolite (ZSM-5) belongs to the MFI structure type [1, 2]. ZSM5 may be a type of crystalline aluminosilicate zeolite belonging to the pentacyl zeolite family. Since amino groups can be strongly attached to metal nanoparticles, zeolites can be attached to Pd metal nanoparticles using amino groups. The general method of making a zeolite catalyst is shown in Figure 1. Zeolite of type (ZSM-5) was dispersed in dry toluene using ultrasonic device and aminoized by the combination of (3-aminopropylethriomethoxysilane) (ZSM-5@NH_2). In the following, the synthesis of the compound (4-pyridine-2- (elimino) methyl) benzaldehyde) from the concentrations of 2-aminopyridine and terephthalaldehyde was performed. Then, amine-activated zeolite is combined (4-pyridin-2- (elimino) methyl) benzaldehyde) was reacted and in the final step, a refined product and a final synthesized catalyst ZSM-5@ATPS/(4-pyridin-2-ylimino) methyl) benzaldehyde) @$PdCl_2$ were formed. Since amino groups can be strongly bound to metal nanoparticles, zeolites can be functionalized into Pd metal nanoparticles using amino groups.



Keywords: ZSM-5, 3-aminopropylethriomethoxysilane, aminopyridine, terephthalaldehyde, Pd-nanoparticles, Suzuki-Miyaura, Heck coupling reaction

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Preparation of MIL-101-En with an ethylenediamine group for immobilizing Pd and its application in Suzuki reactions

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Very recently, design of a heterogeneous catalyst with higher efficiency has been directed towards the development of stable supporting ligands, complexes and other catalytic species onto nanostructured materials [1, 2]. Among nanostructured materials, MOFs They are good support [3, 4]. Ultra-small nano-sized palladium particles were successfully stabilized within the pores of Ethylenediamine groups grafted open metal site metal-organic frameworks of Cr-MIL-101; coordinated diamine groups of ethylene diamine (ED) on the active site of chromium units of Cr-MIL-101. A new correction strategy behind the head is high performance for the Suzuki reaction. Finally, performance catalytic MIL-En-Pd was subsequently investigated in the Suzuki reaction with excellent conversion.

Keywords: MIL-101, Suzuki reaction, MIL-En-Pd, Heterogeneous catalyst.

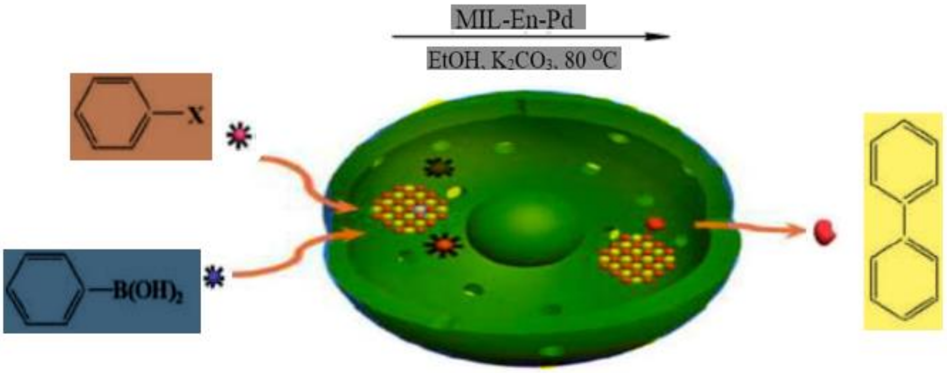

Fig. 1 Schematic view of MIL-101-En-Pd Catalyst for the proposed C-C coupling process.

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Palladium nanoparticles‑decorated Epichlorohydrine@β-Cyclodexterine functionalized UiO-66-NH_2 as a novel and efficient MOF-Catalyst for Suzuki, Sonogashira and Heck Coupling Reactions

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In this study, the new, efficient, and stable strucfture of Uio-66-NH_2@ECH@β-Cyclodexterine@Pd-NPs reported as a heterogeneous catalyst for the types of coupling reactions process under mild conditions. Reaction products were obtained with a high yield percentage. Obviously, electrostatic interaction of palladium with the juctions (Base, Hydroxyl and Carboxyl groups) is strong enough to hold metal ions, so Pd is eefectively stabilized with high stability. Eventually, this tri-fuctional Pd complex can effectively prevent Pd leaching, which is attributed to the exiting joints. Also, analysis of the recycled catalyst was performed after each reuse cycle to evaluate the amount of Pd leaching.[1-3] In addition, the Pd elution determined by ICP analysis after nine (9) recycles was negligible. This research is motivated by excellent results, tried to evaluate and ability to fully measure and identify the newly synthesized MOF-Catalyst as UiO-66-NH_2@1-Chloro-2,3 epoxy- propane@β-Cyclodexterine@Pd-NPs using UiO-66-NH_2 by cross-linking of epichlorohydrine, β-Cyclodexterine and stabilization of Pd-nanoparticles on the above substarte to form a highly efficient and new green MOF-catalyst UiO-66-NH_2@ECH @β-Cyclodexterine@Pd-NPs used as a heterogenous catalyst for promoting Suzuki, Sonogashira and Heck coupling reactions under mild reaction condition. The new synthesized heterogeneous catalyst was studied, identified and investigated using the analysis of various analyzes including XRD, FT-IR, TEM, FE-SEM, EDS-Mapping and ICP.

Keywords: MOF, UiO-66NH_2, ECH, β-Cyclodexterine, coupling reactions

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Palladium nanoparticles‑decorated magnetic Carbon Dot Functionalized on the Cyclodextrin Nanosponges - Biochar Hybrid as a novel and efficient Catalyst for Suzuki, Sonogashira and Heck Coupling Reactions

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This study is motivated by very good and excellent results, attempts to evaluate and the ability to fully measure and identify newly synthesized catalyst Pd@CQDs@Fe_3O_4/Hybrid for the primary time a ternary crossover framework composed of cyclodextrin nanosponges (CDNS), palladated attractive carbon quantum dot (Pd@CQDs@Fe) and Bell-pepper-derived Biochar is designed and arranged through functionalization of CDNS and Biochar and their covalent conjugation taken after by immobilization of Pd@CQDs@Fe. The crossover framework is an attractive heterogeneous catalyst for promoting Suzuki, Sonogashira and Heck coupling reactions under mild reaction condition in aqueous media. Nanocarbon material, can be made from various greens Cheap precursors such as glycerin, chitosan, fruits, etc. Skins and coriander leaves in various ways [1] includes laser ablation, hydrothermal synthesis, pyrolysis, wet Oxidation, ultrasonic and microwave assisted synthesis and Electrochemical etching. Excellent characteristics of [2] CQD such as chemical stability, low toxicity, small size, etc. High solubility and tunability make them suitable Many applications, primarily catalytic candidates. As an example of the catalytic use of CQD is the usefulness of Pd. Supports what is mentioned in the CQDS about the coupling reactions. With evolving natural concerns in mind, the development of bio-based, non-toxic, heterogeneous catalysts is receiving increasing attention. In this framework, carbonization of biomass is presented as a simple and inexpensive strategy for assembling carbonaceous objects, commonly referred to as bio (coal). This includes catalytic purposes, waste management, soil repair, super capacitors, absorbers, fuel production, etc. [3] One of the promising strategies for producing biochar is water treatment of biomass at relatively mild temperatures. The resulting char, known as hydrochar, can be used unmodified or after physical and chemical treatment. It is worth noting that this class of bio-based materials can be combined with other materials.

Keywords: Pd-nanoparticles, Coupling reactions, Cyclodextrin nanosponges, Carbon quantum nanodots (CQDs)

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Metal-organic frameworks stabilized CuI (MIL-En-CuI) for copper-catalyzed azidation/click reaction

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Very recently, design of a heterogeneous catalyst with higher efficiency has been directed towards the development of stable supporting ligands, complexes and other catalytic species onto nanostructured materials [1, 2]. Among nanostructured materials, MOFs They are good support [3]. CuI were successfully stabilized within the pores of Ethylenediamine groups grafted open metal site metal-organic frameworks of Cr-MIL-101; coordinated diamine groups of ethylene diamine (ED) on the active site of chromium units of Cr-MIL-101. A new correction strategy behind the head is high performance for the click reactions. Finally, performance catalytic MIL-En-CuI was subsequently investigated in the click reactions with excellent conversion.

Keywords: MIL-En-CuI, azidation/click, MIL-101, Heterogeneous catalyst.

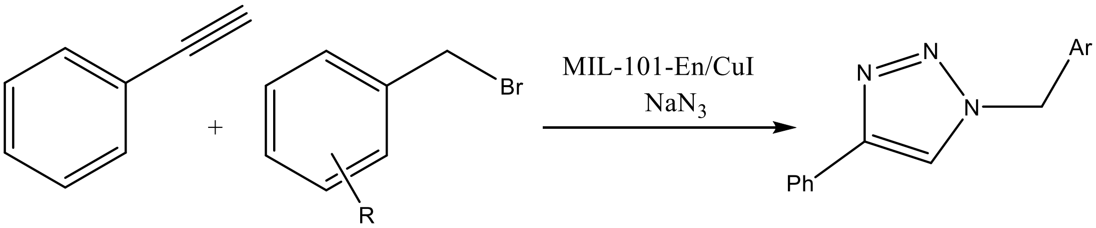

Fig. 1. CuI-Functionalization MIL-En for the click reaction.

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Catalyst-free tandem Michael addition/decarboxylation of coumarin-3-carboxylic acids with imidazopyridine

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Combination of two worthwhile heterocyclic scaffolds in one molecule could construct a new bis-heterocyclic architecture that may increase its therapeutic potential and biological activity than their individual scaffolds via a synergistic effect.[1-4] In this project, the tandem Michael addition/decarboxylation of coumarin-3-carboxylic acids with imidazopyridine has been developed and the biologically important imidazopyridine-3-substituted dihydrocoumarins were obtained in appropriate yields under catalyst-free conditions.(Figure 1) Finally, all ensued products were obtained with good efficiency and their structures were confirmed by Ft-IR, H-NMR, C-NMR and HR-MS. The use of no catalyst or additive, great diversity, sustainable reaction media, clean reaction profile, no column chromatography, thereby avoiding the use of toxic organic solvents, excellent regioselectivity and low E-factor are the notable features of this synthetic route.

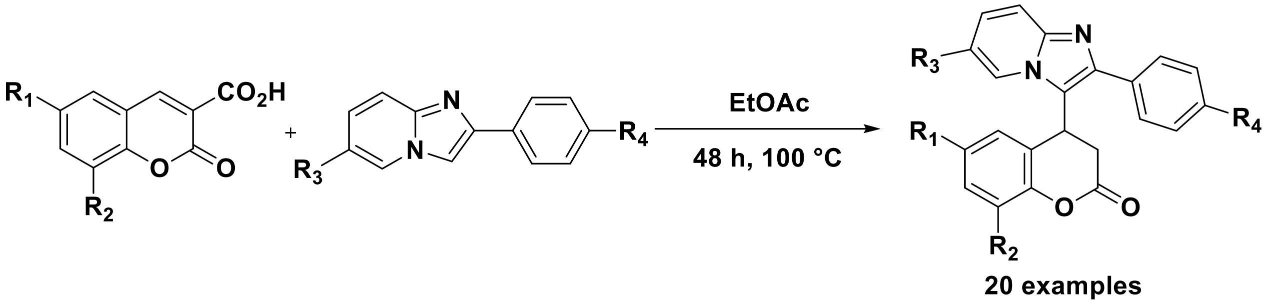

Figure 1. Synthesis of imidazopyridine-3-substituted dihydrocoumarins

Keywords: Coumarin acid, Imidazopyridine, Tandem reaction, Decarboxylation, Heterocyclic chemistry.

References

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Novel probe based on rhodamine B and quinoline as a naked-eye colorimetric sensor for dual sensing heavy metals and hypochlorite

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Rhodamine-based sensors universally reveals a wealth of opportunities for chemosensor and biosensor applications and several small molecules and macromolecules-centered rhodamine B have recently introduced as elevated sensors.[1-3] In this study, a novel colorimetric sensor based on rhodamine B was designed and synthesized to detect metal ions. Rhodamine B hydrazide deraivetives and 2-thioquinoline-3-carbaldehyde were reacted in methanol solvent under refluxed conditions.(Figure 1) The structure of the synthesized sensor was investigated and confirmed by IR and H- and C-NMR spectroscopy. The new chemical sensor demonstrated appropriate sensitivity and selectivity for the detection of Ni ion among all the cations and anions examined in ethanol solution. The measurement was based on the interaction between the synthesized ligands and Ni or hypochlorite and the color of the solution swiftly changed from pale yellow to deep pink which can be rapidly diagnosed by naked eyes. Furhermore, the measurement of details were evaluate by using UV-vis and photoluminescence spectroscopy.

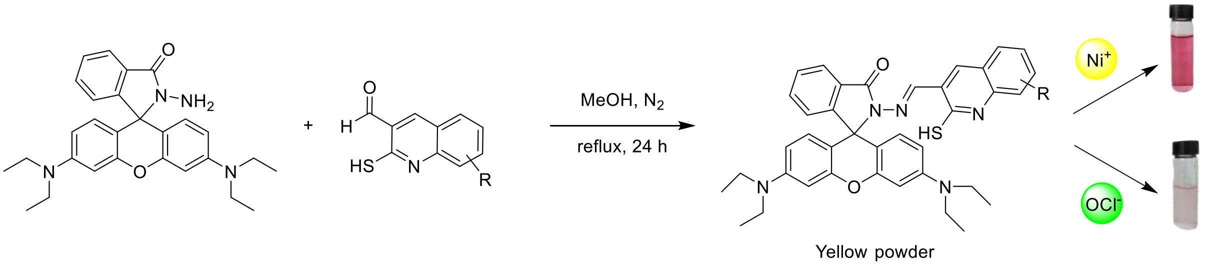

Figure 1. Synthesis of novel colorimetric sensor based on rhodamine B and 2-thioquinoline-3-carbaldehyde

Keywords: Colorimetric sensor, Rhodamine B, Quinoline, Heavy metals, Hypochlorite

References

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Application of ammonium acetate as dual role reagent-catalyst for the synthesis of hybrid pyridines with triazole and sulfonamide moieties

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Pyridine families as the unique *N*-heterocyclic compounds have an important role in many natural products, pharmaceutical active molecules, agricultural compounds, organic synthesis, supramolecular chemistry, functional materials, and catalytic systems [1-2]. The fantastic properties of pyridines such as HIV protease inhibitor and anticancer, anti-inflammatory, are well known for the many of pharmocological researchers [3]. Moreover, sulfonamides as the most important organosulfur compounds by irreplacable properties including high stability and three-dimensional shape, have exceptional advantages such as having good potential in antibiotic compounds, antimicrobials, anti-bacterial, anti-inflammatory and anti-protozoal [4]. On the other hand, triazole scaffolds have several applications in drug systems, dyes, chemosensors, metal complexes, organocatalysts and energetic materials [5]. In our study, we synthesize new hybrid pyridines with triazole and sulfonamide moieties by applying ammonium acetate as dual role reagent-catalyst.

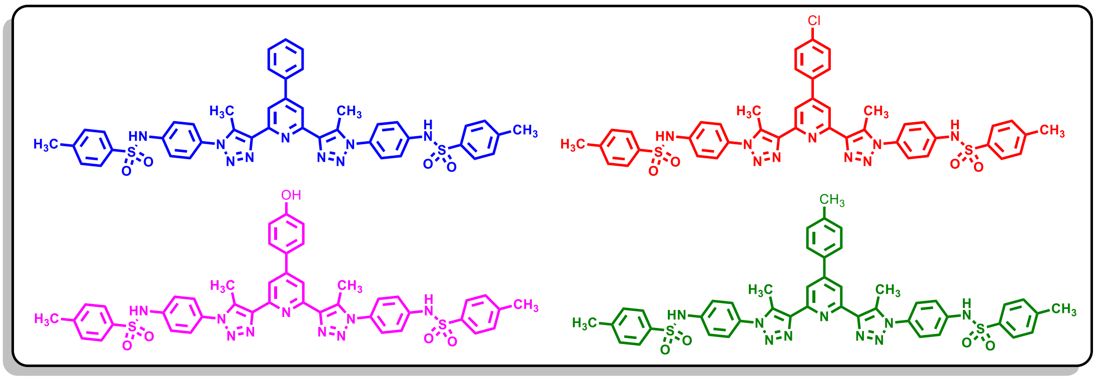
Solvent free, 110 °C, 35-50 min., 78-90 %

Figure 1: Synthesis of pyridine hybrids by using ammonium acetate as dual role reagent-catalyst.

Keywords: Ammonium acetate, Pyridine, Sulfonamide, Triazole.

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Design and synthesis of magnetic nanoparticles supported urea derivatives and its catalytic application for the synthesis of new pyridines via vinylogous anomeric-based oxidation

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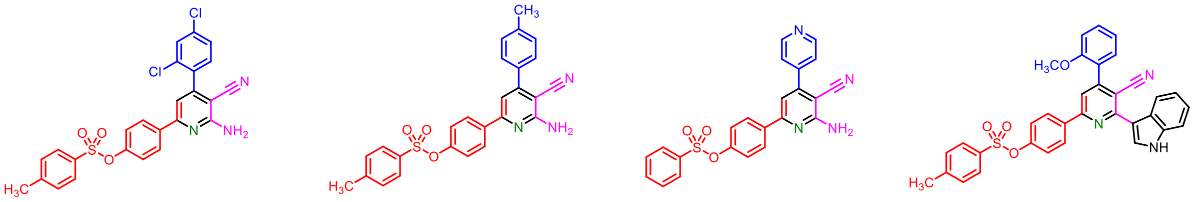
Hydrogen bonding is of paramount importance in many chemical reactions such as reduction, ring closure, selective stereo reactions, and heterocycle synthesis. Hydrogen bonding plays an important role in enzymatic catalysis, arrangement of molecules in crystals, crystal engineering, supramolecular chemistry, and proton transfer reactions [1-2].

Magnetic nanoparticles (MNPs) have been increasingly used in catalysis over the past decade because of their easy recyclable, economical and environmentally safe recovery. In such a case, Fe_3O_4 nanoparticles with strong response to external magnetic field and high surface area, provide proper conditions to anchoring catalytically active organic linkers [3-4].

Pyridine, a heterocyclic compound, is used as a medicine for treatment of diseases such as depression [5].

In this study, we applied a synthetic system for the synthesis of sulfonates linked pyridines *via* vinylogous anomeric-based oxidation in the presence of novel urea-functionalized MNPs as a heterogeneous hydrogen bonding catalyst.



Reaction conditions:
Solvent free, Temperature: 110 °C, Time: 30-45 min, Yield: 80-92%

Scheme 1: Catalytic synthesis of pyridine derivatives in the presence of novel nanomagnetic hydrogen bond catalyst *via* vinylogous anomeric-based oxidation

Keywords: Hydrogen bonding, Nanomagnetic Catalyst, Pyridine,

References

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Direct synthesis of novel symmetrical 1,3-diynes via Cu-catalyzed Glaser homocoupling reaction

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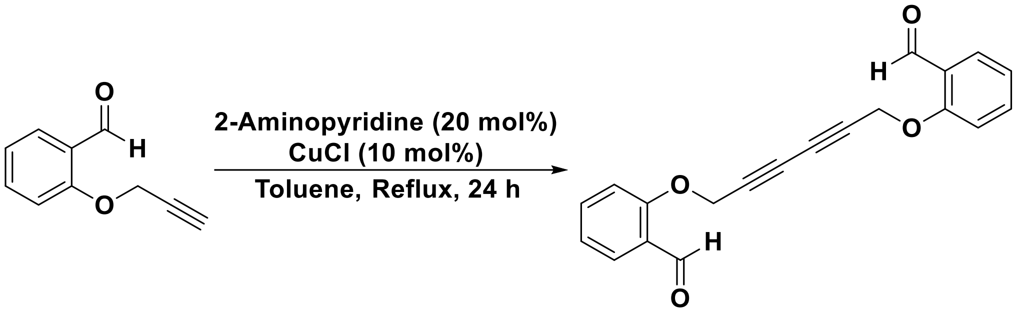
Glaser coupling is one of the most pivotal modern organic tools for the formation of carbon-carbon triple bond and has also been extensively used for the synthesis of polymers, macrocycles and oligomers.[1,2] In continuation of our research toward the development of metal-mediated organic transformations,[3,4] herein we report an efficient and straightforward procedure for the synthesis of novel symmetrical 1,3-diynes. 2-aminopyridine has been established as an efficient ligand in Cu-catalyzed cross-coupling of terminal alkynes to form final product using CuCl as the catalyst under base-free condition. Significantly, we hope that the final products will be deployed as privileged reactants for the preparation of macrocycles and polymers.



Keywords: Cross coupling reactions, Glasser reactions, Diynes, Copper catalyst

References

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Catalytic application of a porous polymer functionalized magnetic nanoparticles for the synthesis of 1,2,4-triazoloquinazolinone

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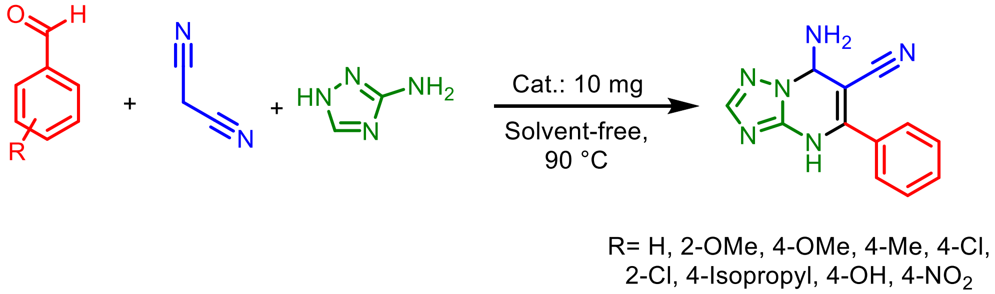
Organic polymers due to having diverse properties such as excellent thermal stability, large surface areas and synthetic designability have been found several applications in the areas of catalytic systems. [1-2]. Furthermore, magnetic nanoparticles have excellent magnetic properties and ultra-comfortable separation processes. These compounds are used as heterogeneous support and active site for modification of many catalytic systems and were applied in organic synthesis domains such as photocatalysis, photoelectrochemical catalysis, oxidation reactions, multicomponent reactions, enzyme catalysis, coupling reactions and chiral catalysis [3-4]. 1,2,4-triazoloquinazolinone as the major important fused *N*-heterocycle compounds have tremendous pharmacological applications and are in many of natural products [5]. In this study, catalytic application of porous organic polymer functionalized magnetic nanoparticles was investigated for the synthesis of 1,2,4-triazoloquinazolinones (Scheme 1).



Scheme 1: Synthesis of 1,2,4-triazoloquinazolinones by using organic polymer functionalized magnetic nanoparticles as catalyst.

Keywords**:** Polymer, Magnetic nanoparticles, 1,2,4-triazoloquinazolinone.

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A one-pot four-component approach to synthesis of epiminomethanoimino-indeno[1,2-b]pyrrol-4-one derivatives

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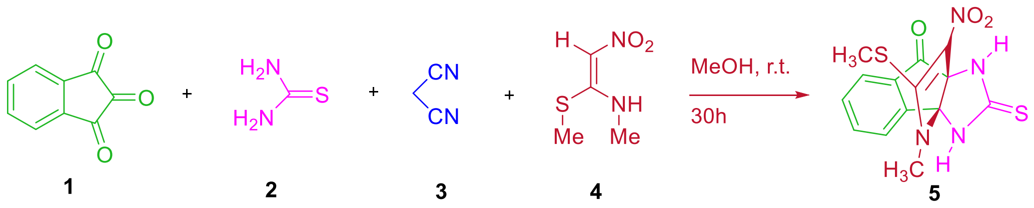
Ninhydrin has been used in many heterocyclic preparations and considered as an crucial building block in organic synthesis. There is plenty of reactions that include ninhydrin in the synthesis of heterocyclic compounds.[1]

Heterocyclic compounds with embedded nitrogen atoms are privileged structural entities found in natural products, pharmaceuticals, and material sciences.[2]

Propellants with three non-zero bridges and a zero bridge between a pair of carbon atoms at the top of the bridge attracted the attention of organic chemists and because of their unusual shapeو physical properties and their existence, important artificial targets.[3]

The three-component reaction of ninhydrin **1**, thiourea **2**, malononitrile **3** and nitroketene dithioacetal **4** in methanol at room temperature for 30 h, afforded a series of epiminomethanoimino-indeno[1,2-b]pyrrol-4-one **5** in 75 % yields (Scheme 1).



Scheme**1**: Synthesis of epiminomethanoimino-indeno[1,2-b]pyrrol-4-one

Keywords: Ninhydrin, thiourea, heterocyclic compounds, nitroethen, CH acid

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Effect of polymerization time on monomer conversion in a semi-batch emulsion polymerization of styrene and butyl acrylate

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Due to a low reactivity and solubility in water and steric hindrance of benzene ring, styrene (St) has a low tendency to introduce in to polymer chain in an emulsion polymerization with butyl acrylate (BA) [1,2]. This issue lead to a low St monomer conversion and made air pollution because of remaining pollutant monomer in the polymer latex product. In a conventional semi-batch seeded emulsion copolymerization of St and BA using hybrid surfactant namely, dioctyl sulfosuccinate (DOSS) as an anionic and nonylphenol ethoxylate (KENON20) as a non-ionic surfactant, Increasing final polymerization time (the time after complete addition of the monomers) (from 40 min. to 70 min.) lead to rise the conversion (from 93.0% to 99.7%). Solid content and monomer conversion determined by gravimetrical method.

Keywords: Emulsion polymerizatin, Semi-batch, Styrene, Butyl acrylate

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A one-pot four-component approach to synthesis of novel epiminoethano-indeno[1,2-b]naphtho[1,8-ef][1,4]diazepin-12-one derivatives

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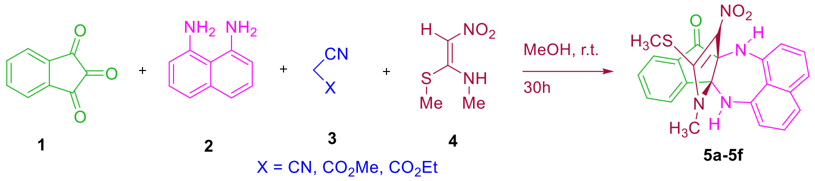
Multi-component reactions (MCRs) have emerged as a highly efficient synthetic tool in organic and medicinal chemistry because of their ability to synthesis pharmaceutical compounds and their productivity, high atom economy, step efficiency, molecular diversity, and operational simplicity [1]. In the past decade, new MCRs have been developed and used for the construction of important complex molecules[2].

Nitrogen-containing heterocycles, are able to insert into DNA and disrupt undesirable cellular processes[3] which result in this wide range of biological properties that include antitumor, antibacterial, antiparasitic, antiviral, antifungal[4].

The four-component reaction of ninhydrin 1, naphthalene-1,8-diamine **2**, malononitrile derivatives **3** and nitroketene dithioacetal **4** in methanol at room temperature for 30 h, afforded a series of epiminoethano-indeno[1,2-b]naphtho[1,8-ef][1,4]diazepin-12-one derivatives **5a-5f** in 65-85 % yields (Scheme 1).



Scheme1: Synthesis of epiminoethano-indeno[1,2-b]naphtho[1,8-ef][1,4]diazepin

Keywords: Ninhydrin, naphthalene-1,8-diamine, diazepin, heterocyclic compounds, CH acid

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A new magnetic organic polymer: catalytic application for the synthesis of 4,6-diarylpyrimidin-2(1*H*)-one

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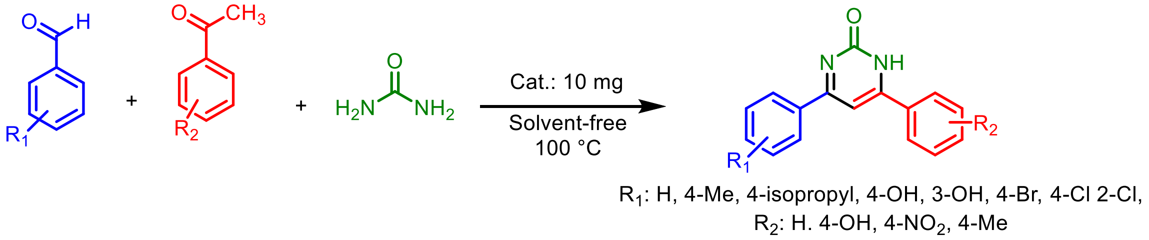
Heterogeneous catalysts due to their significant benefits such as chemically tunable properties, high thermal and chemical stability and easy reusability, have been emerged the attention of many chemists [1]. Magnetic heterogeneous catalysts as a fantastic subset of heterogeneous catalytic systems, are considerable research area in catalysis. These materials have small size in the range of nano scale. Moreover, magnetic catalysts can be modified by ionic liquids, polymers and etc. Therefore, magnetic catalysts are a bridge between heterogeneous and homogeneous catalysis [2]. Dihydropyrimidinone moieties as one of the greatest families of heterocyclic compounds, have various biological activities and are a kind of modulators for the transport of calcium ions. These materials have good potential as active antihypertensive agents, adrenoceptor-selective antagonists, and kinesin Eg5 inhibitors. As a result, 4,6-diarylpyrimidin-2(1*H*)-one gained great attention in organic synthesis [3,4]. In this investigation, we are going to synthesis 4,6-diarylpyrimidin-2(1*H*)-one derivatives by using a new magnetic organic polymer as catalyst (Scheme 1).



R_1: H, 4-Me, 4-isopropyl, 4-OH, 3-OH, 4-Br, 4-Cl 2-Cl,
R_2: H. 4-OH, 4-NO_2, 4-Me

Scheme 1: Catalytic application of a new magnetic organic polymer for the synthesis of 2,3-dihydroquinazolin-4(1*H*) ones.

Keywords: Dihydropyrimidinone, Magnetic nanoparticle, Organic polymer.

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Synthesis of magnetic organic polymer as new heterogeneous catalyst and its application for the synthesis of 2,3-dihydroquinazolin-4(1*H*) ones

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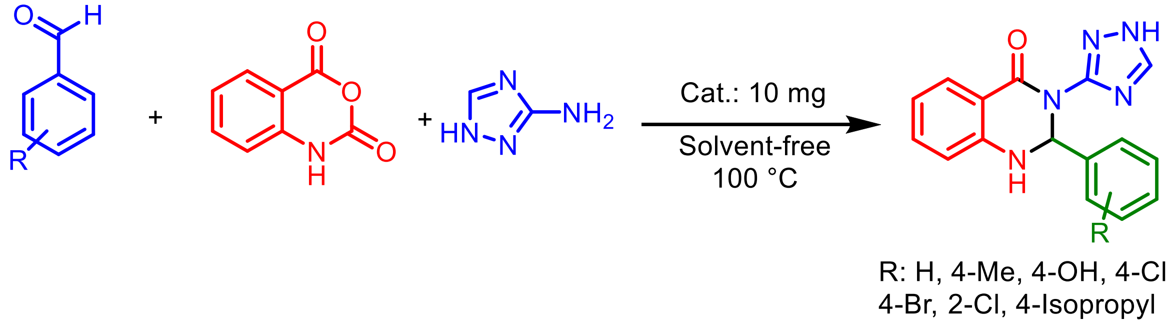
In the last decades, magnetic nanoparticles (MNPs) as versatile compounds have been widely applied in modern technological fields such as catalyst, medicine, environmental perspectives and drug delivery. MNPs have variety benefits such as good thermal stability, easy separation and reusability, high surface area and low toxicity [1-2]. Moreover, modification of magnetic nanoparticles with polymers creates a unique outlook for catalytic investigations [3]. 2,3-Dihydroquinazolins as one of the most important nitrogen-containing heterocycle compounds were profoundly studied by relevant chemists and have several benefits in medicinal researches. Anti-inflammatory, anti-depressant and HIV protease inhibitors are just a few of the medicinal applications of 2,3-dihydroquinazolins derivatives [4-5]. Herein, we investigated the catalytic application of magnetic organic polymer for the synthesis of 2,3-dihydroquinazolin-4(1*H*) ones (Scheme 1).



Scheme 1: Catalytic application of acidic magnetic porous organic polymer for the synthesis of 2,3-dihydroquinazolin-4(1*H*) ones.

***Keywords*:** 2,3-Dihydroquinazolin, Magnetic nanoparticles, Polymer.

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Catalytic application of magnetic nanoparticles anchored deep eutectic solvent for the synthesis of pyranopyrazoles

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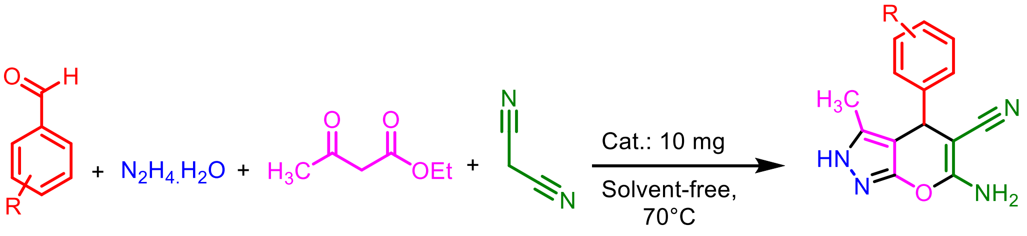
Nowadays, the design of biological catalysts which are in line with the environment and green chemistry is an appreciable perspective and deserve more attentions. Deep eutectic solvents supported on the nanomagnetic particles are an example of this catalytic systems. These materials because of their dual acidic and hydrogen bonding functional groups and ability of chelation to the metals can be used as robust multifunctional catalytic systems [1-2]. There are several advantages for these systems which are including of the synthesis of high-efficiency products, short reaction time and ease of operation [3]. Pyranopyrazoles as one of the most preeminent classes of heterocyclic compounds have a key role in biological and pharmacological domains. Several medicinal applications such as antimicrobial, anticancer, anti-inflammatory and inhibitors of human Chk1 have been devoted for pyranopyrazole derivatives [4-5]. In this study, catalytic application of magnetic nanoparticles anchored deep eutectic solvent as catalyst was investigated for the synthesis of pyranopyrazole derivatives (Scheme 1).



R= H, 2-OMe, 4-OMe, 4-Me, 4-Cl, 2-Cl, 4-Isopropyl, 4-OH, 4-NO_2

Scheme 1: Synthesis of pyranopyrazoles by using magnetic nanoparticles anchored deep eutectic solvent

Keywords: Deep eutectic solvent, Magnetic nanoparticles, Pyranopyrazole.

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Improving properties of inside tire paint by amphiphilic polyurethane as a dispersant to extend the life of the bladder into the tire production process

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In the production of tires, an emulsion is commonly used to prevent the green tire from sticking to the bladder, which is commonly called pre-cure inside paint. Despite the existence of new water-based internal paint, due to the ventilation of bias green tires, the use of new water-based systems is not suitable, so the use of inside emulsion paints based on solvents, as internal lubricants of the tire can be suitable options[1]. These emulsions are a combination of clay (talc, mica and bentonite) in organic solvent[2]. However, the colloidal particles in these paints are not stable enough in the organic solvent and clot over time, causing the spray gun head to clog and not spraying evenly on the inner and outer surfaces of tire.

We have recently reported the preparation and characterization of a novel amphiphilic polyurethane that was able to disperse a variety of hydrophilic and hydrophobic dyes [3]. In the present study, this polymer with hydrophilic and hydrophobic parts on theire surface was used as dispersing and emulsifying and improves the inside and outside paints properties by reducing surface tension and coagulation of dispersed particles (Figure 1). In addition, these paints increased the green tire slip and reduced the tire adhesion to the bladder , and ultimately increased the life of the bladder and reduced the mold's dirty.

Keywords: Amphiphilic polyurethane, inside tire paint, dispersant, bladder, bias tires.

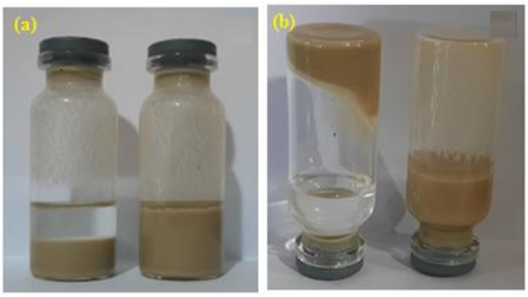

Figure1: (a) Solubility and stability of colloidal mineral particles in hydrocarbon solvents after 10 minutes in the presence of the amphiphilic polyurethane(right-side tube) and in the absence of this polymer (left-side tube); (b) Inverted the same samples after ten minutes.

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Synthesis of 3-phenethyl-5-(benzoylmethylene)-4-oxo-2-thioxo-1,3-thiazolidine derivatives via solvent-free reaction between arylglyoxals and rhodanines

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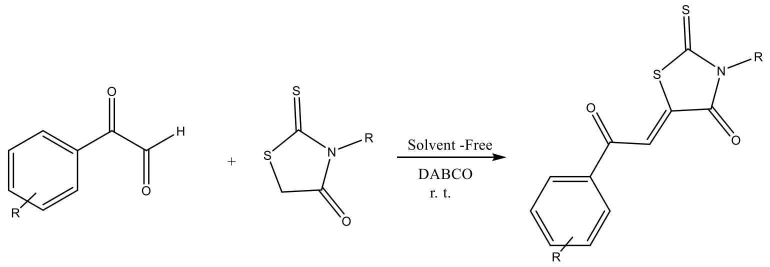
The arylidene rhodanine-based compounds are considerable heterocyclic molecules with diverse pharmacological activities such as anticancer, anti-bacterial, anti-diabetic, antifungal and anti-HIV. These molecules also inhibit numerous targets such as aldose reductase [1]. Recently, rhodanine -based molecule supported on nano-magnetic particles has also been used to remove heavy metal contamination or used as a catalyst for organic transformations [2]. Evidence suggests that the activity of the rhodanine derivative correlates with the size and the nature of the substituents at C-5 and N-3 positions [3]. In this study, we synthesized 3-phenethyl-5-(benzoylmethylene)-4-oxo-2-thioxo-1,3-thiazolidine derivatives via the solvent-free reaction between arylglyoxals and rhodanine rings in the presence of a catalytic amount of DABCO at room temperature.

Keywords: Rhodanines, solvent-free reactions, green chemistry, glyoxals.



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$ZnFe_2O_4$@SiO_2@l-Lisin@Cr-EDTA-MOF: Synthesis, characterization and its catalytic applications for the chemoselective Oxidation of sulfides

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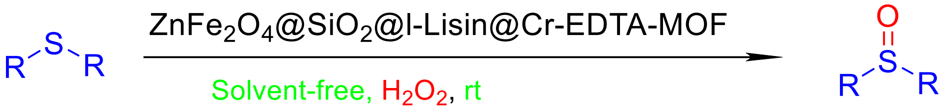
In this research, the design, and synthesis of $ZnFe_2O_4$@SiO2@l-Lisin@Cr-EDTA-MOF magnetic nanocatalyst nanoparticles as a novel, the recyclable, and heterogeneous catalyst was developed. The magnetic nanocatalyst was analyzed using various spectroscopic methods such as Fourier transform infrared spectroscopy (FTIR), scanning electron microscopy (SEM), powder X-ray diffraction (XRD), and energy dispersive X-ray (EDX), thermogravimetric analysis (TGA), vibrating sample magnetometer (VSM). The prepared magnetic nanoparticles exhibit excellent catalytic activity in synthesizing the oxidation of sulfides to the sulfoxide under green conditions **(Scheme 1)**. The heterogeneous nature of the catalyst was confirmed via the hot filtration experiment. Furthermore, the activity of the recycled nanocomposite was examined for at least five cycles with a negligible loss of its activity [1]

Keywords: sulfoxide, $ZnFe_2O_4$@SiO_2@l-Lisin@Cr-EDTA-MOF, $ZnFe_2O_4$, l-Lisin, EDTA, MOF.



Scheme 1 Oxidation of sulfides to sulfoxides catalyzed by $ZnFe_2O_4$@SiO_2@l-Lisin@Cr-EDTA-MOF.

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Regioselective Synthesis of *β*-Amino Acid Derivatives Containing Cyclooctane Ring

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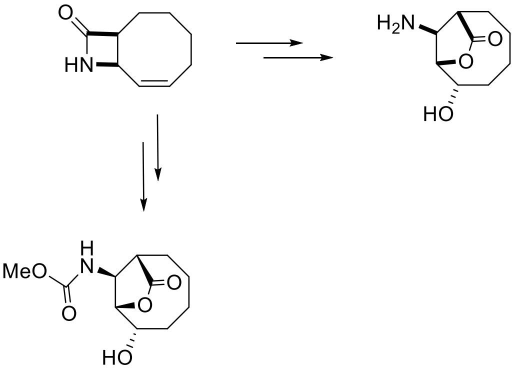
Cyclic *β*-amino acids have for the past few decades aroused widespread synthetic interest owing to their diverse biological activities, especially applications in the field of medicinal chemistry. They can be used as starting substances for different heterocycles, as precursors for the synthesis of polymers, as potential pharmacons, for the synthesis of natural products or analogues, and also as building blocks in drug research [1-2]. Therefore, in this work we focused synthesis of some *β*-amino acid derivatives containing cyclooctane ring [3].



Cyclooctane amino acids derivatives were synthesized from *β*-lactam *via* cycloaddition of chlorosulfonyl isocyanate to *cis*,*cis*-1,3-cyclooctadiene, by selective transformation of the C-C double bond, stereoselective epoxidation and regioselective oxirane ring opening with HCl(g)-MeOH, $NaHSO_4$, or NaN_3. Density-functional theory (DFT) computations were used to explain the reaction mechanism for the ring opening of epoxide and the formation of five-membered lactones. The configuration of methyl 6-hydroxy-9-oxo-8-oxabicyclo[5.2.1]decan-10-yl)carbamate was confirmed by X-ray diffraction.

Keywords: Cyclic β-Amino Acids; Bicyclic β-lactam; Aminocyclitol; Azides.

Acknowledgments: This study was funded by the Research Fund of the Atatürk University (project number: 2014/54).

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Novel Preparation of Modified Biochar as Bronsted acid catalysis for Biginelli Synthesis of 3,4-Dihydropyrimidin-2(1*H*)-one

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Carbon-based materials have long been used in heterogeneous catalysis reactions due to their desired properties for catalyst support and carbon-based materials act as direct catalysts in many industrial applications. Along with the use of biochar as produced, researchers have currently devised various modification approaches to further expand its activation capacities [1]. Certain catalytic reactions require strong acid sites. To this end, biochar was sulfonated (i.e., introducing a sulfonate group ($–SO_3H$) onto biochar) using a simple and efficient procedure [2]. 3,4-dihydropyrimidin-2(1H)-ones and their derivatives have an important role in synthetic organic chemistry and natural products due to their extensive range of biological and pharmacological properties[3]. Here in an environmentally benign Biginelli synthesis of 3,4-dihydropyrimidine-2(1H)-ones by one-pot three-component reaction of aromatic aldehydes, ethylacetoacetate and urea in the presence of sulfonated biochar as recyclable nanocatalyst have been reported.

Keywords: Biginelli, nanocatalyst, bichar sulfonic acid.

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FDU@n-Pr-chromotropic acid organic-inorganic hybrid mesoporous nanocatalyst: as a highly efficient and reusable promoter for the synthesis of chromeno[2,3-d] pyrimidine-8-amine and tetrahydrobenzo[b]pyran derivatives

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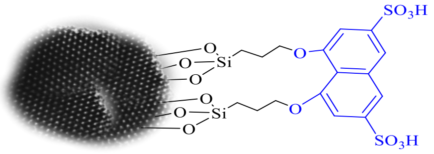
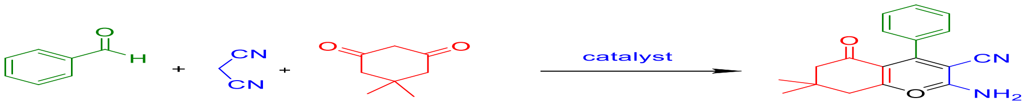
In this work, a convenient, efficient, and practical heterogeneous acid-catalyzed multicomponent synthesis of industrially important compounds including chromeno[2,3-d] pyrimidine-8-amine and tetrahydrobenzo[b]pyran has been developed using an FDU-supported tris- chromotropic acid as a catalyst. The prepared mesoporous organic-inorganic hybrid was characterized by XRD, TGA, EDS, ICP, X-ray mapping, and SEM techniques. The catalytic activity of described nanocatalyst was considered for the synthesis of chromeno[2,3-d] pyrimidine-8-amine and tetrahydrobenzo[b]pyran derivatives. The catalytic activity of FDU@n-Pr-chromotropic acid nanoparticles for both of the mentioned reactions was excellent in short reaction times. The reaction works in ethanol as a green solvent and a catalyst that can be easily recovered via a simple filtration process and recycled up to five times without apparent loss of activity and promises economic and environmental benefits. Therefore, the use of commercially available materials, eco-friendly procedure, operational simplicity, ease of separation by simple filtration, cheap and chemically stable reagents, good reaction times, simple practical methodology, and ease of use make the prepared catalyst a promising candidate for potential applications in some organic reactions[1–3].

Keywords: chromeno[2,3-d] pyrimidine-8-amine; tetrahydrobenzo[b]pyran; FDU@n-Pr-chromotropic acid; FDU.



FDU-12

Scheme 1. Synthesis of chromeno [2,3-d] pyrimidine-8-amines catalyzed by FDU@n-Pr-chromotropic acid.



Scheme 2. Synthesis of tetrahydrobenzo[b]pyran catalyzed by FDU@n-Pr-chromotropic acid.

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Titanium metal and Hexane Recovery From Catalyst Slurry In the Polyethylene Production Process

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Metals like Ti, Ni, Mo, Rh, Pt, Pd, etc., are widely used as a catalyst in chemcal and petrochemical industries. They are generally supported on porous materials like through precipitation or impregnation processes. In many of the cases, the metals are in the form of oxides, however, in other cases, they are reduced into active metals for catalyzing the appropriate reactions. After periodical use of the catalysts, due to poisoning effect of foreign material and impurities, which deposit on the surface of the catalyst, they will become inactive. In such cases, fresh catalysts have to be substituted and spent catalyst will be discareded as waste material.[1] Disposal of such catalyst materials, which contains appreciable amounts of heavy metals, is enviromentally hazardous. Therefore, a suitable and economically viable method is required for recovery of metals at the same timemethod should not pose the risk of environmental hazardous.[2] The purpose of this study is the extraction of TiO_2 using digestion of spent catalyst with various inorganic acids as well as hexane distilation. Leaching process has done with different concentrations of H_2SO_4, HCl, HNO_3 , and after sepration, liquid phase dried by heating under specific temperature. The results of XRF analysis showed that the recovery of TiO_2 obtained was 94% through acid digestion.

Keywords: Hexane,Titanium, Catalyst, Polyethylene

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Study of Difficulties in the Expanded Poly Styrene Coating Process and Suggestion to Overcome Agglomeration of Final Product

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Expanded polystyrene is one of the products of Bead foaming technology. Production of polystyrene beads are categerized into different fractions such as 100, 200, 300, 400 and 500 based on the size of expansion polystyrene beads in the classification and sieving stage then after coating and packaging, products deliver to downstream companies.[1] The presence of mineral contaminants, electrostatic charges and adhesion between expanded polystyrene beads causes the beads to accumulate in the pre-expansion process and this creates problems in downstream industries.[2] Coating agents are used to prevent the beads from lumping together and to prevent the expanding agent from penetrating outside the cell structure. To evaluate the effect of coatings such as monoglycerol Stearate, Zinc Stearate and Calcium Stearate on reducing clumping, weight concentrations of 0.1, 0.3 and 0.5% of the above coatings, added to 50 grams of 300 and 400 grade polystyrene samples. A total of 18 samples, numbered from 1 to 18, were completely subjected to clumping test (lumping test). All samples were prepared at the same time and kept under the same conditions. Samples 6, 12 and 13 showed the best result (A) from a lumping point of view. Zinc Stearate and Calcium Stearate showed the best results and Glycerol mono Stearate showed the worst results. To investigate the effects of pentane shelf life as a foaming agent inside the expanded polystyrene cell structure, gas chromatographic test of superior samples of clotting test (6, 12 and 13) was used. This test was repeated for all three samples after 40 days from the time of sample preparation and then 65 days after sample making. The results of this test showed that Zinc Stearate in grade 300 expanded polystyrene showed a weaker result compared to the effect of both coatings of Zinc and Calcium Stearate in grade 40. The results were reported after the above period for samples 13, 12 and 6 as 5.58, 4.57 and 4.116 wt%, respectively.

Keywords: Expansion Polystyrene, Coating, Agglomeration, Electrostatic, Pre - Expansion

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A Narrative and Proficient MOF Catalyst of Gold-Nanoparticles-Decorated Epichlorohydrine@Poly dopamine functionalized UiO-66-NH_2 as a novel and efficient MOF-Catalyst for A^3-Coupling recation

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In this study, the new, efficient, and stable strucfture of Uio-66-NH_2@ECH@Poly dopamine@Au-NPs reported as a heterogeneous catalyst promoting A^3 coupling reactions process under mild conditions. Reaction products were obtained with a high yield percentage. Obviously, Au is effectively stabilized with high stability. Eventually, this Au-MOF-catalyst can effectively prevent Au leaching, which is attributed to the exiting joints. Also, analysis of the recycled catalyst was performed after each reuse cycle to evaluate the amount of Au leaching.[1-2] In addition, the Au elution determined by ICP analysis after six recycles was negligible. This research is motivated by excellent results, tried to evaluate and ability to fully measure and identify the newly synthesized MOF-Catalyst as UiO-66-NH_2@1-Chloro-2,3 epoxy- propane@polydopamine@Au-NPs using UiO-66-NH_2 by cross-linking of epichlorohydrine, polydopamine and stabilization of Au-nanoparticles on the above substarte to form a highly efficient and new green MOF-catalyst UiO-66-NH_2@ECH polydopamine @Au-NPs used as a heterogenous catalyst for promoting A^3 coupling reactions under mild reaction condition. The new synthesized heterogeneous catalyst was studied, identified and investigated using the analysis of various analyzes including XRD, FT-IR, TEM, FE-SEM, EDS-Mapping and ICP.

Keywords: Au-nanoparticles, UiO-66-NH_2, MOF, Polydopamine, A^3-Coupling reaction

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Fe_3O_4@SiO_2@DABCO as a Magnetically Separable Nanocatalyst for Highly Efficient Knoevenagel Condensation Under Clean Condition

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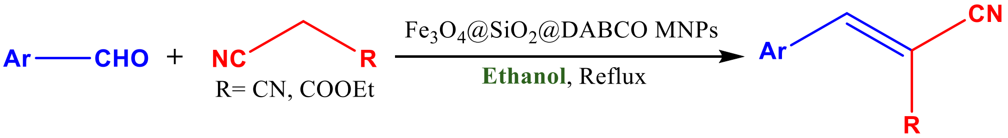
Recently, Fe_3O_4@SiO_2 supported heterogeneous catalysts was designed and widely used as traditional magnetically separated metal catalysis in the large variety of organic transformations, organocatalysi, and even enzyme catalysis. [1] Knoevenagel condensation is one of the most significant transformation for formation of C–C double bond in organic synthesis.[2] It carries out via the nucleophilic addition of an active methylene group to an aldehyde functional group followed by water loss. This condensation reaction is suitable for the proper synthesis of different structural alkenes that can be applied as intermediates in multiple reactions.[3] In addition, the Knoevenagel condensation can be utilized as a benchmark reaction to synthesize benzylidenemalononitriles (BMNs) and ethyl cyanoacrylates. BMNs have several properties in the pharmaceutical and biological fields including anti-cancer, anticonvulsant, anti-inflammatory and antioxidant activities.[4] Ethyl cyanoacrylate is used for gluing various materials. It is also used in medicine and polymeric industrial.[5] In this work, we wish to develop a new type of magnetic catalyst (Fe_3O_4@SiO_2@DABCO) that can be effective for Knoevenagel reaction. Therefore, the DABCO supported Fe_3O_4@SiO_2 nanoparticles was used as a novel and reusable nanocatalyst for the one-pot synthesis of benzylidenemalononitrile in water as a green solvent.

Keywords: Fe_3O_4@SiO_2@DABCO NPs, Organometallic catalyst, Nanocatalyst, Knoevenagel Condensation.



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A Convenient Synthesis of Functionalized Tricyclic Frameworks Containing an Azocine Moiety

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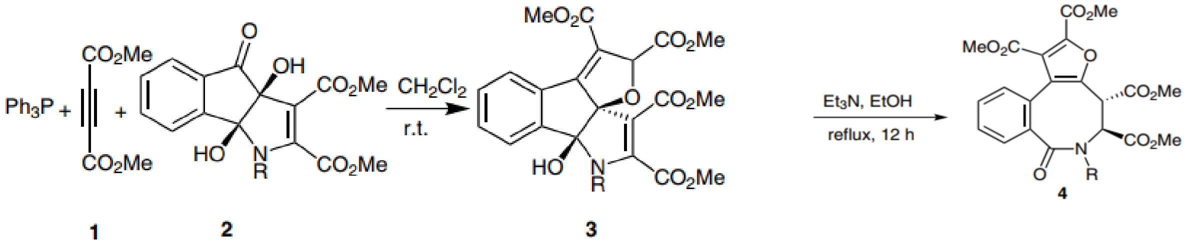
Tetrahydro-3a,8b-dihydroxy-oxoindeno[1,2-*b*]pyrroles, prepared from ninhydrin and enamines, are subjected to intramolec- ular Wittig reactions to afford dihydro-1*H*-furo[2′,3′:2,3]cyclopen- ta[1,2-*b*]pyrroles. These fused 5,5-ring systems undergo Et$_3$N-mediated fragmentation to afford tetrahydrobenzo[*c*]furo[3,2-*e*]- azocines in good yields.



Keywords: Acetylenic ester, Ninhydrin, Multicomponent reactions, Intramolecular wittig reaction, Azocine

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Nanofibrous electroconductive scaffolds based on poly(vinyl alcohol), polyaniline, and polythiophene for skin tissue engineering applications

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Tissue engineering (TE) has been suggested as a powerful alternative for conventional treatment approaches (*e.g.*, artificial prostheses, mechanical devices, and surgical repair) for regeneration or healing of damaged and failed tissue/organ [1]. This strategy combines molecular biology and materials engineering to develop biological substitutes consisting living cells, bioactive molecules, and scaffold. In this context, scaffold provide physicochemical cues for living cells for their adherence, proliferation, as well as differentiation. The most important features of a proper scaffold are biocompatibility, biodegradability, high porosity, proper hydrophilicity, and good mechanical properties [2]. Electrical conductivity has important role in some biological functions (*e.g.*, cell adhesion, cell migration, cell differentiation, and DNA synthesis) particularly for the electrically excitable cells, including osteoblast, myoblasts, and fibroblast. Therefore, electrically conductive polymers (ECP) such as polyaniline (PANI) is considered as a potential candidate to afford conductive biomaterials [3].

The aim of this study was to design and develop electrically conductive nanofibrous scaffolds based on poly(vinyl alcohol)-*grafted* polyaniline (PVA-*g*-PANI) for skin TE applications. For this purpose, PVA is functionalized with *p*-anthranilic acid in the presence of *p*-toluene sulfonic acid as the catalyst, and then aniline monomer is grafted to the functionalized PVA by an oxidative chemical polymerization method. The solutions of the synthesized polymers and pure PVA and fibrinogen natural protein were electrospun to produce uniform, conductive, and biocompatible nanofibers. Some physicochemical properties of these nanofibers such as morphologies, electrical conductivities, hydrophilicities, and mechanical properties were investigated. The cytocompatibilities of the fabricated nanofibers were confirmed by MTT and assessing the adhesion, using scanning electron microscopy (SEM).

Keywords: Electrospinning, Polymer scaffolds, Polyaniline, Poly(vinyl alcohol)

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Preparation and characterization of Fe_3O_4@SiO_2/APTPOSS core–shell composite nanomagnetics and their application in the one-pot synthesis of 4H-pyrans derivatives

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During the past few decades, magnetic nanoparticles (MNPs) have received a lot of interest owing to their unique features such as easy synthesis, good stability, low toxicity, high activity, efficient recovery, high surface area and facile separation from mixtures using an external magnet.[1] Meanwhile, MNPs (Fe_3O_4) can be used as a versatile support for functionalization of N-heterocyclic carbenes, metals, organocatalysts and chiral catalysts. Inorganic–organic hybrid polyhedral oligomeric silsesquioxanes (POSSs) have attracted much attention in recent years, due to their unique cage-shaped structures, nanometre-sized structures and easy chemical modification.[2] These hybrid nanoparticles have been used in several applications including drug delivery, dental materials, medical devices, anti-tumour agents, tissue engineering scaffolds, semiconductors devices, optical devices, binders for ceramics, catalysis and solar cells.[3]

It is well known that pyrans are important core units in a number of natural products and photochromic materials. Compounds with a pyran ring system have many pharmacological properties and play important roles in biochemical processes. Therefore, preparation of this heterocyclic nucleus has gained great importance in organic synthesis.

Octakis[3-(3-aminopropyltriethoxysilane)propyl]octasilsesquioxane (APTPOSS) as a polyhedral oligomeric silsesquioxane derivative was prepared and used as a reagent to obtain a core–shell composite using magnetic iron oxide nanoparticles as the core and the inorganic–organic hybrid polyhedral oligomeric silsesquioxane as the shell. Fe_3O_4@SiO_2/APTPOSS were confirmed using Fourier transform infrared spectroscopy, scanning electron microscopy, energy dispersive spectroscopy, dynamic light scattering, thermogravimetric analysis, X-ray diffraction and vibrating sample magnetometry. The inorganic–organic hybrid polyhedral oligomeric silsesquioxane magnetic nanoparticles were used as an efficient new heterogeneous catalyst for the onepot three-component synthesis of 4H-pyrans under solvent-free conditions. Moreover, these nanoparticles could be easily separated using an external magnet and then reused several times without significant loss of catalytic activity.

Keywords: 4H-pyran, Nanomagnetic, One-Pot Synthesis

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Functionalized HMS as efficient mesoporous catalyst for synthesis of tetrahydrobenzo[b]pyran and 1,4-dihydropyrano[2,3-c]pyrazole derivatives

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Mesoporous compounds are the most popular materials, due to their structural characteristics, such as high surface areas and pore volumes and have found variety applications, such as adsorbents, catalyst supports, drug delivery systems and biosensors [1]. Among theme, hexagonal mesoporous silica (HMS) with wormlike mesoporosity, uniform and narrow pore size distribution, high surface area and pore volume, short channel, thermal stability, easily synthesis and functionalization has found promising applications as a support for synthesis of heterogeneous catalysts [2]. Pyranopyrazole and benzopyran derivatives, have become important due to their pharmacological and biological properties such as anti-inflammatory, antioxidant, anti-bacterial, in perfumes and cosmetics and in food as additives [3,4]. The present study describes the synthesis, characterization, and investigation of catalytic activity of xanthine-Ni complex incorporated into functionalized HMS (HMS/Pr-Xa-Ni) in synthesis of tetrahydrobenzo[b]pyran and 1,4-dihydropyrano[2,3-c]pyrazole derivatives.

Keywords: HMS, Mesoporous, Pyranopyrazole, Benzopyran

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The incorporation of indometharin drug to 2-hydroxyethyl methacrylaten ethacrylate Hydrophile and hydrophobe copoly mers by esterification reaction and Study of itsreleasing in physiologic conditions

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Acrylic – type polymeric system having degradable ester bonds linked to indomethacin were synthesized and evaluated as materials for drug delivery[1]. The drug release of the polymer prodrugs of indomethacin (IND) was not only dependent on the property of the polymers but also dependent on the solubility of the prodrugs. Indomethacin was linked to 2-hydroxyethyl methacrylate by N,N-dicyclohexyl carbo imid to obtain metachryloyloxy ethyl indomethacin. The resulting acrylic derivative of indomethacin was copolymerized with 2-hydroxyethyl methacrylat and 2- hydroxypropyl methacrylate by free radical polymerization method in N,N-dimethyl formamid , utilizing benzoyl peroxide as an initiator at 70 °C[2]. The obtained polymeric prodrugs were characterized by various spectroscopy techniques. Gel permeation choromatography was used for determination of average molecular weights of polymers bearing drug units as side substituents of the acrylic backbone. Release studies of indomethacin were performed into dialysis bags by hydrolysis buffered solutions (pH=1 , 7 , 10) at 37 °C. Detection of hydrolysis by UV spectroscopy at selected interval showed that the drug can be released by selective hydrolysis of the ester bond at the side of drug moiety. The release profiles indicated that the hydrolytic behavior of polymeric prodrugs in strongly based on the hydrophobicity of polymer and the pH of the hydrolysis solution[3].

Keywords: Indomethacin, Polymeric, Prodrug, Hydroxyethyl, Polymer.

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Synthesis novel 1,3,4-thiadiazoles with homotaurine moiety

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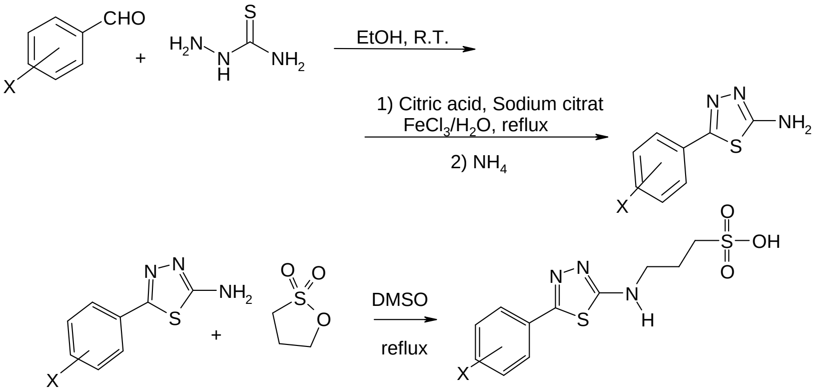
Heterocyclic compounds are one of the most exciting groups in organic chemistry. Due to the multiple benefits of heterocyclic compounds, they have always been considered by chemists, and they have become the subject of various investigations[1,2]. Among the wide world of heterocyclic compounds, 1, 3, 4-thiadiazoles are attractive groups of heterocyclic compounds. Thidiazole rings are bioisosteres of pyrimidines and oxadiazoles[3].In this work, we synthesized 1,3,4- thiadiazole derivatives with a homotaurine chain. Due to the mesoionic character of heterocyclic parts in newly synthesized molecules, it is expected that they can have biological activity[4]. The first reaction was the addition reaction between thiosemicarbazide and various phenyl aldehyde. Then in the presence of $FeCl_3$, the thiosemicarbazone has a cycloaddition reaction and forms the 1,3,4-thiadiazole ring. The resulting product attacks to1,3-propane sultone as a nucleophile in the next step.



Keywords: 1,3,4-thiadiazole, heterocycle, homotaurine

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Synthesis of magnetofluid containing metal oxides and their application in Suzuki and Heck reactions

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Due to the bulk state of solid compounds, they have a lower specific surface area than nanoparticles (NPs) and have low dispersion in solvents. Today, the synthesis of catalysts at the nanoscale has been used and this study focuses on the functionalization of magnetic (Fe_3O_4) NPs. Also, expected to this property, these particles orient in the presence of an external magnetic field. Most catalysts synthesized in chemical reactions are made with a binder, which prolongs the synthesis process, and the characteristic of the catalyst is that it does not have a binder. An active and heterogeneous Fe_3O_4-CuO nanocatalyst was synthesized using a simple method and inexpensive precursors. According to the importance of coupling chemistry in organic syntheses, the use of catalysts based on magnetic NPs has been considered. Finally, this catalyst was used in Suzuki–Miyaura reaction and also Heck–Mizoroki reaction which has shown good efficiency.

Keywords: Functionalization, heterogeneous catalyst, Suzuki–Miyaura reaction, Heck–Mizoroki reaction.

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A New Bis(NHC)-Pd(II) Complex Supported on Magnetic Mesoporous Silica, SBA-15, for Dehalogenation of Aryl Halides

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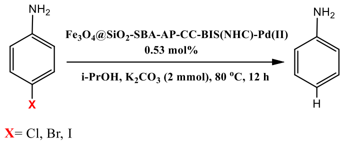
Dehalogenation of aryl halides, represents an important chemical transformation in organic synthesis. A plenty of dehalogenating systems have been developed for the reduction of haloarenes [1-2]. Herein, the synthesis and characterization of a new magnetic catalyst, e.g. SBA-AP-CC-bis(NHC)-Pd(II), have been reported. Magnetic SBA-15 was subsequently treated with (3-aminopropyl)triethoxysilane (APTES), cyanuric chloride (CC), imidazole, and 2-bromopyridine. The modified magnetic SBA-15 was then further reacted with separately prepared trans-[Pd(Cl)$_2$(SMe$_2$)$_2$] complex to give Fe_3O_4@SiO_2-SBA-AP-CC-bis(NHC)-Pd(II) as a supported bis(NHC) complex (Fig. 1). The obtained catalyst was characterized using solid ^{13}C NMR, X-ray diffraction spectroscopy (XRD), energy-dispersive X-ray analysis (EDS), and X-ray photoelectron spectroscopy (XPS). Atomic absorption revealed that the Pd content of the product is 2.83 %wt. (0.266 mmol/g). The supported complex was used in dehalogenation of aryl halides after finding optimal reaction conditions. The reaction parameters such as solvent, base, and catalyst dosage were optimized. The recycling experiments revealed that the magnetically retrived catalyst can be used at least in 7 consuective runs.

Keywords: Magnetic SBA-15, Supported complex, Dehalogenation



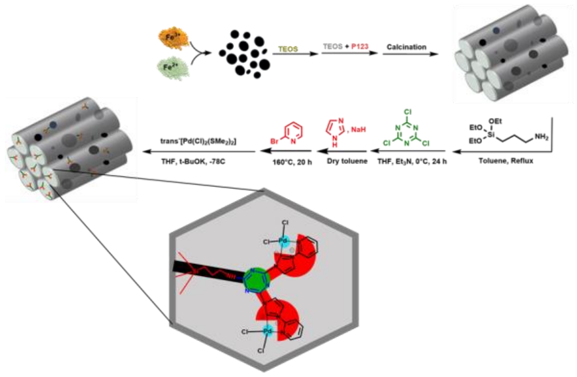


Fig.1: Synthesis of the Fe_3O_4@SiO_2-SBA-AP-CC-bis(NHC)-Pd(II)

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Multi-component synthesis of the 2′-aminobenzothiazolomethylnaphthols by using a new magnetic porous polymeric catalyst

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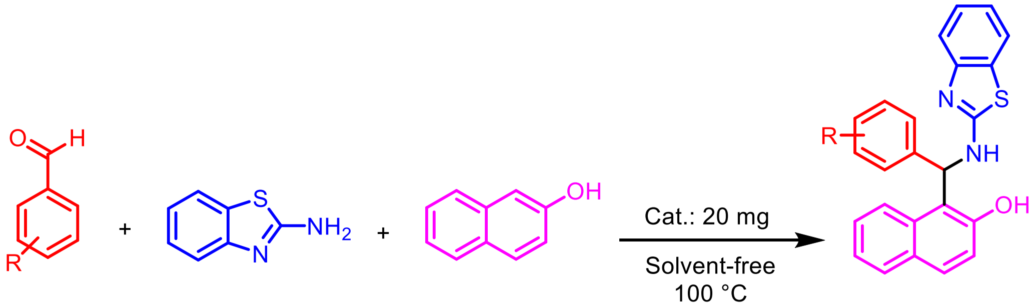
In chemistry, a multi-component reaction (MCRs), or multi-component assembly processes (MCAPs), are a chemical reaction which three or more compounds react together to form a single product. Multicomponent reactions have privileged properties such as selectivity, simplicity, high atom economy, synthesis of complex molecules, and efficiency of the protocol. This strategy is robust methods for the synthesis of pharmaceuticals and biological compounds and has a decisive role in polymer synthesis, supramolecular systems and etc. [1-2]. Polymeric systems due to theirs high reactivity, selectivity, recovering and reusability and adjustable shapes, have an excellent catalytic potential in multicomponent reactions. A major method for the synthesis of 2′-aminobenzothiazolomethylnaphthols is the multicomponent concentration of aromatic aldehydes with 2-aminobenzithiazole and *β*-naphthol in the presence of a catalyst. The resulting products represent widespread usages as pharmaceutical active structures [4-5]. Herein, a new porous polymeric catalyst was synthesized and used in the synthesis of 2′-aminobenzothiazolomethylnaphthols.



R= H, 4-Cl, 4-Br, 4-Me,
4-Isopropyl, 4-OH, 2-OH,
Pyridine-4-carbaldehyde,

Scheme 1: Synthesis of the 2′-aminobenzothiazolomethylnaphthols by using a new porous polymeric catalyst.

***Keywords*: Multi-component reaction, 2′-aminobenzothiazolomethylnaphthols, Polymer.**

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One-Pot Synthesis of 1,4-Dihydropyridines via the Catalyzed Hantzsch Three-Component Reaction by [Fe_3O_4@- SiO_2@$(CH_2)_3$-AP-SO_3H/HCl

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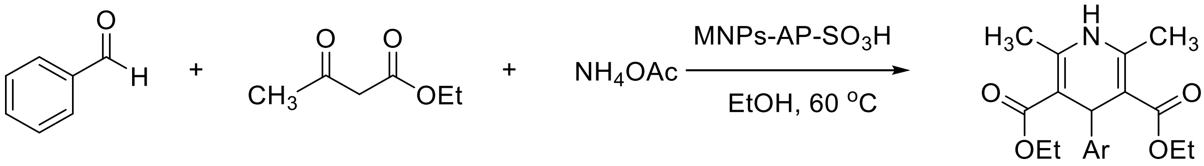
1,4-Dihydropyridine derivatives exhibit a large range of biological activities [1]. They have been used as anticonvulsant, antidepressive, antianxiety, analgesic, antitumoral, hypnotic, vasodilator, bronchodilator, and anti-inflammatory agents [2]. Some of them, such as amlodipine, felodipine, isradipine, lacidipine, and nifedipine, are drugs effective as calcium-channel blockers for the treatment of cardiovascular diseases and hypertension [3]. 1,4-Dihydropyridines are also good precursors of the corresponding substituted pyridine derivatives [4] and constitute useful reducing agents for imines in the presence of a catalytic amount of Lewis acid. Hantzsch first reported in 1882 the one-pot, three-component condensation of an aldehyde with ethyl acetoacetate (or 1,3-dicarbonyl compounds) and ammonia (or ammonium acetate) in acetic acid or refluxing alcohol [5]. We decided to explore the catalytic application of [Fe_3O_4@- SiO_2@$(CH_2)_3$-AP-SO_3H/HCl] as a magnetically recoverable solid acid catalyst in the synthesis of 1,4-Dihydropyridin derivatives, as portrayed in Scheme 1.



Scheme 1. The reaction between benzaldehyde with ethyl acetoacetate and ammonium acetate

Keywords: 1,4-Dihydropyridin, [Fe_3O_4@-SiO_2@$(CH_2)_3$-AP-SO_3H/HCl], Ethyl acetoacetate, Ammonium acetate

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(Copper ferrite nanoparticles catalyzed formation of β-Ketophosphonates via oxyphosphorylation of styrenes with H-phosphonates: A DFT study on UV–vis absorption spectra)

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Typical copper ferrite nanoparticles ($CuFe_2O_4$) were used as a catalyst for one-pot synthesis of β-ketophosphonates via the reaction of alkenes with H-phosphonates under conventional heating conditions.These compounds are important intermediate for the synthesis of many biological active compounds and natural products [1-3]. The catalyst was prepared by using the coprecipitation method and was analyzed by physiochemical techniques. By using this catalyst system, several types of useful and new β-ketophosphonate products were obtained in very good to excellent yields under optimized reaction conditions in a novel way. Furthermore, the catalyst is recyclable and reusable from the reaction.

Keywords: *Oxyphosphorylation, $CuFe_2O_4$, Styrenes, β-Ketophosphonates, Heterogeneous catalyst*

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Preparation and properties of biobased amphiphilic random polyurethane

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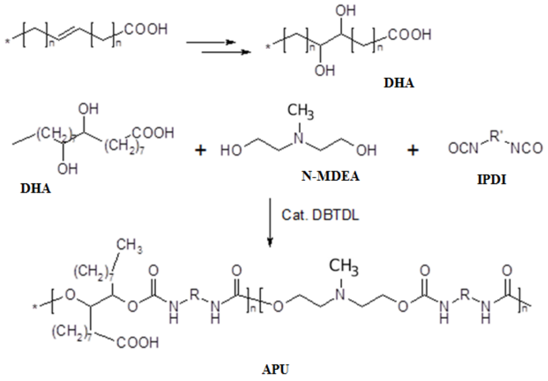
Biobased Amphiphilic Polyurethans (APU)s from renewable resources have been widely studied over the past decades[1]. APU can be synthesized via polycondensation reaction between diisocyanates and diols with lipophilic and hydrophilic constituents that are alternately or randomly distributed along the polymer backbone. Plant oils derived from sunflower, olive, palm, corn, canola, castor, soybean and linseed have a raw material used to synthesize PUs and a great potential to replace petroleum for the production of diols[2].
We have recently reported the preparation and characterization of a renewable, green and scalable dihydroxy acid from olive oil [3]. In this work, The biobased amphiphilic random polyurethane was prepared by the reaction of N-Methyl diethanolamine (N-MDEA), isophorone diisocyanate (IPDI), dihydroxy acid (DHA) and one drop of dibutyl tin dilaurate (DBTL) as a catalyst (Scheme1). The chemical structure of APU was ascertained by FT IR and ^{1}H NMR spectroscopies. APU showed self-assembled structures in aqueous media by direct dissolution method. The CMC value of the amphiphilic random polyurethane in aqueous solution were analyzed by fluorescence spectra using pyrene as a hydrophobic prob. Particle size and the morphology of nanoparticles of the APU were investigated by Dynamic Light Scattering (DLS) and Tranamitance Electron Microscopy (TEM), respectively. The results showed a narrow distribution with small particle diameters of nanoparticles and spherical shape.

Keywords: Amphiphilic Polyurethan, Biobased polymer, Self-assembly, Nanoparticles.



Scheme1: Structure of amphiphilic invertible polyurethane

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A Cu-Ni bimetallic magnetic nanocatalyst: a novel, efficient, magnetically and recyclable catalyst for Sonogashira reaction

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The Sonogashira C–C cross-coupling reaction is one of the most applicable types of C–C cross-couplings, which involves the coupling of vinyl or aryl halides or triflates with terminal alkynes (Csp^2–Csp) [1]; since its vital application for the construction of complex biological and pharmaceutical molecules from simple precursors, the Sonogashira reaction has had significant importance in the field of synthetic organic chemistry [2]. Various methodologies have been reported in the literature for the Sonogashira cross-coupling reactions catalyzed by nickel and copper, due to the lower cost and easy availability of these metals [3]. In recent decades, bimetallic catalysts as an important class of active catalysts have attracted much of attention in academic and industrial applications. The bimetallic catalyst procedure is different from single metal catalysts because both metals use special cycles that refer to transmetalation [4]. Stabilized catalysts on the surface of Fe_3O_4 NPs are noteworthy within the industrial applications because of providing the opportunity of precious metals recovery while capability for acceptable elimination of metal contamination in chemical and pharmaceutical products [5]. MNPs have high surface area that causes them to stick together and eventually agglomerate; therefore, they are usually covered with compounds such as silica. This modification allows for suitable functionalization of the NPs with various compounds to achieve a specific goal. In our study, we synthesized a magnetically recyclable Copper/nikel bimetallic nanocatalyst (Fe_3O_4@SiO_2/Cu-Ni) with high performance for the Sonogashira reaction.

Keywords: Bimetallic catalyst, Fe_3O_4@SiO_2/Cu-Ni, Heterogeneous catalysis, Sonogashira reaction

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Synthesis Novel N-substituted 1,2,4-thiadiazole derivatives

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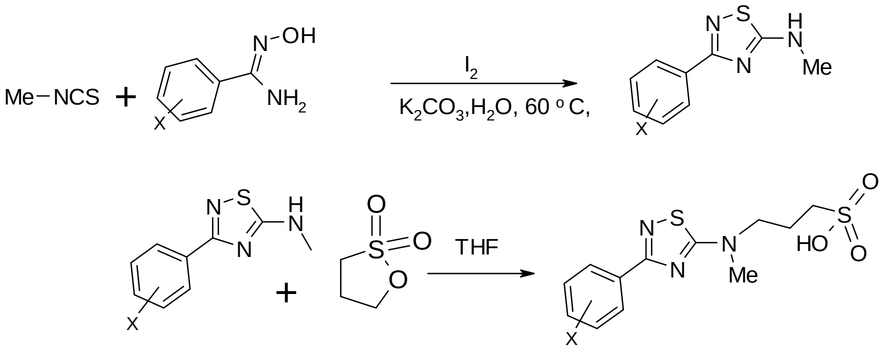
Sulfur-containing structural motifs can be fined in natural products, biologically active compounds, and synthetic intermediates. Consequently, 1,2,4-thiadiazole derivatives have varied biological and pharmaceutical properties, and the synthesis of new 1,2,4-thiadiazole derivatives has received considerable attention[1,2].

In this study, novel 3-(methyl(3-phenyl-1,2,4-thiadiazol-5-yl)amino)propane-1-sulfonic acid derivatives have been synthesized in excellent yield from N-methyl-3-phenyl-1,2,4-thiadiazole-5-amines and 1,3-propane sultone. 1,2,4-thiadiazole compounds have been synthesized from methyl isothiocyanate and N-hydroxy-benzamidine in the presence of I_2 as the catalyst[3]. The resulting products reacted with 1,3- propane sultone through the amine group as a nucleophile, and novel N-substituted1,2,4-thiadiazoles derivatives have been achieved.



Keywords: 1,2,4-Thiadiazole, Heterocycle, 1,3-Propane sultone

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Biginelli-type synthesis of new dihydropyrimidinones in the presence of a porous polymer functionalized Fe_3O_4 nanoparticles

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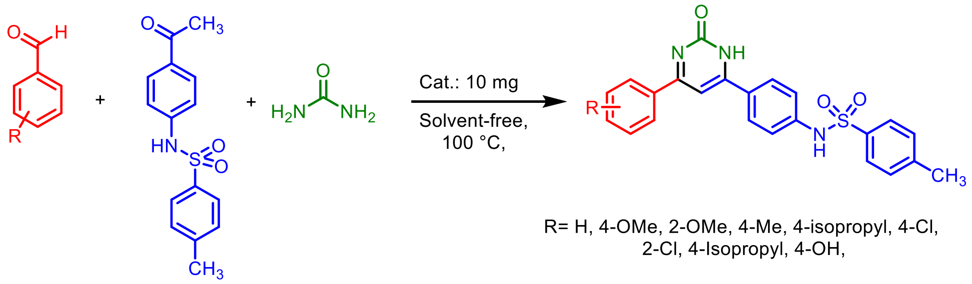
Design and synthesis of novel and efficient catalysts in organic transformations constantly is a developing trend and an attractive challenge in chemical reactions. This perspective is a promising approach among chemists. Heterogenization of organic catalysts by using solid supports is an attractive and benefit strategy for the design of novel and lucrative catalytic systems. Magnetic catalysts are one of the most important categories of heterogeneous catalysts [1-2]. As a sequence, Fe_3O_4 nanoparticles have excellent adjustable functionality, large surface area ratio, excellent magnetic properties and can be modified by many organic compounds. Hereupon, magnetic catalysts are applied in photocatalysis, chiral catalysis, oxidation reactions, photoelectrochemical catalysis, multicomponent reactions, enzyme catalysis and coupling reactions [3]. Dihydropyrimidinones as a prevalent family of *N*-heterocycle compounds have been incorporated in many areas of chemistry such as materials science, medicinal chemistry, chemical biology and chemistry of metal complexes of ligands. These materials have been created intensive progress in pharmacological researches [4-5]. In this study, we focused on the synthesis of Biginelli-type of dihydropyrimidinones in the presence of porous polymer functionalized Fe_3O_4 nanoparticles (Scheme 1).



Scheme 1: Synthesis of dihydropyrimidinones in the presence of porous polymer functionalized Fe_3O_4 nanoparticles.

***Keywords*: Dihydropyrimidinones, Fe_3O_4, Magnetic nanoparticle.**

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Magnetic copper oxide/polysaccharides bio-nanocomposite as a pH-sensitive and targeted 5- fluorouracil delivery vehicle

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To date, various nanocarriers have been designed and evaluated as an anticancer drug delivery system [1]. Among them the polysaccharide based nanocomposites are more favorable. Chitosan (CS) is a naturally cationic polysaccharide obtained from chitin with amino groups in its structure which is of great importance in biomedical areas due to its biodegradability and biocompatibility. Cross-linking of CS with κ-carrageenan (κ-Car) which is contain the anionic sulfate groups results in hydrogels with high mechanical strength and controlled drug release [2-3]. By concidering these, in this work, the basil plant extract was used for the biosynthesis of copper oxide nanoparticles (CuO NPs). Presynthesized magnetite was hybridized with CuO NPs (mCuO). After coating of mCuO with κ-carrageenan, the 5-fluorouracil (5-Fu) was loaded on it (mCuO bio NPs@Car/5-Fu). Finally pH-sensitive magnetic composite hydrogel was synthesized via physical crosslinking throuth the electrostatic interactions between κ-Car and CS (mCuO bio NPs@Car/5-Fu@CS). The chemical structure and morphology of synthesized mCuO bio NPs@Car/5-Fu@CS hydrogel were characterized by FT-IR, XRD, SEM, EDX, MAP and VSM analysis. Encapsulation efficiency showed a 72% of loading capacity. The in vitro release behavior of 5-Fu from mCuO bio NPs@Car/5-Fu@CS in pH 1.2 and pH 7.4 was investigated and most of the loaded drug was released gradually at acidic pH. Furthermore, the antibacterial activity of synthesized mCuO bio NPs@Car/5-Fu@CS was evaluated and the MBC and MIC values were determined. The antibacterial assessment confirmed the high antibacterial activity of CuO bio nanoparticles and synthesized hydrogel against *Staphylococcus aureus* (*S. aureus*) and *Escherichia coli* (*E. coli*).

Keywords: Green chemistry, Chitosan, κ-carrageenan, Magnetic CuO bio nanoparticles, Controlled release, Antibacterial.

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Copper Anchored onto Functionalized MCM-41 as a New and an Efficient Heterogeneous Nanocatalyst for the Synthesis of Benzothiazoles

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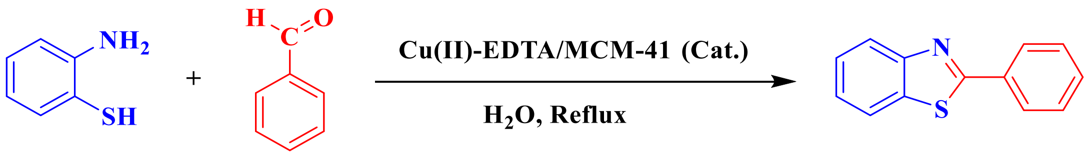
In the past decades, the use of heterogeneous catalysts as green, economic, and reusable catalysts has attracted much attention in industrial and academic purposes.[1] Benzothiazols are the most important structure of heteroaromatic compounds in organic chemistry[2] that are used to create drugs, for example antiulcer, antiviral, antibacterial, anti-diabetes, anticancer, antioxidant, and enzyme inhibition.[3,4] In this study, Mesoporous Si-MCM-41 was synthesized via Sol-gel method according to the literature way.[5] Hydroxyl (OH) groups of MCM-41 pore walls in MCM-41 can be functionalized with APTES by a silane coupling reagent which it introduces amine agent into the nanopores. Thus, MCM-41-APTES was functionalized with activated EDTA using thionyl chloride. Alternatively, the MCM-41@APTES@EDTA@Cu was also synthesized by immobilized copper complex on EDTA-functionalized nanostructured MCM-41. Then, we would report a facile method for the synthesis of benzothiazoles derivatives from aminothiophenol and various aldehydes catalyzed by using a novel heterogeneous nanocatalyst (MCM-41/EDTA-Cu(II)) as a highly efficient and reusable nanocatalyst in H_2O green solvent under reflux.

Keywords: Mesoporous silica, Copper, Benzothiazoles, Green reaction conditions.



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Cu-Ethylene glycol Complex Anchored onto Functionalized Si-MCM-41: as Promise, Reusable and Regioselective Nano-catalyst for Click Reaction

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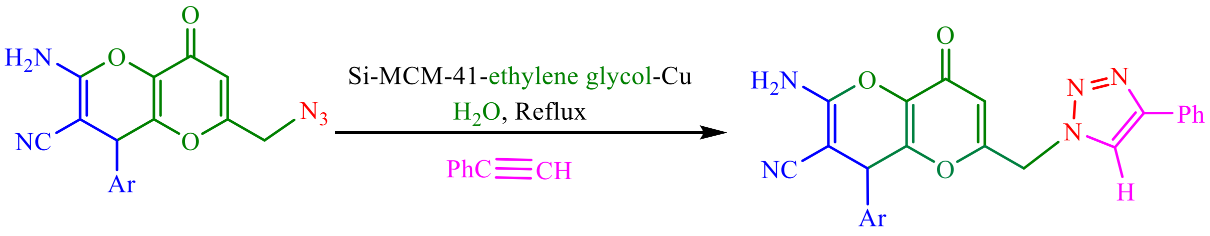
Mobile Crystalline Material (MCM-41) of the family M41S is constructed via a liquid templating mechanism and hydrothermal synthesis [1, 2]. They are an interesting molecular sieve for use in catalysis because of the large surface area, homogeneous pores, and good thermic stability. The properties of Si-MCM-41 are improved by incorporating other functional groups via deposition of active species on the internal surface of the material or the silica walls. Considering that the heterocyclic 1*H*-1,2,3-triazole compounds are structures with different features (chemical, technical and biological). Recently, the Click reaction between an organic azide and a terminal alkyne (CuAAC) has found many applications in organic synthesis [3, 4]. Thus, we became interested in the development of a simple, clean, eco-friendly, excellent yielding, and efficient method using a novel catalyst for the synthesis of triazoles. Based on this, the Cu^{II} complex on ethylene glycol-functionalized the nano Si-MCM-41 has been immobilized. Then, it is utilized as a good regioselective nanocatalyst in the synthesis of 1,4-disubstituted 1*H*-triazoles by Click reaction of various 2-amino-4-aryl-6-(azidomethyl)-8-oxo-4,8-dihydropyrano[3,2-*b*]pyran-3-carbonitriles with phenylacetylene in water as clean solvents.

Keywords: Si-MCM-41-ethylene glycol-Cu, Nanocatalyst, Click reaction, 1,2,3-Triazole.



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Anchored Ni- ethylene glycol complex in functionalized Fe_3O_4@Si-MCM-41 nanoparticles: magnetically new and effective heterogeneous catalysts for the clean synthesis of dicoumarols

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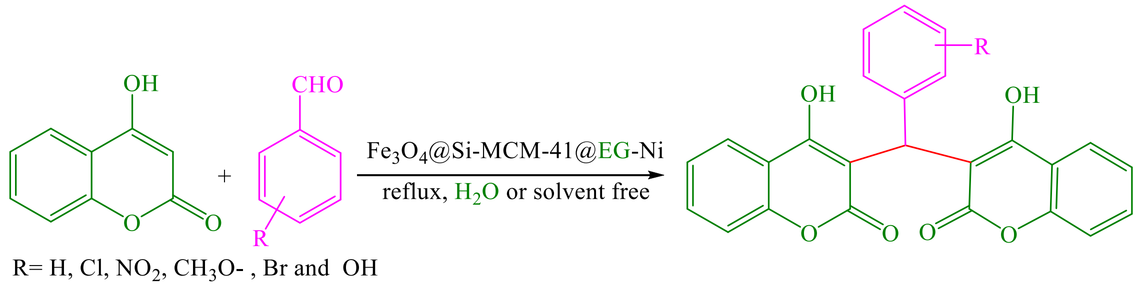
Recently, magnetite nanostructures have attracted much attention for researchers due to their small size distribution, being surface-functionalizable, stability, strong magnetic nature, low-cost synthesis features, biocompatibility, etc [1, 2]. Mesoporous silicate coatings can improve the features of magnetic nanostructures by preventing the aggregation of nanoparticles [3]. Dicoumarol is a natural function and anticoagulant like warfarin as a vitamin K antagonist. Many coumarols and coumarin derivatives have biological activities such as antioxidant, antifungal, antimicrobial, antibacterial, and antibiotic [4]. Hence, due to the importance of re-use and recoverability of solid heterogeneous catalysts, the development of new magnetic recyclable nanocatalysts is also desired [5]. Then, given our interest in studying the synthesis of heterocyclic compounds by using nanocatalysts. we became concerned with the synthesis, confirmatory characterization, and applications of Fe_3O_4@silica-MCM-41@Ethylene glycol@Ni as recyclable, solid, new, and magnetic nanocatalyst for the synthesis of dicoumarols via reaction of two equivalents of 4-hydroxycoumarin with one equivalent of aldehydes in water and also under solvent conditions.

Keywords: Fe_3O_4-Si-MCM-41-ethylene glycol-Ni, Nanocatalyst, Dicoumarol.



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Preparation of $NiCuFe_2O_4$ NPs and use as a reusable magnetic nanocatalyst for synthesis of xanthene derivatives under ultrasound conditions

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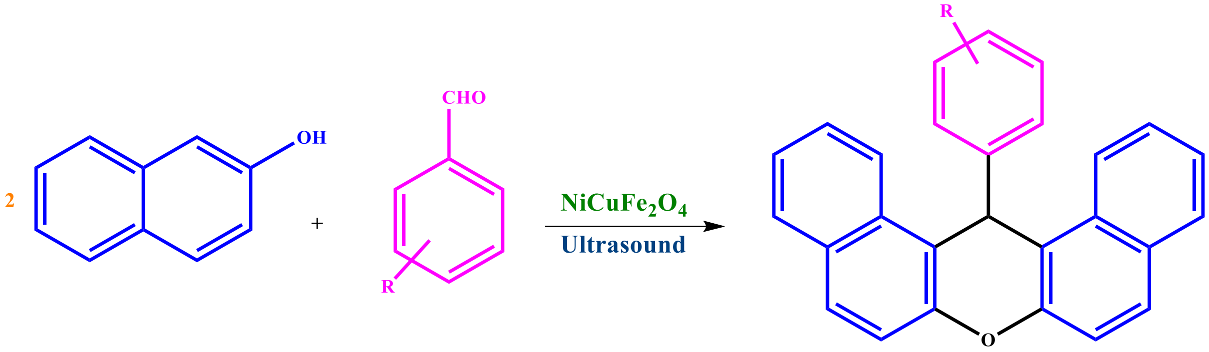
Von Bayer synthesized xanthene derivatives for the first time in 1871. 14-Aryl-14-H-dibenzo [a,j] xanthene derivatives are valuable and widely used in various industries. Because of their properties and biological activities, these compounds have different medicinal properties such as; antiviral [1], antioxidant, anti-tumor [2], anti-stress [3] and anti-hypertensive [4].

Many chemical processes can be performed using nanoparticle catalysis. Catalysts are often required for industrial-scale synthesis for optimal efficiency and effectiveness. The authors utilized $NiCuFe_2O_4$ to synthesize xanthene derivatives. The three-metallic catalyst used in this reaction enhances the yield of the reaction compared to one or two metal catalysts due to its synergistic effect. Also, optimizing the reaction under ultrasound conditions made these compounds reach faster, easier, and higher efficiency.

In this research, we hope to report the preparation of magnetic $NiCuFe_2O_4$ NPs and their application as reusable nanocatalysts to synthesize xanthene derivatives from the reaction of 2-naphthol with aldehydes under ultrasound conditions in high yields and short reaction times. The catalyst was characterized by FT-IR, XRD, SEM, EDX, and VSM techniques, and the obtained products were identified by FT-IR and ^{1}H NMR spectra.



Keywords: Xanthene, Nanoparticles, $NiCuFe_2O_4$, 2-Naphthol.

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Efficient synthesis of magnetic MCM-41 nanoparticles with zirconium complex and its application for C-S bonds formation

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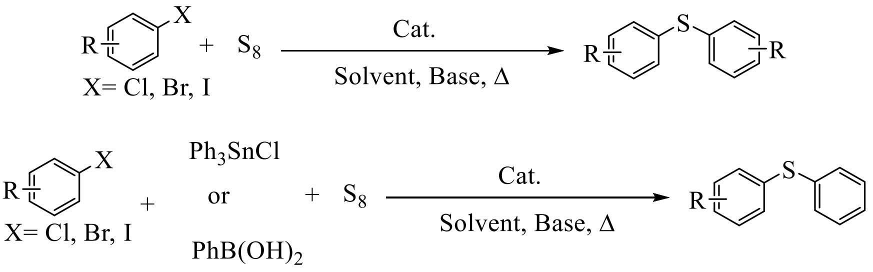
Nowadays, to combine the advantages of both homogeneous and heterogeneous catalysts, nanoparticles have been used as excellent and efficient supports as catalysts. Among the various nanoparticles, nanoporous MCM-41 has been widely used as catalyst in many organic reactions because of some unique properties such as high specific surface area (>1000 m^2/g), homogeneous hexagonal pore arrays (diameter 1.5–10 nm), relatively hydrophobic nature, ease of functionalization, large number of silanol groups that contribute to high catalyst loading, high thermal stability (900 ºC) and facile separation [1–2]. The C–S coupling reactions are of high importance in organic synthesis, the pharmaceutical industry as well as material science [3]. Sulfides are used as valuable intermediates in the production of several potent drugs for the treatment of Alzheimer's and Parkinson's diseases, diabetes, inflammatory and immune diseases [4]. We decided a new system for the synthesis of unsymmetrical and symmetrical diaryl sulfides in the presence of zirconium oxide-modified-MCM-41 as nanostructure catalyst (Scheme 1).



Scheme 1. Zirconium complex supported on magnetic MCM-41 nanoparticles for the synthesis of unsymmetrical and symmetrical diaryl sulfides

The advantages of prepared catalyst, is simple separation and reusable for several times without significant loss of its catalytic activity.

Keywords: Mesoporous silicas, Sulfide, Nanocatalyst

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Hybrid nanofibrous scaffolds for cutaneous tissue engineering: Preparation, characterization, and antibacterial properties

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Since polymeric nanofibrous scaffolds have been widely used in medical applications, the risk of bacterial contamination must be eliminated. In the present study, PCL/SESM/CS nanofibrous scaffolds were fabricated via electrospinning method for cutaneous regeneration [1]. The composition, Morphology, hydrophilicity, and mechanical features of prepared nanofibrous scaffolds were characterized using FTIR, SEM, water contact angle, and tensile tests. Besides, cell attachment and proliferation of BCCs and differentiation of BCCs toward keratinocyte-like cells were evaluated using MTT analysis. All results revealed that prepared nanofibrous scaffolds are good candidates for cutaneous regeneration. And could be used in further in-vivo uses .Finally, antimicrobial tests against three types of microorganisms (E. coli, S. aureus, and C. Albicans) were carried out according to the disc diffusion method. Antimicrobial test results proved that nanofibers containing chitosan show inhibition against S. aureus [2].

Keywords: Electrospinning; Antibacterial; chitosan; Tissue engineering

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An efficient catalyst-free synthesis of novel pyrimidoquinolines and spiroindoline pyrido-dipyrimidines

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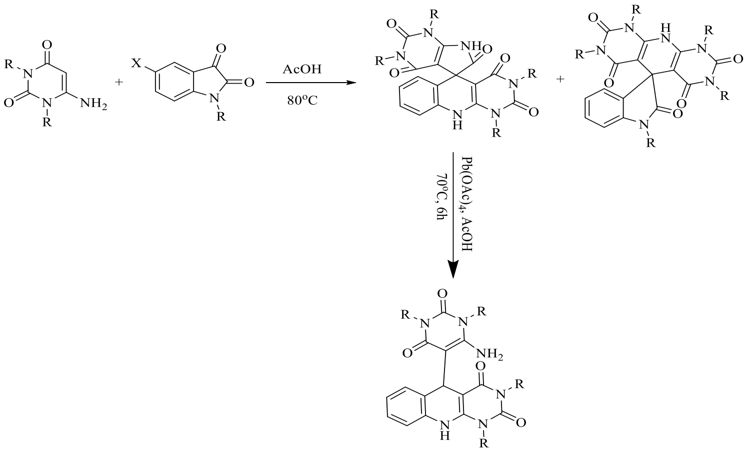
Due to their widespread biological and medicinal properties, N-containing heterocyclic compounds [1] specially isatin [2] and pyridopyrimidine [3] derivatives have received much attention in recent years and considerable efforts have been made to develop their synthetic methods in organic chemistry.

In this article, a number of spiro derivatives of pyridoxinoline and pyridopyrimidine were prepared from the single-dish, single-step reaction of aminouracil derivatives with isatin or substituted isatins on nitrogen atoms in acetic acid during 6 hours without using of catalyst. In the following, pyrimidoquinolines were prepared by treatment of them with $Pb(OAc)_4$ in the acetic acid. In addition to the simplicity of procedure, our method has appropriate reaction time, simple work-up, and excellent isolated yields.



Scheme 1: synthesis of pyrimidoquinolines and spiroindoline pyrido-dipyrimidines

Keywords: pyrimidoquinoline, Pyridodipyrimidine, 6-aminouracil, isatin

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Palladium (0)-functionalized magnetic MCM-41 nanoparticles: as an efficient and reusable catalyst for carbon-carbon bonds formation

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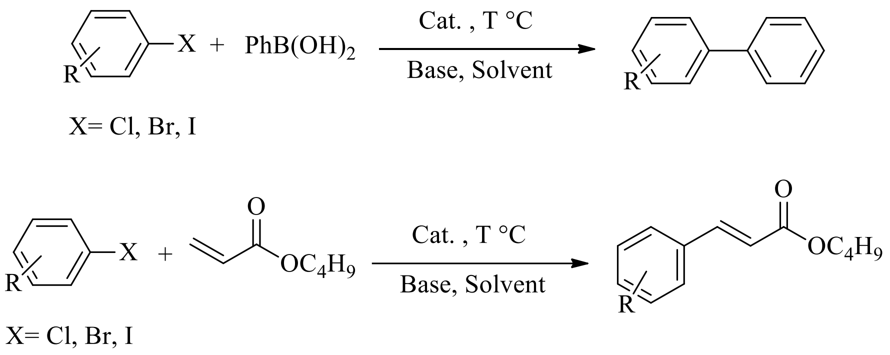
In 1992 mesoporous material was introduced by Mobil Oil Company researchers. In this class MCM-41 with hexagonal arrangement of the mesopores is highly grace through large specific surface area, presence of the spread network of uniform pores and pore volume [1]. Application of modified MCM-41 as a catalyst has advantages like high stability under severe condition such as high temperature and organic solvent and easy separation process [2]. Suzuki–Miyaura and Heck–Mizoroki cross-coupling reactions are versatile and important methods for C–C bonds formation in organic synthesis. These reactions have many applications in industrial processes such as the synthesis of natural products, organic building blocks, biologically active compounds, pharmaceuticals, and agricultural derivatives [3–4]. Herein, we report the formation of carbon-carbon bonds in the presence of a catalytic amount of palladium(0)-modified- MCM-41 (Scheme 1). In this method isolation and reusability of catalyst have been investigated.



Scheme 1. Palladium complex supported on magnetic MCM-41 nanoparticles for carbon-carbon bonds formation

The significant advantages of the designed system include simple and inexpensive procedure, eco-friendly, high stability, good to excellent yields of products in relatively mild conditions, and short reaction time.

Keywords: Nanostructure, Suzuki reaction, Heck reaction, Cross-coupling reactions

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Synthesis of Novel 2-amino-5-oxo-4-phenyl-4,5,7,8,9,10-hexahydrobenzo[4,5]thiazolo[3,2-*a*]pyrano[2,3-*d*]pyrimidine-3-carbonitrile via One-pot Three-component Reaction.

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Pyrimidine derivatives have properties that are potentially useful in combating diabetes. Pyrimidine derivative-containing heterocyclic compounds in combination with other moieties play several roles in biological processes and have significant chemical and pharmacological importance in the industry. In addition, pyrimidines in conjugation with a thiazole nucleus have gained prominence in medical and clinical applications. Thiazolopyrimidines have been gaining popularity in recent years for their outstanding use as components of pharmacological compounds such as bioavailable CXCR$_2$ antagonistand anti-diabetic agents, antimicrobial agents, antioxidants, anti-inflammatory agents, antimalarials, and antitubercular activities, antiviral, anti-Parkinson disease and anticancer agents [1].

Pyranopyrimidines are a class of heterocyclic compounds comprising a pyrimidine ring with two nitrogen atoms at "1,3-positions" fused to a pyran ring with one oxygen atom. Alternatively, pyranopyrimidine heterocycles have significant and confidential biological and physiological potency since this class of compounds demonstrated antibacterial, antitumor, antimicrobial, anti-inflammatory, antioxidant, antidiabetic, tyrosine phosphatase inhibitors, antitubercular, Hh signaling inhibitors in NIH$_3$T$_3$ cells, antihypertensive, antimalarial, antiviral, anticancer, and cardiotonic agents [2].

A new and efficient method for the synthesis of hitherto unreported 2-amino-5-oxo-4-phenyl-4,5,7,8,9,10-hexahydrobenzo[4,5]thiazolo[3,2-*a*]pyrano[2,3-*d*]pyrimidine-3-carbonitrile was developed via the Domino Knoevenagel condensatione Michael additione intermolecular cyclization sequences of aldehyde derivatives, malononitrile, and 6,7,8,9-tetrahydro-2*H*-benzo[4,5]thiazolo[3,2-*a*]pyrimidine-2,4(3*H*)-dione in PEG 400 as a green solvent.

Keywords: Multicomponent reactions, Thiazolo[3,2-*a*]pyrano[2,3-*d*]pyrimidine, Malononitril

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Synthesis of novel spiro[chromeno[2,3-d][1,3,4]thiadiazolo[3,2-a]pyrimidine-10,3'-indoline]-2',9,11-trione via three component reaction

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A new and efficient method for the synthesis of hitherto unreported spiro[chromeno[2,3-d][1,3,4]thiadiazolo[3,2-a]pyrimidine-10,3'-indoline]-2',9,11-trione was developed via the Domino Knoevenagel condensatione Michael additione intermolecular cyclization sequences of isatin derivatives, cyclohexane-1,3-diones, and 2-phenyl-5H-[1,3,4]thiadiazolo[3,2-a]pyrimidine-5,7(6H)-dione, employing 12-tungstophosphoric acid (H3PW12O40) as an effective and inexpensive catalyst.

Spirooxindole, a unique and versatile scaffold, has been widely studied in some fields such as pharmaceutical chemistry and synthetic chemistry. Especially in the application of medicine, quite a few compounds featuring spirooxindole motif have displayed excellent and broad pharmacological activities. Many identified candidate molecules have been used in clinical trials, showing promising prospects [1].

Thiadiazolopyrimidine derivatives are an important class of fused heterocyclic moieties with widespread biological effectiveness. The thiadiazolo-pyrimidine nucleus and its derivatives, belonging to the pseudo purine class, show interesting biological profiles, including antiviral, anticancer, antibiofilm, antitumor, antitubercular, antiglycation and antioxidant activities [2].

Keywords: Multicomponent reactions, thiadiazolo[3,2-a]pyrimidine-dione, Spirooxindole

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Preparation of new hybrid azabenzene systems in the presence of magnetic nanoparticles as catalyst

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Azabenzene, a simple six membered heterocycle containing one nitrogen (N) atom in the ring, has been found in a variety naturally occurring compounds, and in therapeutics such as niacin (nicotinic acid) and NAD^+ acting as a substrate or cofactor in biological processes [1]. Pyridines are attractive scaffolds for drug design and development. Many currently used anticancer drugs contain these privileged structures. Such anticancerdrugs acting at various drug targets were designed and developed [2]. Recently, a number of substituted pyridines have been synthesized and reported for their anticancer activities [3,4].

In this investigation, we synthesized some new hybrid azabenzene systems by the use of magnetic nanoparticles (Figure 1).

Keyword: Azabenzene, Hybrid azabenzenes, Magnetic nanoparticles, Pyridine systems,

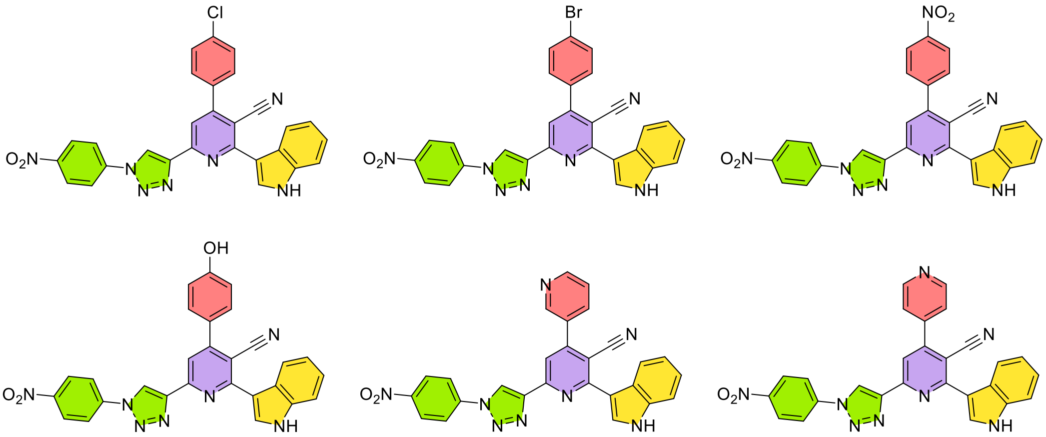

Figure 1: Synthesis of new hybrid azabenzenes in the presence of magnetic nanoparticles

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Vivid catalytic application of magnetic nanoparticles (MNPs) at the synthesis of linked imidazo[1,2-a]pyridine ring systems

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Magnetic nanoparticles have gained a great deal of attention from both academic and industrial point of view, owing to their unique properties including high surface area, and superparamagnetism, which enable them to be suitable for modification with many compounds and employing them as a catalyst in organic reactions [1].

Carbon-carbon and carbon-heteroatom bond-forming reactions are at the center of organic synthesis. Multicomponent cascade reactions have become a powerful tool in modern organic synthesis for the drug discovery processes [2,3].

Bridgehead nitrogen heterocycles are of interest because they constitute an important class of natural and unnatural products and many of them are useful as biological compounds [4]. Saturated and partially saturated imidazo[1,2-a]pyridine ring systems exhibit pharmacological properties such as antiviral [5], antimalarial [6] and antiulcer activities [7].

In this research, we have synthesis and take application of surface-modified magnetite nanoparticles as magnetically recoverable catalyst in the prepration of some novel imidazo[1,2-a]pyridine ring systems under mild and solvent-free condition.

Keyword: Imidazo[1,2-a]pyridine, Magnetic nanoparticles, Multicomponent reaction,

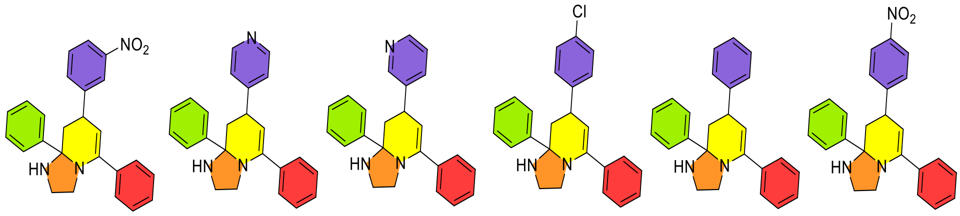

Figure 1: Synthesis of substituted imidazo[1,2-a] pyridines in the presence of magnetic nanoparticles

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Synthesis and antioxidant properties of benzylic acid derivative bromophenols including natural products

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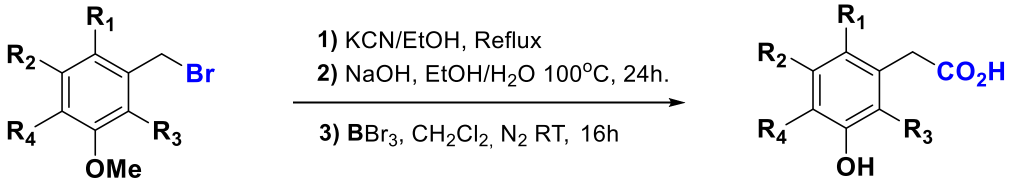
Natural bromophenols, commonly found in marine, have many biological activities such as antioxidant antimicrobial and inhibition effects on carbonic anhydrase enzymes. In addition to the natural benzylic acid derived bromophenols 6 and 7, their derivatives were also obtained by substitution, hydrolysis and demethylation reactions of the corresponding four benzyl bromides (Scheme 1).[1-4]



1 $R_1 = R_3 = H$, $R_2 = Br$, $R_4 = OMe$
2 $R_1 = R_2 = Br$, $R_3 = H$, $R_4 = OMe$
3 $R_1 = R_3 = Br$, $R_2 = OMe$, $R_4 = H$
4 $R_1 = R_2 = R_3 = Br$, $R_4 = OMe$

5 $R_1 = R_3 = H$, $R_2 = Br$, $R_4 = OH$
6 $R_1 = R_2 = Br$, $R_3 = H$, $R_4 = OH$
7 $R_1 = R_3 = Br$, $R_2 = OH$, $R_4 = H$
8 $R_1 = R_2 = R_3 = Br$, $R_4 = OH$

Scheme 1. Synthesis of bromophenols **6-7** and their derivatives

The antioxidant potentials of benzylic acid derived bromophenols were, for the first time, appraised by several outstanding bioanalytical methods. Besides these, we estimated the antioxidant effects were studied using by the methods of DPPH·, $ABTS^{\bullet+}$ scavenging activities, ferric (Fe^{3+}) and cupric (Cu^{2+}) ions and Fe^{3+}-TPTZ reducing capacities.

Keywords: Antioxidant activity, Bromination, Bromophenol, Radical scavenging, Natural product, Benzylic acid.

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2-[(2*E*)-2-(3-chloro-4-fluorobenzylidene)hydrazinyl]pyridine: Synthesis, Spectroscopic, Structural Properties and Theoretical Analysis

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Hydrazones are the condensation product of hydrazines or hydrazides with aldehydes or ketones. Some acid catalysts and techniques can increase the yield of this reaction [1]. Hydrazones are small organic molecules with the structure $R_1R_2C=NNH_2$, where R_1 and R_2 represent different substituent groups. Hydazones are easily synthesized compounds with sharp melting points and crystallize well. and can be used as valuable building blocks for synthesis of functional materials. Hydrazones can be used as important building blocks for synthesis of functional compounds in drug design. Because, the C=N double bond in hydrazone molecules act as ligands for metal complexes, organocatalysis and synthesis of organic compounds [2]. Hydrazones compounds are also very effective organic compounds in their own right. When hydrazones are used as intermediates for the synthesis of other substances, the -CONHN=CH- azomethine group plays an active role [3]. The chemical properties of hydrazone derivatives have been widely studied in many fields such as chemistry, technology and medicine for long years. Of these, studies in the biomedical aplications have become very popular in the last few decades.

In this study, hydrazone compounds, namely, 2-[(2*E*)-2-(3-chloro-2 fluorobenzylidene)hydrazinyl]pyridine (3C*l*4FH) thought to be used in medicine, technology and analytical chemistry was synthesized and single crystals of compound was obtained. The crystal structure of this compound was resolved with XRD method. Its structure was characterized using elemental analysis, FT-IR, ^{1}H-NMR, ^{13}C-NMR and UV–VIS spectroscopic methods. The substituent effect on their absorption spectra was explored. Optimized geometrical parameters were carried out by the density functional theory (DFT) at B3LYP method with 6-311++G(*2d,2p*) basis set. The theoretical and experimental results were compared and found to be in good agreement.

Keywords: Crystal structure, X-Ray diffraction, Spectroscopic analysis , DFT, Hydrazone

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C-C Coupling Reaction of Ketones with Alcohols in the Presence of Nickel Nanocatalyst

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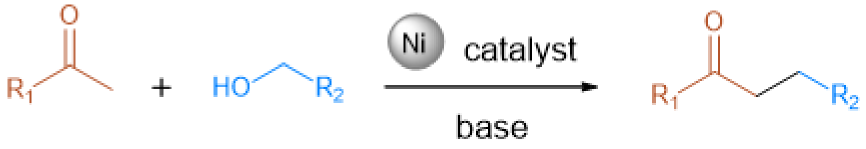
In the present era, metal-magnetic nanoparticles have been increasingly appreciated in hetrogeneous catalysis and organometallic chemistry owing to their easy preparation, low toxicity, and large surface area, supermagnetic power and high stability. The magnetic material Fe_3O_4 is able to separate from the reaction mixture by using an external magnet without applying the traditional filtration methods.[1,2] Carbon−carbon bond-forming reactions are fundamental in organic synthesis to synthesize complex and functionalized molecules from readily available substrates. The direct α-alkylation of ketones with alcohol, to synthesize important α-alkylated ketones and enones is an attractive procedure for C−C bond formation. On the other hand selectivity represents one of the most important issues for catalysis.[3] As α-alkylation of ketones with primary alcohols can produce two kinds of valuable chemicals, it will be interesting if product selectivity can be well controlled. Therefore, herein we report synthesis of nickel NPs, which is applied as effective, clean, good stability, and recoverable magnetic nanocatalyst for the synthesis of important C-C coupling reaction of ketones with alcohols.



Keywords: α-alkylation, ketones, primary alcohols, Heterogeneous catalyst, C-C activation

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Molecular dynamic simulations and quantum chemical calculations of adsorption dronic acid derivatives and hydroxyapatite

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Bisphosphonates are analogues of inorganic pyrophosphate. Some bisphosphonates, such like etidronate, clodronate and pamidronate, more than 40 years are being used clinically in the treatment of osteoporosis and malignant bone diseases such as Paget's disease, tumor-induced osteolysis, and are potent inhibitors of farnesyl pyrophosphate synthase. The main problem of these compounds is their little absorption after oral consumption; only a few percent of the dose is absorbed[1-4]. Therefore, the design and synthesis of new derivatives as a possible prodrug of etidronate seems very necessary.

In recent years, computational chemistry has obtained an important role in the design and analysis of new drugs with the help of existing software. Various computational methods have strongly reduced the time and cost of drug discovery [5]. In this study, some new dronic acid derivatives were designed and then the molecular docking studies and toxicity of designed ligands were evaluated. The proposed structures were designed in ChemDraw professional 17.1 software. The risk of toxicity, drug-likeness, solubility, TPSA, CLogP, and drug score was obtained by OSIRIS software for each of the structures. Then, the structures were transferred to MATERIAL STUDIO software to get geometric optimization. Next, molecular docking studies were performed using Molegro Virtual Docker software and the results were analyzed by Discovery Studio software. Due to the interaction of bisphosphonates with bone tissue, in this modeling study, hydroxyapatite crystals were used to evaluate the binding energy of bisphosphonates. The results were shown that the total energy of the system decreases when bisphosphonate adsorb on the surface. The negative binding energies were indicating that a good interaction was established between the bisphosphonate and hydroxyapatite.

Keywords: Bisphosphonates, Hydroxyapatite, Dronic acid, Molecular docking

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Synthesis of a new bionanocomposite hydrogel based on β-cyclodextrin - Metal-Organic Framework

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In recent years, metal organic framework have received much attention from researchers due to their special properties such as high porosity, large specific surface area, biocompatibility, adjustable and functionalizable structure, easy synthesis, special topology, high thermal and mechanical stability. Also β-cyclodextrin is a biocompatible polymer due to its properties, high adsorption capacity, ability to trap compounds in its cavities, the possibility of preparing functionalized polymers to increase the absorption and loading of drugs, excellent chemical stability [1,4]. In this study, β-CDCA polymer was synthesized using direct melt polycondensation method between β-CD and citric acid(CA) that was performed at an approximately temperature 200 °C and in the absence of organic solvents and harmful additives. The presence of carboxylic groups in the β-CD hydrogel network has been effective in adsorbing drugs, organic and inorganic pollutants. Then, a hydrogel nanocomposite containing a metal-organic framework was prepared insitu from the reaction between the β-CDCA polymer suspension with different amounts of $FeCl_3.6H_2O$ / terephthalic acid and then prepared by microwave irradiation. Their structures were characterized by Fourier transform infrared (FT-IR), X-ray diffraction (XRD) , thermal analysis (TGA), Dynamic Light Scattering (DLS), and SEM analysis. The effects of pH on the swelling ratio and adsorption properties of nanocomposite hydrogels were investigated.

Keywords: bionanocomposite, hydrogel, β-cyclodextrin, Metal-Organic Framework

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Preparation and characterization of functionalized GO@Fe3O4 nanocomposite and its application as catalyst for synthesis of naphthopyranopyrimidines compounds

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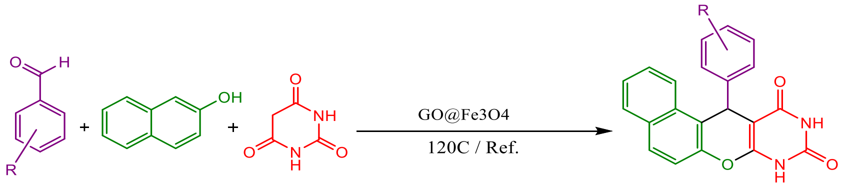
Presented protocol is a safe, eco-friendly and convenient method for the synthesis of benzochromenopyrimidines is described using a one-pot multi-component reaction of b-naphthol, 1,3-dimethylbarbituric acid, and various aryl aldehydes in the presence of GO@Fe_3O_4 nanocomposite, an effective and recyclable heterogeneous catalyst, under reflux conditions. Pyran and pyrimidines are present in a number of natural products and many synthetic compounds and have lots of medicinal properties and therapeutic applications [1,2]. Multicomponent synthesis of pyran and pyrimidine derivatives has been developed using a variety of catalysts such as $ZnFe_2O_4$@alginic acid[2], and MNPs@$NHC(O)CH_2CH_2PPh_2Py$ [3].

Pranopyrimidines possess an array of biological and physiological properties such as antibacterial, antifungal, antimicrobial, antitumor, analgesic, anticonvulsant, and antihypertensive [4]. GO is mechanically, electronically, and physically unique nanomaterial for a diverse domain of applications such as catalysis [5]. In case of catalysis, reaggregation of graphene based sheets is a major concern and lead to catalyst deactivation. For solving this problem, we suggested the addition of surfactant to exfoliate the GO sheets properly during the catalysis. Then, GO nanosheets were applied to support Fe_3O_4 nanoparticles (Fe_3O_4@GO) using co-precipitation method in the presence of GO sheets. This strategy led to formation of uniform particles of Fe3O4 on the surface of GO sheets.Preparation of catalyst was performed through a simple and convenient method and characterized using FTIR, FESEM, TGA and EDX techniques.

Keywords: benzochromenopyrimidines, GO nanosheets, nanocomposite, magnetic.



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Synthesis of tetrazole-based high energetic nitrogen-rich polymers

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High-energy substances are a group of substances with high stored chemical energy, which can release energy during a reaction. [1]. The new capabilities of tetrazole derivatives with high nitrogen content determine the great interest in polymers containing tetrazole rings. Poly (5-vinyl- (1H) -tetrazole) is one of the most attractive polymers containing the tetrazole ring. Due to its high internal energy, efficient and unique physical and chemical properties, polyvinyl-tetrazoles are the most important candidates among tetrazole polymers as a high-energy substance [2,3]. Also, high-energy tetrazole-based polymers produce more clean, low molecular weight N_2 gas as a combustion product due to their low carbon and hydrogen content. As a result, tetrazole-based energetic substances are green energetic substances that do not cause any harm to the environment [1]. In this work, in the first step, poly-5-vinyltetrazole was synthesized using polyacrylonitrile. The obtained polymer structure was confirmed by FT-IR, ^{1}H NMR, and ^{13}C NMR. In the next step, poly-5-vinyltetrazole salts were synthesized with ammonia, hydrazine, hydroxylamine, and aminoguanidine. The structure of the synthesized polymers was confirmed by FT-IR, DSC, TGA, and SEM, and their thermal stability was studied.

Keywords: Nitrogen-rich polymers; Tetrazole; Explosives; Energetic materials.

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Silica Nanospheres KCC-1 As A Good Catalyst for The Preparation of 2-Amino-4H-Chromenes by Ultrasonic Irradiation

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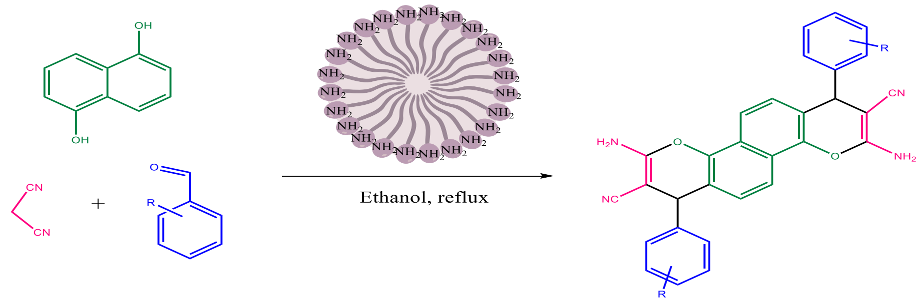
Chromenes have biological properties including anti-cancer, antivirus, antibacterial, antidiabete, antioxidant, antipyretic and anticonvulsant [1-3]. These properties make chromenes appealing goals in organic synthesis. In this work, we used KCC-1@NH_2 nanosilica as a basic catalyst for the preparation of chromenes under ultrasonic irradiation conditions for the first time. The recyclability, nontoxicity and high stability of the catalyst, combined with low reaction times and excellent yields, make the present protocol very useful for the synthesis of the title products under ultrasonic conditions. The produced products were confirmed via ^1H NMR, ^{13}C NMR, FT-IR analysis.

In the synthesis of fibrous nano-silica (KCC-1), we can control particle size, fiber density, surface area and pore volume of KCC-1 and tune by changing various reaction parameters, such as the concentrations of urea, CTAB, 1-pentanol, reaction time, temperature, solvent ratio, and even outside stirring time.[4] Furthermore, it is the fibrous morphology of KCC-1 that produces better accessibility of the active sites for enhanced catalytic activities and recovery efficiencies.[4] In this regard, we chose an easy, fast and green method for the synthesis of 2-amino chromenes with modified dendritic silica nanosphere (KCC-1@NH_2) by the ultrasonic route. Also, we managed to synthesize some new derivatives of 2-Amino-4H-Chromenes.

Keywords: Fibrous nanosilica, Spheres; KCC-1, Chromenes, multi-component.



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Molecular Structures, Biological Activities and Molecular Docking Studies of Halogenated Inositol Derivatives

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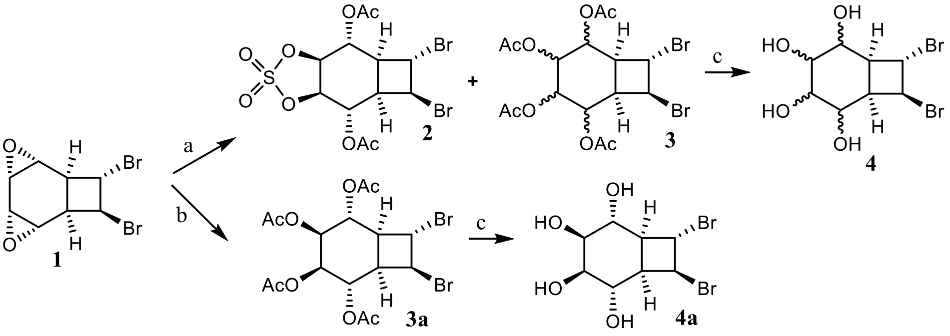
Cyclitols and their halogen derivatives have attracted attention, especially as building blocks for natural product synthesis [1]. The ring-opening reaction of the bisepoxide 1 led to cyclic sulfate 2 and conduritol (A, B and F) tetraacetate 3. The structures of tetraacetates 3 and cyclic sulfate 2 were established on the basis of 1D and 2D NMR spectra, X-Ray analysis and further supported by the IR and HRMS data as spectroscopic evidence. Removal of the acetate functionalities of conduritols 3 gave the expected tetrols pruducts 4 in almost quantitative yield (Scheme 1). The structure of conduritol-B tetraacetate, cyclic sulfate 2 and conduritol-A derivatives 4a has been confirmed by X-ray crystal structure analysis [2].

All compounds showed moderate antioxidant activity, they have a highly effective anti-inflammatory effect when compared to the standard drug ibuprofen. Also, we performed the molecular docking studies with cyclic sulfate and inositol on AChE and BuChE enzymes for therapeutic Alzheimer's patients and α-glucosidase enzymes for type-2 diabetes patients for enzyme inhibition. Cyclic sulfate has the best binding energies against AChE, BuChE and α-glucosidase enzymes compared to acarbose and galantamine drugs. Having the best binding energy revealed that their energies were -8.22 kcal/mol (AChE), -7.58 kcal/mol (BuChE), and -6.59 kcal/mol (α-glucosidase) [3].



Scheme 1. a) Ac_2O / H_2SO_4 b) *i)* H_2SO_4 / H_2O, 75 °C, 24h *ii)* AcCl / DCM, rt, 15h c) NH_3(g), MeOH

Keywords: Halogenated cyclitols, Anti-cholinesterase, Molecular docking

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Bio-synthesis and characterization of the magnetic iron nanoparticles using Mentha extract and evaluation of its antibacterial properties

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There are many medicinal plants in Iranian traditional medicine with significant therapeutic properties [1]. In recent years, the experiments have revealed that plants raise the cytotoxicity and anticancer potentials of iron nanoparticles (Fe NPs) against several cell lines especially tumor cell lines. Metal NPs have unique properties owing to their large surface area to volume ratio, a large fraction of surface atoms, surface energy, and crystalline nature with low imperfections and differ significantly from their respective bulk materials, Such unique properties have enabled them to be appropriate candidates for a variety of applications such as bio sensing , catalysis, drug delivery, food science, electrochemical sensing, water purification, nano device fabrication, agriculture, amongst others. Among the various biological sources, plant extracts are safe, easily available, biocompatible, and provide good control over morphology and resistance. Mentha is a plant determined by various pharmacological properties, such as antiviral, antibacterial, and antifungal activity [2-3]. By concidering these, in this work, the mentha plant extract was used for the bio-synthesis of Fe NPs and presynthesized magnetite was hybridized with Fe NPs (mFe bio NPS). The chemical structure and morphology of synthesized mFe bio NPs was characterized by FT-IR, XRD, SEM, EDX, MAP and VSM analysis. Furthermore, the antibacterial activity of synthesized mFe bio NPs was evaluated and the MBC and MIC values were determined. The antibacterial assessment confirmed the high antibacterial activity of Fe bio nanoparticles against *Staphylococcus aureus* (*S. aureus*) and *Escherichia coli* (*E. coli*).

Keywords: Green chemistry, Magnetic Fe bio nanoparticles, Antibacterial.

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High energetic nitrogen-rich polymers based on triazole; Synthesis and characterization

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The need for new high-energy material has led to the study of high-energy polymers. High-energy polymers are used as binders in propellants and explosives [1]. Nitrogen-rich compounds based on heteroaromatic rings with high nitrogen content are the leading high-energy materials in research. Triazine, heptazine, triazole, tetrazine and tetrazole are some of these heteroaromatic compounds with high nitrogen content. The important point about high-energy polymers based on heterocycle rings is that they are environmentally friendly. Heterocyclic ring-based energetic substances are known as green energetic substances, and when decomposed, release CO_2, N_2, and CO gaseous products [2-3]. Due to the increasing usage of these compounds, in this research work, some examples of nitrogen- rich monomers containing 1,3,5- triazine and tetrazole rings were synthesized by the reaction of aromatic nucleophilic replacement. Then the polymerization reaction on the monomers was carried. In the following the FT-IR, NMR, DSC, TGA analysis were performed, and also their thermal stability was studied.

Keywords: Green chemistry; Nitrogen-rich polymers; Triazine; Energetic materials.

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Ion-exchanged zeolite Y as a heterogeneous catalyst for synthesis of some derivatives of 1, 8-dioxo-octa-hydro xanthenes

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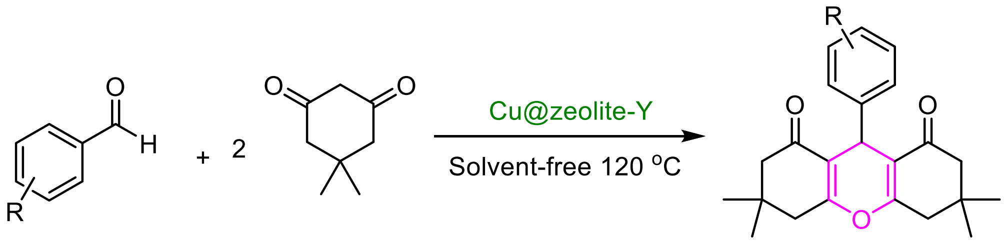
Xanthenes are important oxygen ring and its main application is in medicinal chemistry such as antibacterial, antiviral, anti-inflammatory and analgesic activities [1]. They are also used differently as dyes in lasers [2-3]. Zeolites are crystalline compounds that have a porous, spherical structure and large internal cavities composed of aluminum and silicate. Their origin is both natural and artificial [4].

In this paper, a simple method for the synthesis of some derivatives of xanthenes using ion-exchange zeolite Y with copper cation as heterogeneous catalyst was reported. Synthesis of xanthenes was performed using 2 mmol of dimedone and 1 mmol of aromatic aldehydes with 97 % yield. The catalyst used in this study is ion-exchange zeolite with metal ions, which due to having holes in its structure, has a high activity level that can increase the amount of product production and reduce its time. Ease of preparation, reusability, facile work-up, high activity, stability, applicability to a wide variety of substrates, and being cheap are the catalyst advantages.

Keywords: Xanthene, Heterogeneity, Zeolite Y, Catalyst



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Synthesis of substituted cyclohexanol derivatives

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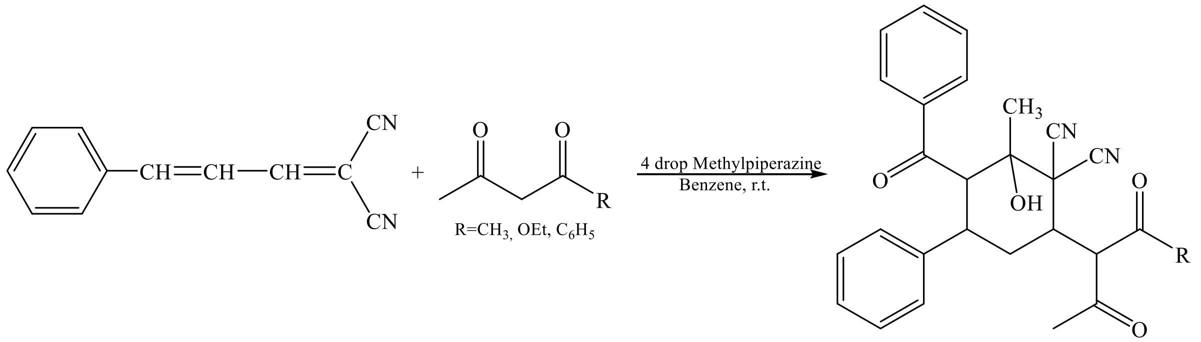
Michael C-C alkylation has an important role in the formation of cyclohexanol derivatives. In the literature, there are various synthesis methods for these types of compounds [1, 2]. Also, there are a lot of sources about the antimicrobial, antifungal, cytotoxicological and etc activities of cyclohexanol derivatives [3, 4].

Considering the above, by the Michael addition of various active methylene compounds to 2-(3-phenyl-allylidene)malononitrile in the presence of methylpiperazine catalyst in benzene medium, the synthesis of cyclohexanol derivatives has been carried out.



Structures of synthesized compounds confirmed by ^{1}H, ^{13}C NMR and X-Ray methods.

Keywords: malononitrile, benzoylacetone, methylpiperazine, Michael addition

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A convenient catalytic method for the synthesis of pyridines with henna and pyrazole moieties via a cooperative vinylogous anomeric-based oxidation

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In this work, $[Fe_3O_4@SiO_2(CH_2)_3][DABCO\text{-}H][C(CN)_3]_2$ was synthesized and fully identified by various techniques. Then, $[Fe_3O_4@SiO_2(CH_2)_3][DABCO\text{-}H][C(CN)_3]_2$ was used as a nanomagnetic heterogeneous catalyst for the synthesis of henna-based benzopyrazolo[3,4-*b*]quinolindiones *via* cooperative vinylogous anomeric based oxidation under solvent-free condition. This method tolerates most of the substrates and has the advantages of high yields, short reaction times, and eco-friendly. Moreover, some of these compounds are new and reported for the first time. Multi-component reactions show a significant role in chemical procedures due to their ability to produce complex molecules with high atomic economies and efficacy. They are also simpler than multi-step reactions and because they are achieved in one step, isolation of intermediates during the reaction is not required, so they can help to save time, and energy and diminish the use of organic solvents [1-3]. To enhance the functionality and impact of the method and to diminish the time, energy, and raw materials in chemical methods, the use of catalysts is recommended as one of the principles of green chemistry. One of the types of catalysts used in synthetic procedures is solid acids. These catalysts can be applied several times in chemical reactions. Also, nanomagnetic catalysts as a type of solid catalysts today attract much attention. These catalysts can be quickly collected and isolated from the starting materials and product by an external magnet to reuse used repeatedly. Lawsone (2-hydroxynaphthalene-1,4-dione) or hennotannic acid which has a red-orange color, is extracted from the leaves of the plant henna. Henna has been applied for dyeing skin, hair, fingernails, fabrics, silk, wool, and leather [4].

Keywords: Anomeric Effect; Heterogeneous catalyst; Nanomagnetic catalyst; Solvent-free;

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One-pot synthesis of sulfur-containing heterocycles through the reaction between alkyl cyanoacetates and carbon disulfide in the presence of propargyl bromide

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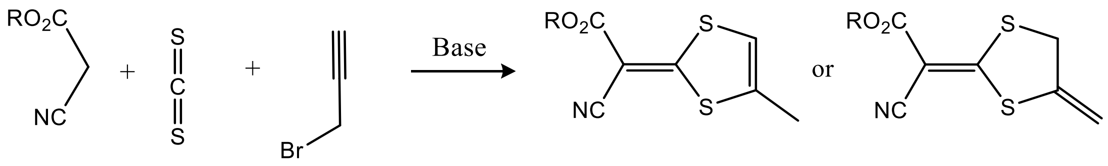
1,3-Dithiolanes bearing electron-acceptor substituents are applied in the synthesis of compounds with valuable optical and electronic properties. For this reason, searching for rational synthetic approaches to such 1,3-dithiolanes is an urgent problem [1]. Over the past few decades, a-oxo ketene (S,S)-acetals have been emerging as versatile intermediates in organic synthesis [2]. The sulfur atoms exercise a stabilizing effect on neighboring positive as well as negative charges, an extremely useful feature for organic synthetic purpcses [3].

In this project, we prepared a new derivatives of 1,3-dithiolanes through the one-pot reaction between alkyl cyanoacetate, carbon disulfide and propargyl bromide in the presence of a catalytic amount of base.

Keywords: 1,3-Dithiolane. One-pot reactions. Ketene dithioacetals.



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Synthesis of spiro[indolo[2,1-*b*]quinazoline-6,4'-pyrano[2,3-*c*]pyrazole]-5'-carboxamide

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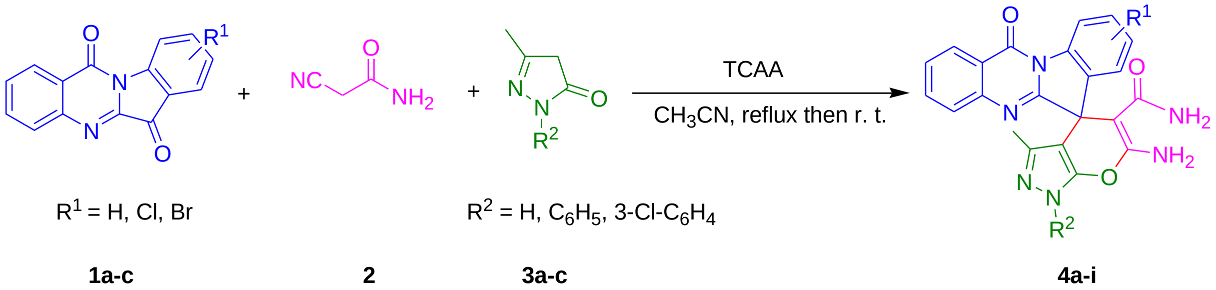
Pyranopyrazoles are known as important and functional heterocyclic compounds which have many applications in the field of medicinal chemistry. These compounds exhibit significant biological and pharmacological properties including antibacterial, anticancer, antiviral, anti-inflammatory, and human Chk1 kinase inhibitor activity [1-3].

Previously, we reported the synthesis of spiro[indolo[2,1-*b*]quinazoline-pyrano[2,3-*c*]pyrazole] compounds [4]. In continuation of the interest in the synthesis of these structures, we explored the synthesis of spiro[indolo[2,1-*b*]quinazoline-6,4'-pyrano[2,3-*c*]pyrazole]-5'-carboxamides through a reaction of tryptanthrins, cyanoacetamides and 3-methyl-pyrazol-5(4H)-ones in CH_3CN, using trichloroacetic acid (TCAA) as a catalyst (Scheme 1).



Scheme 1. Synthesis of spiro[indolo[2,1-b]quinazoline-6,4'-pyrano[2,3-c]pyrazole]-5'-carboxamides

Keywords: Tryptanthrin, Cyanoacetamide, 3-methyl-pyrazol-5(4H)-one.

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SYNTHESIS OF VINYL ESTERS OF SOME AROMATIC CARBOXYLIC ACIDS FROM VINYL ACETATE

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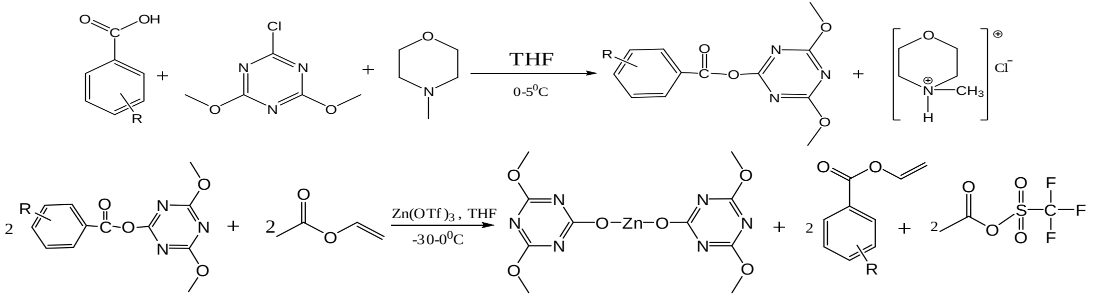
In this work the synthesis of vinyl esters of aromatic carboxylic acids with various substituents was carried out by the reaction of 2-chloro-4,6-dimethoxy-1,3,5-triazine with vinyl acetate in the presence of N-methylmorpholine and zinc trifluoromethylsulfonate ($Zn(OTf)_2$)), 3,3′-diphenylbinaphthalate dilitium (3,3′-Ph_2BINOL-2Li), tertiary potassium butylate ($KO^{tr}Bu$) and butylithium (BuLi). The influence of the nature initial reagents and temperature on the product yield was determined. From aromatic carboxylic acids 4-methoxybenzoic, 4-tert-butylbenzoic, 3,4-dimethoxybenzoic, 4-methylbenzoic, 4-fluorobenzoic, 2-bromobenzoic, 4-bromobenzoic, 3-trifluoromethylbenzoic, 3-nitrobenzoic, 4-nitrobenzoic, benzoic acids have been synthesized according to following scheme.



where: *I=C_6H_5COOH; II=$C_6H_5CH_2COOH$; III= 4-CH_3-$C_6H_4COOH_5$;*
IV=4-CH_3O-C_6H_4COOH;V=3,4-CH_3O-C_6H_3COOH; VI=2-Br-C_6H_4COOH; VII=4-Br-C_6H_4COOH,
VIII=4-F-C_6H_4COOH, IX=3-O_2N-C_6H_4COOH, X=4-O_2N-C_6H_4COOH, XI=4-$(CH_3)_3C$-C_6H_4COOH

Based on the results obtained, a series of activities of the reagents used in the synthesis of vinyl esters were established. It was found that the product yield increases in the following order: 3,3'-Ph_2BINOL-2Li/TGF<BuLi/TGF<$KO^{tr}Bu$/ TGF<$Zn(OTf)_2$/TGF was found. In this case an exchange reaction of vinyl groups has been carried out between the triazine active carboxylic acid ester and vinyl acetate. Since the formation of vinyloxy ion from vinyl acetate is a reversible process, than increasing of temperature leads to a decreasing the yield of vinyl ester [1].

At a temperature of -30 °C in the presence of the $Zn(OTf)_2$/TGF reagent, the maximum yield of vinyl esters are I - 69; II - 72; III - 75; IV - 82; V-74, VI-44; VII-60; VIII-66; IX-62; X-59; XI-78%. The yield of vinyl esters of aromatic carboxylic acids increases according to following raw: *2-Br-C_6H_4COOH < 4-O_2N-C_6H_4COOH < 4-Br-C_6H_4COOH < 3-O_2N-C_6H_4COOH < 4-F-C_6H_4COOH < C_6H_5COOH < $C_6H_5CH_2COOH$ < 3,4-CH_3O-C_6H_3COOH < 4-CH_3-C_6H_4COOH<4-$(CH_3)_3C$-C_6H_4COOH<4-CH_3O-C_6H_4COOH.*

Keywords: Vinylacetate, aromatic carboxylic acid, vinyl ester, 2-chloro-4,6-dimethoxy-1,3,5-triazine, N-methylmorpholine.

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One Pot and Catalyst Free Synthesis of Cis-dihydroxy-Indenopyrazolone

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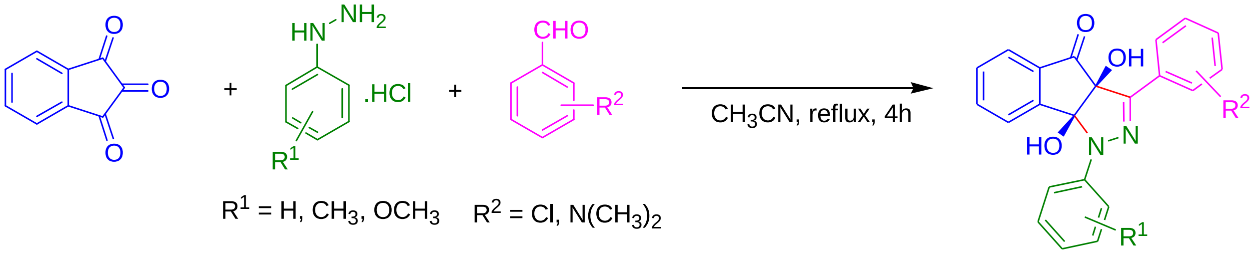
Cis-diol containing structures are an important class of compounds which have significant biological and clinical importance in bioanalysis and dye fields [1-2].

Pyrazolones and their fused derivatives, as one of the most important heterocyclic compounds, play an essential role in the medicinal chemistry and possess a broad range of pharmacological activities including anticancer, antiviral, and antibacterial [3-5].

Taking the advantages of these structures, bringing new enhancement properties, and increasing their medicinal performance, we are interested in the synthesis of cis-dihydroxy-Indenopyrazolone derivatives.

Herein, we develop the catalyst free synthesis of a series of functionalized cis-dihydroxy-indenopyrazolone derivatives through a reaction of ninhydrin, various arylhydrazin hydrochlorides, and different aldehydes in CH_3CN, under reflux condition (Scheme 1). This method benefits some advantages such as mild reaction condition, simple purification, and no chromatographic process which make it attractive.

Keywords: Arylhydrazin hydrochloride, Cis-diol, Pyrazolones



1 **2a-c** **3a-b** **4a-e**

Scheme 1. Synthesis of cis-dihydroxy-Indenopyrazolone derivatives

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One Pot and Catalyst Free Synthesis of Cis-dihydroxy-Indeno[1,2-d]imidazolone

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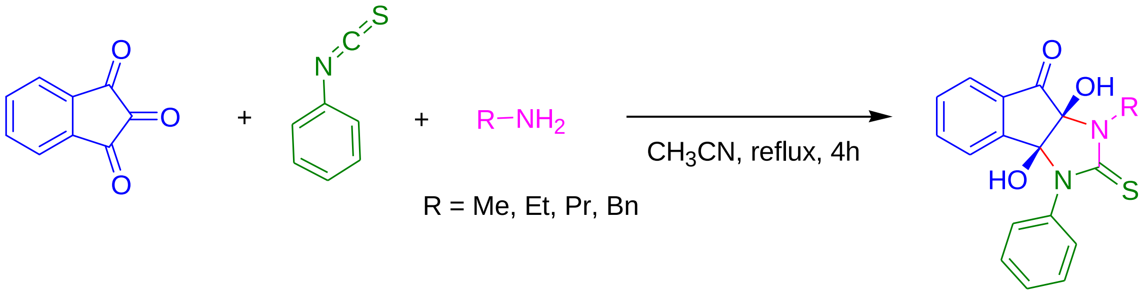
Imidazolone derivatives are found to be the most commonly used bioactive heterocycles. They are potent for their pharmacological and biological activities, as imidazolone-based drugs have a wide range of applications in many areas of clinical medicine [1-2].

On the other hand, cis-diol structures have important roles in different biological processes, including inter and intracellular signaling, molecular recognition, immune response [3-5].

Considering the importance of two above structures, we developed an efficient process for the synthesis of cis-dihydroxy-indeno[1,2-d]imidazolone derivatives. In this work, ninhydrine, phenylisothiocyanate, and aliphatic primary amines in CH_3CN reacted to obtain the corresponding products (Scheme 1).



1 **2** **3a-d** **4a-d**

Scheme 1. Synthesis of cis-dihydroxy-indeno[1,2-d]imidazolone derivatives

Keywords: Imidazolone, Ninhydrine, Phenylisothiocyanate.

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Vitamin B_3-SO_3H supported on magnetic nanoparticles as a green catalyst for efficient synthesis of *α*-aminonitriles

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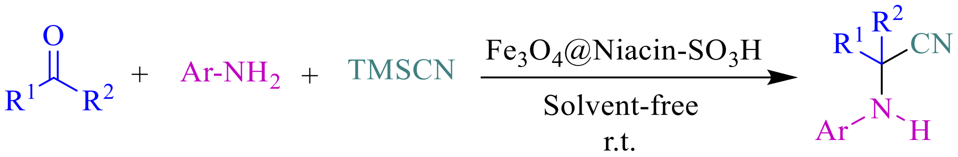
Organocatalysis has developed a new catalytic strategy in organic synthesis and the potential of this concept as a powerful tool is attractive in organic transformations [1]. *α*-Aminonitriles are among the most important units in organic transformations. They are useful intermediates in the synthesis of *α*-amino acids, nitrogen-containing heterocycles, amides, diamines, and various nitrogen-containing heterocycles such as imidazoles and thiadiazoles [2].

In this study, magnetic vitamin B_3-SO_3H nanoparticles (Fe_3O_4@Niacin-SO_3H) is prepared by grafting vitamin B_3 on Fe_3O_4 nanoparticles, followed by sulfonation, then characterized by XRD, EDX, FT-IR, SEM, and VSM. The catalytic activity of Fe_3O_4@Niacin-SO_3H is probed through Streaker reaction, where efficient green synthesis of *α*-aminonitriles is achieved under mild conditions. The classical procedure for their synthesis is treatment of an aldehyde or a ketone with amine in the presence of various cyanide sources [3,4]. This bio-catalyst is easily recovered and reused many times without significant loss of its catalytic activity.



Scheme 1. Catalytic synthesis of *α*-aminonitrile derivatives over Fe_3O_4@Niacin-SO_3H.

Keywords: Vitamin B_3, Streaker, *α*-aminonitriles, Magnetic Nanocatalyst

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Synthesis of Indenone Derivatives via Metal Free Double C–H Activation/Annulation Reaction of Aldehydes with Alkynes

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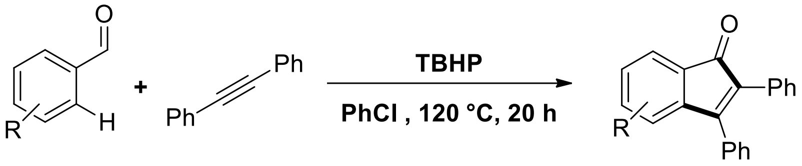
Because of the indenone frameworks importance in materials and medicinal chemistry, a great deal of efforts have been devoted to indenones synthesis thus far [1]. Considering the drawbacks of traditional and transition-metal catalyzed approaches, scientists have accepted the necessity of innovating new methods to yield indenones [2]. In recent years, there has been a growing interest in metal free synthetic strategies as a practical alternative to aforementioned methods [3].

In this study, a controlled radical reaction for indenones synthesis has been developed. The reaction proceeds via a metal free double C–H activation/annulation reaction of aldehydes with alkynes. Simple reaction process, wide substrate scope, and employing commercially available starting materials with no requisite for prefunctionalizations via an economically and environmentally benign procedure are the benefits of this strategy.



Keywords: Annulation, C-H activation, Metal free, Indenone, Radical oxidant

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Synthesis of triarylpyridine compounds by using phosphonium ionic liquid as catalyst via cooperative vinylogous anomeric based oxidation

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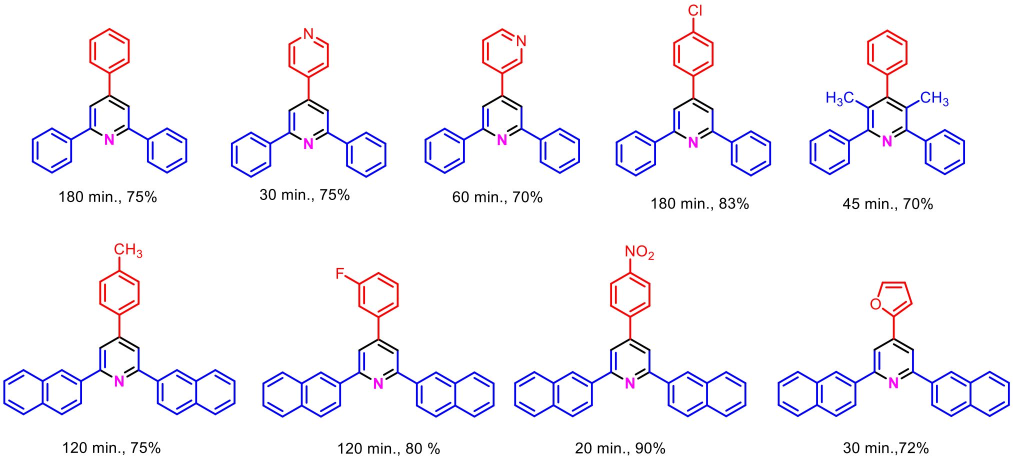
Ionic liquids (ILs) as one of the most important classes of chemical compounds, have attracted the great deal of interest. Many of researchers are engaged in exploration of exceptional properties of these versatile systems [1]. The cationic section of ILs have a key role in viscosity, solubility, melting point, density and other characteristic properties of ionic liquids. Among varied type ILs, phosphonium-based ionic liquid (PILs) due to its thermal and chemical stability and less viscosity in comparison of other ILs, have a tremendous attention. PILs have low cost and simplicity of synthesis and an excellent potential for diverse chemical processes [2-3]. Pyridine families are one of the most substantial building blocks of *N*-heterocycle compounds and are well known for any relevant chemistry researchers. For many years, these compounds by fantastic properties and diverse benefits, have garnered great attentions [4]. In this study, we focus on the catalytic application of phosphonium ionic liquid for the synthesis of triaryl pyridine systems (scheme 1).



Scheme 1: Synthesis of triaryl pyridines by using phosphonium ionic liquid as catalyst.

Keywords: Ionic liquids, Pyridine, Phosphonium ionic liquid.

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Investigation of the influence of Calix[4]arene on the performance of nickel oxide sensors to identify Ascorbic Acid

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Ascorbic acid is a biomolecular compound that exists in the human body, and due to changes in its amount in a healthy and sick person, it is necessary to measure its amount by a sensor. A sensor is made up of various components, one important part is metal oxide, which acts as a electrocatalyst, and another important part is the conductive organic molecule which cause increasing the sensitivity of the sensor. Calixarenes are supramolecular host molecules with versatile applications [1,2]. Otherwise, nickel oxide has high sensing power and is cheap and available. In this study, nickel oxide was synthesized under hydrothermal conditions using nickel cations and organic compounds like urea as precipitating agent. Calixarene was used as conductive compound of the sensor. Results showed that the sensitivity of this non-enzymatic sensor is favorable (Fig. 1) [3,4].

Keywords: Ascorbic Acid, Calixarene, Nickel oxide, Sensor

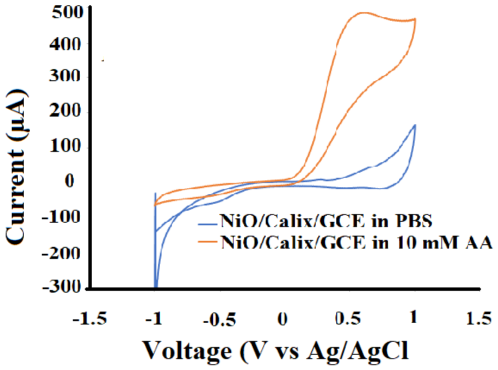

Fig. 1: CV of the NiO/Calix

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Investigation of Water Soluble Calix [4] Arene as an Adsorbent for the Removal of Acid Red 88 From waste Water

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Azo dyes are widely used in different industries such as: textiles, papers, printing and etc. Since azo dyes have toxic effect on living organisms and some of them are released into the environment via wastewater, it is necessary to remove these organic compounds from wastewater. The development of macrocyclic receptors, such as calixarenes made it possible to extract these dyes. Tetra sulfonic acid calix[4]arene has been used as an effective molecular host in adsorption of azo dyes in the aqueous environment. Firstly, para-tert-butyl calix[4]arene compound was synthesized. Then, ipso sulfonation reaction was carried out on para-tert-butyl calix[4]arene to give tetra sulfonic acid calix[4]arene . Sample characterization was performed by various spectroscopic techniques such as IR, ^{1}H-NMR and ^{13}CNMR. Since this compound has stable and inflexible cone conformation, it can be a suitable host in host-guest interactions. Acid Red 88 was used as absorptive guest to study complexation properties of the host molecule. Complexation was characterized by use of adsorptive spectrophotometric method. By comparison of the absorption intensity, the formation constants for SCX4/Acid Red 88 complex was estimated to be 5.2×10^{4}. The stoichiometric ratio of the complexes was determined to be 1:1 by use of Benesi-Hildebrand plots. All these results demonstrate a strong interaction between the host tetra sulfonic acid calix[4]arene and the guest Acid Red 88 (Fig. 1)[1,2,3].

Keywords: Azo dye, Calix arene

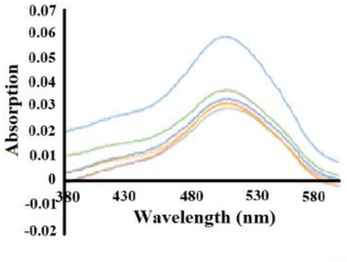

Fig. 1: Absorption spectrum of Acid Red 88

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Novel heterogeneous catalyst, copper acetylacetonate supported on 3-aminopropyl triethoxysilane functionalized halloysite (Cu $(acac)_2$/AMPTSi/ HNTs) for the synthesis of propargylamines

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Novel heterogeneous catalyst, copper acetylacetonate supported on 3-aminopropyl triethoxysilane functionalized halloysite (Cu $(acac)_2$/AMPTSi/ HNTs) for the synthesis of propargylamines.We have successfully synthesized a catalyst on halloysite nano composites as a very stable and recoverable nano-catalyst for the green production of propargylamines derivatives under solvent free conditions. The H-AP-Cu is an effective catalyst to be considered for A^3 -coupling reaction of Aldehyde, amine, and phenylacetylene to the following properties: nontoxic, perfect durability, reusability, shorter reaction time, and also excellent products yields. The MCRs are becoming significantly important in organic chemistry due to accessing wide range of structures from different components in a single step[1–3]. Among those MRCs, the A^3 -coupling of aldehydes, amines and alkynes has received considerable attention in recent years and known as an effective way to reach propargylamines derivatives, which are versatile key intermediates of biological and heterocyclic compounds and structures such as acrylamidines, oxazoles, and pyrrole.[4]

Keywords: copper acetylacetonate, on 3-aminopropyl triethoxysilane, nano-catalyst, A^3 -coupling

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A Simple and Environmentally Friendly Method for The Synthesis of Amides via the Reaction of the Corresponding Carboxylic Acids and Amines by Kaolin@Dextrin-Zn as Catalyst

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Due to the various applications of amides in various fields of research and industry, providing a green method with appropriate efficiency is considered.[1,2] Since the synthesis of amides has always been of interest to organic chemists due to their application in various industrial applications, researchers have helped to synthesize greener over time by providing better methods Many of the previous methods were inefficient and costly,[3] and we tried to use materials that were readily available in the composition of the catalyst, a new catalyst with an organic-mineral approach that, in addition to being effective and useful,[4] has a good percentage of efficiency and performance. We prepared a catalyst that is effective in performing amid reactions between amines and aliphatic and aromatic carboxylic acids. The accuracy of our catalyst synthesis was also confirmed using IR/SEM/TGA/EDX/XRD/TEM analyzes.

Keywords: Kaolin, Dextrin, Zn, Amidation

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Solubility and Phase Transfer of Poorly Organic Soluble Dyes in Organic Solvent by Amphiphilic Invertible Polyurethane Reverse Micelle

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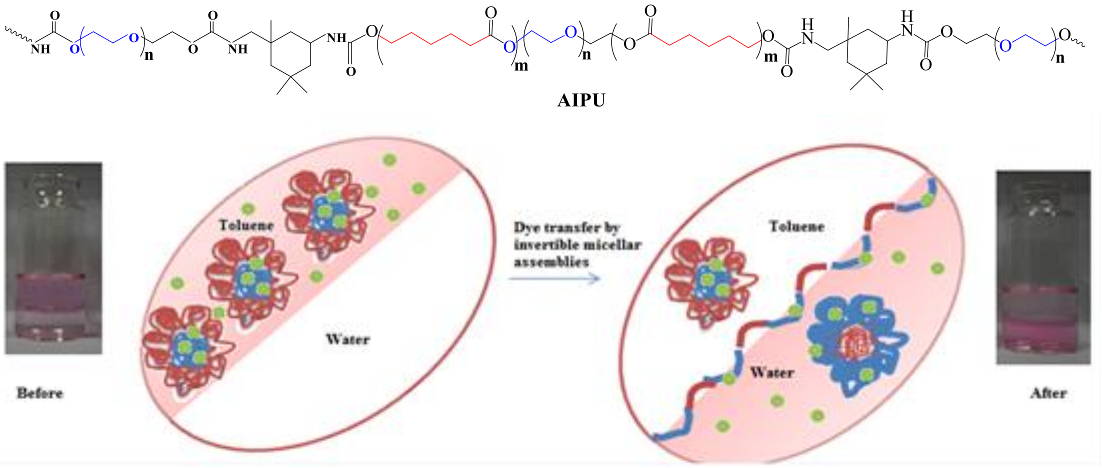
Amphiphilic invertible polymers (AIPs) are a new class of smart polymers with hydrophilic and hydrophobic moieties that their invertibility is considered to be a fast-conformational change of the macromolecules in response to solvent changes. They were mainly explored as systems for nanoencapsulation, phase transfer, nano-reactors and catalysis[1-4]. Their amphiphilic core-shell structure provides good solubilization for hydrophobic or hydrophilic guest molecules in their micellar structure in polar aqueous or nonpolar organic media, respectively [5]. We have recently reported a synthesis of amphiphilic invertible polyurethane (AIPU) with hydrophilic and hydrophobic moieties (Scheme 1). Such architecture can induce the polymer to behave like a micellar host in a nonpolar solvent. Hence, the self-aggregation and reverse micelle formation of the AIPU and the morphologies of the nanoparticles were investigated using dynamic light scattering (DLS) and field emission scanning electron microscopy (FE SEM). The ability of the copolymer to encapsulate, solubilize and transfer a hydrophilic molecule (Fuchsine was used as probe) through polar/nonpolar interface was evaluated.

Keywords: amphiphilic polymer, Invertibility, Self-assembly, reverse micelle, Nanoparticles.



Scheme 1: Structure of amphiphilic invertible polyurethane and conventional mechanism of delivery.

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Catalytic application of urea-functionalized magnetic nanoparticles in the synthesis of novel pyridine-triazole hybrids via an anomeric-based oxidation

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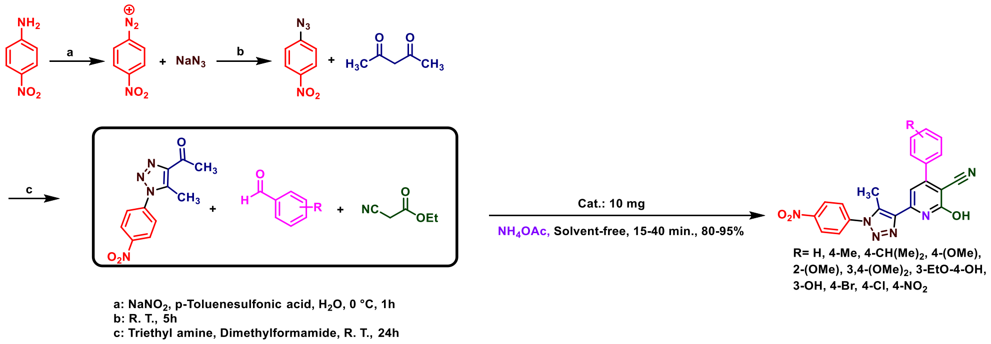
Magnetic nanoparticles have been studied in various fields such as medicine, drug delivery and catalyst due to their high potentials [1]. The most prominent features of multi-component reactions include good selectivity, high atomic economy, synthesis of complex molecules with the least possible by-product, simplicity and efficiency of the protocol. Multi-component reaction strategy has been able to provide powerful methods for the synthesis of drugs and biological compounds, polymers, supramolecular systems and molecular machines [2].

We used urea-containing magnetic nanoparticles as a highly efficient recyclable acid-hydrogen bond catalyst in the synthesis of new pyridine compounds. Catalyst characterization was performed using a variety of techniques, including FT-IR, ^{1}H-NMR, ^{13}C-NMR, EDS, FE-SEM, TEM, TGA, VSM, and elemental mapping analysis. Then the multi-component reaction is performed using catalyst under solvent-free conditions. This method has the advantages of high efficiency, short reaction time, mild reaction conditions for the synthesis of pyridine compounds and suitable recyclability.

Keywords: Multicomponent reaction, Nanomagnetic catalyst, Pyridine, Triazole, Vinylogous anomeric-based oxidation.



Scheme 1: Catalytic synthesis of pyridine derivatives *via* anomeric based oxidation process.

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Application of deep eutectic solvent-magnetic nanoparticles activated with urea derivatives as new catalyst for the synthesis of new hybrid pyridones

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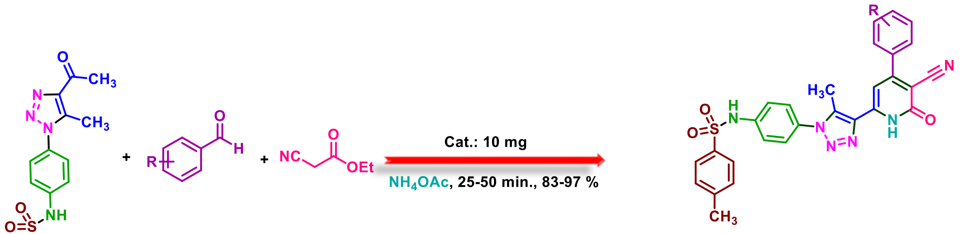
Magnetic nanoparticles are significant because of their wide range of applications as catalysts [1]. Also, deep eutectic solvents play a strong catalytic role in accelerating organic reactions including epoxidation, coupling reactions, and multicomponent reactions [2]. Multiparticle reactions are also common reactions for the synthesis of pyridone rings [3].

In this study, we used deep eutectic solvent-magnetic nanoparticles activated with urea-dithiocarbamic acid as an efficient and potent recyclable catalyst for the synthesis of new component hybrid pyridones. This catalyst was fully characterized using several techniques such as FT-IR, NMR, EDS, elemental mapping, FE-SEM, TEM, TGA/DTG and VSM analysis. Then, the application of this catalyst in the synthesis of new hybrid pyridones with sulfonamide and triazole sections was performed. According to the results, the reactions were performed under mild green reaction conditions with high efficiency.

Keywords: Anomeric-based oxidation (ABO), Deep eutectic solvent, Magnetic catalyst, Pyridone, Sulfonamide, Triazole.



R= H, 4-Me, 4-Isopropyl, 3-OH, 4-OMe, 2-OMe, $3,4\text{-(OMe)}_2$, 4-OH-3-OEt, Pyridine-4-carbaldehyde, Pyridine-3-carbaldehyde Thiophene-2-carbaldehyde, 4-Cl, 2-Cl, 4-Br

Scheme 1: Catalytic synthesis of pyridone derivatives *via* anomeric based oxidation process

References

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Ecofriendly and Fully bio-based Supramolecular Gel based on Cellulose Nanowhisker gallate by Cyclodextrin Host-Guest Chemistry

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In this research work, cellulose nanowhisker gallate (CNW-GA) in an aqueous solution and β-Cyclodextrin (β-CD) grafted on cellulose nanowhisker (CNW-g-β-CD) using toluene diisocyanate (TDI) as cross-linker were prepared. The mixture of CNW-GA and CNW-g-β-CD in an aqueous medium by sonication and mechanical agitation formed supramolecular hydrogel through host-guest interaction. The host-gust gel formation was approved using IR, XRD, EDX, and SEM techniques. Also, UV-Vis titration spectrophotometry confirmed successful complexation between gallic acid pendant groups with β-CD side groups. Moreover, it showed CNW-g-Ga compared to phenolphthalein gallate pendant groups has stronger host-guest interaction with CNW-g-β-CD proving and consequently could replace phenolphthalein with grafted gallate in β-CD cavity. Finally, the possibility of complex formation between β- CD and gallic acid was theoretically investigated. It was found gallic acid be able to complex with β-CD through its both head and tail

Keywords: Gallic acid. Cellulose nanowhisker. Cyclodextrin. Supramolecular gel

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Design and preparation $Fe_3O_4@SiO_2$-LT-Cu(II) nanocatalyst:A novel magnetic recoverable catalyst for the Biginelli reaction

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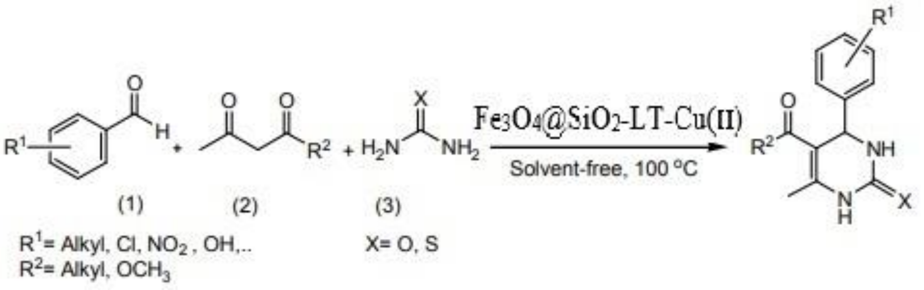
In this work, a new magnetically $Fe_3O_4@SiO_2$-LT-Cu(II) nanocatalyst was prepared from inexpensive starting materials [1]. A novel magnetic catalyst has been introduced. The prepared catalyst was fully characterized by various spectroscopic analyses such as XRD, SEM, FT-IR, VSM and EDX. After characterization, its activity was evaluated as a supported transition metal catalyst in the multi-component Biginelli reaction [2,3,5]. The novel catalyst acts as an efficient heterogenized catalyst for the synthesis of 3,4-dihydropyrimidin-2(1H)-one/thione derivatives in solvent-free conditions [1-5]. A wide range of biologically active dihydropyrimidin-2(1H)-one/thiones were synthesized in the presece of the novel catalyst in low time and high yields (Scheme 1). In addition, the reusability of catalyst was tested by an external magnet. Investigation showed that no notable reduction of yields was observed after reusing over ten runs, proving its stability over recycling processes.



Scheme 1. The Biginelli reaction between aromatic aldehyde, urea, and ethyl acetoacetate to synthesize dihydropyrimidinones (DHPMs)

Keywords: Biginelli reaction, Dihydropyrimidinones, Nanocatalyst Cu(II), Solvent-free

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Evaluation of antioxidant properties of supramolecular bio-gels of cellulose nanowhisker gallate and cellulose nanowhisker cyclodextrin in an aqueous medium

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Oxidative stress caused by free radicals is one of the most causes of many chronic diseases. The most important defense against free radicals is antioxidants. Gallic acid is one of the strongest and most effective natural antioxidants in plants [1]. However, biodegradable biopolymers such as cellulose and cyclodextrin are needed to take advantage of the antioxidant properties of gallic acid [2]. In this project, the antioxidant properties of gallic acid, cellulose nanowhisker gallate (CNW-GA), β-cyclodextrin grafted to cellulose nanowhisker (CNW-g-β-CD) and CNW-GA and CNW-g-β-CD supramolecules using UV-vis technique in aqueous solvent was investigated [3]. The results showed that by using DPPH radical as oxidant agent, the host-guest interaction of the CNW-g-β-CD with CNW-GA enhances the antioxidant properties of gallic acid [4,5]. The forming of bio-hydrogel was confirmed using IR, SEM, and XRD techniques

keywords: Antioxidant properties. Supramolecules. Host-guest interaction. Biodegradable polymers

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Synthesis of 2, 4, 5-trisubstituted imidazole derivatives in the presence of Lewis acid as catalyst in different conditions

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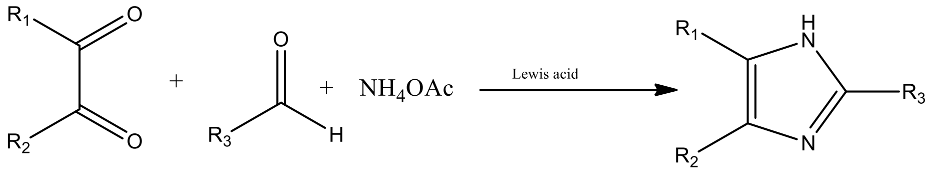
Imidazole derivatives are an essential group of ring compounds with many biological effects and pharmacological activities [1]. The structure of imidazole derivatives is a five-membered ring with two neutrons[2]. They are widely used in pharmaceutical compounds such as analgesics, anti-tumor, anti-inflammatory, pesticides, and fungicides. Various derivatives of triaryl imidazole are also used in photography[3]. Due to the toxic nature of many organic solvents, such as chloroform and carbon tetrachloride, it is suggested to design processes rooted in green chemistry[4]. The synthesis of 2, 4, 5-trisubstituted imidazole derivatives from the past until now has been done under different conditions and using various catalytic systems. As a new reusable and green heterogeneous catalyst, a lewis acid was used to synthesize 2, 4, 5-trisubstituted imidazole derivatives. As a new catalyst, we have performed several tests under different conditions to evaluate the catalyst's performance. Using benzyl derivatives, 1, 2-dicetone, aromatic aldehydes, and ammonium acetate salt, a multicomponent reaction in the presence of Lewis acid as catalyst leads to the one-pot synthesis of 2, 4, 5-trisubstituted imidazole[5], and after the work up derivatives of imidazole characterized by ^{1}H-NMR, ^{13}C-NMR and FT-IR. Short reaction time, simple workup, high yields, and environmentally friendly catalysts are advantages of this protocol. Lewis acid catalyst is prepared and characterized by FT-IR, XRD, SEM, TEM, XRF, EDS, and TGA. Using microwave, thermal, and ultrasonic methods to synthesize 2, 4, 5-trisubstituted imidazole derivatives shows the high efficiency of catalyst in different conditions.



Synthesis of 2, 4, 5-trisubstituted imidazole

Keywords: Trisubstituted imidazoles, Multicomponent reactions, One-pot synthesis, Green chemistry, Heterogeneous catalysis

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Tetrachloroperylene tetracarboxy dianhydride as a selective sensor for cyanide anion

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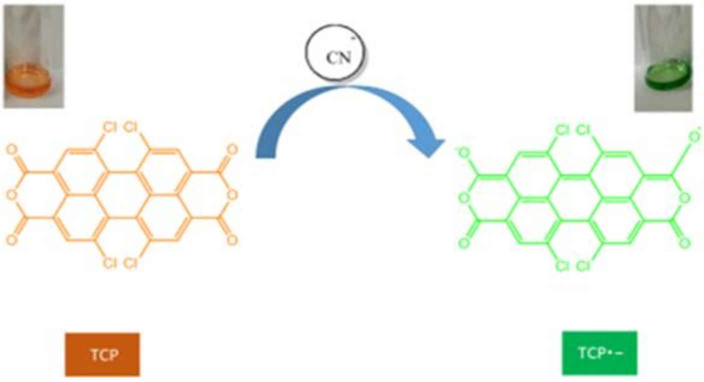
Currently, development of molecular probes for anions has been a subject of intense research interest, because more anions play important roles in biological systems and also constitute some pollutants in our environment [1, 2]. Cyanide is an extremely toxic anion and can affect many functions in the human body [3].

Herein, sensing utility of tetrachloroperylene dianhydride (TCP) and its diimide derivatives was investigated for CN^-. After characterization of the synthesized TCP and diimide derivatives, their chemical interactions in the organic medium with various anions were explored. Experimental and computational methods were used together to study the reaction pathway. TCP showed a rapid chromogenic response change to only cyanide anion between various anions. Single electron transfer from cyanide anion to TCP produces stable radical anion under ambient conditions with unique multidimensional signal radical anion that can be studied by various spectroscopic techniques.

Keywords: Electron transfer, Radical anion,Sensor,Cyanide



Scheme1: chromogenic response of TCP to cyanide anion.

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Synthesis of thiourea-peptoids via Ugi reaction in presence of Fe/MWCNT@TiO$_2$ nanocomposite az a heterogeneous catalyst

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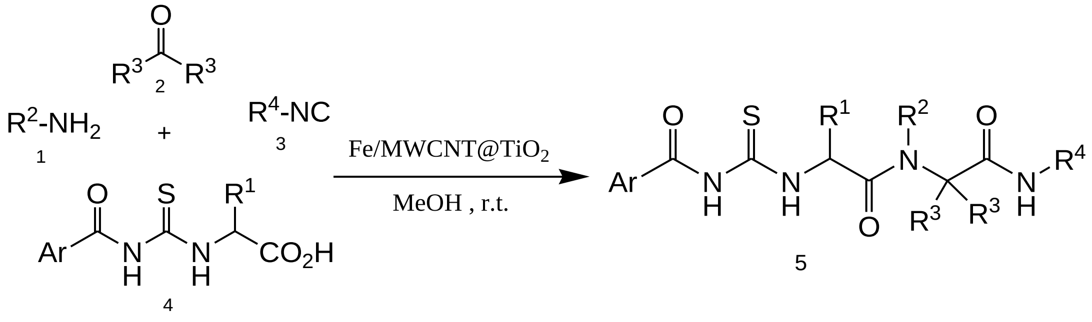
One of the important Multicomponent reaction is th Ugi four-component reaction, which is of considerableinterestowning to its exceptional chemistry [1-2]. Benzoylthioureidocarboxylic acids **4**, prepared from benzoyl chlorides, potassium thiocyanate, and α-aminoacids, are used as acid components in the Ugi reaction to produce thiourea-peptoids **5** in moderate to good yields [3]. In this research, preparation of a magnetic nanocomposite based on multi-wall carbon nanotubes (MWCNT) are described. This nanocomposite was prepared by immobilization of Fe_3O_4 nanoparticles on the nanotubes and then coating by TiO_2 nanoparticles through a sol-gel process. The activity of Fe/MWCNT@TiO$_2$ nanocomposite was evaluated in the synthesis of thiourea-peptoids.



Keywords: Ugi reaction, thiourea-peptoids, magnetic nanocamposite

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Synthesis and characterization of pyrimidine-based azo dye ligands and their metal complexes: photophysical and electrochemical properties

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Heterocyclic azo dyes are important chromophores which have received much attention due to feature favorable properties such as strong absorption in the entire visible region, chromic and photochromic properties bond to ion metals and etc [1]. Recently, Metal complexes of these dyes are considered to be important stereochemical models in transition metal coordination chemistry due to their preparative accessibility and structural variety [2].

In the present study, we designed and synthesized several samples of new pyrimidine-based azo-heterocyclic dyes as ligands. After coordination with an intermediate metal center, these ligands act as a dual chelating species with nitrogen atoms of the azo and oxygen atoms of the carbonyl fraction. In addition, benzoylation of one of the oxygen groups attached to the pyrimidine ring increases the electron-killing property of the ring as well as its absorption wavelength [3]. Also, the presence of oxygen carbonyl group to create a more stable complex than the oxygen attached to the pyrimidine ring, Which become shorter in the formation of the bond with the metal, have the ability to increase the wavelength and absorption intensity for the ligands. Structures were identified using various analysis techniques such as elemental analysis, IR spectrum and 1H-NMR.

Keywords: Heterocyclic azo dyes, Pyrimidine, Metal complexe, Benzoylation , Coordination chemistry.

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STUDY ON THE SYNTHESIS OF NOVEL ALKYLTHIO-PYRIDO[2,3-*d*]PYRIMIDINE DERIVATIVES

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The importance of functionalized pyridopyrimidines, a common source for the development of new potential therapeutic agents, is well known [1]. Furthermore, the replacement of the oxygen with a sulfur atom may induce changes in the properties of the nucleobases and the ability to stabilize the DNA [2]. Also, the thiouracil derivatives are of particular significance in medicinal chemistry due to their broad scope of remarkable antiviral, anticancer, and antimicrobial activities [3].

On the other hand, multi-component reactions as a creditable methodology have been developed for the synthesis of heterocycles in medicinal and combinatorial chemistry. One-pot character, construction of diverse structural scaffolds, fewer reaction and purification steps, high atom economy, quantitative yields of products, time and energy-saving are some pros of this procedure. Therefore, the application of this synthetic pathway in organic chemistry has been a matter of considerable interest [4].

Similarly, one of the major principles of green chemistry is the utilization of a set of principles that reduces or eliminates the use or generation of hazardous substances in the design, manufacture and application of the chemical products. Based on this fact, designing new methods by employing multi-component reactions (MCR) without using any harmful organic solvents is an essential need in the synthesis of pyridopyrimidine scaffolds [5].

In the present study, a novel method for the synthesis of 7-amino-5-aryl-4-oxo-2-alkylthio-3,4,5,8-tetrahydropyrido[2,3-*d*]pyrimidine-6-carbonitriles by a three-component reaction of 6-amino-2-alkylthio-pyrimidin-4(3*H*)-one, malononitrile and several aryl aldehydes in H_2O at 80 °C with excellent yield and short reaction time, in the presence of nanocatalyst is reported.

Keywords: Pyrido[2,3-*d*]pyrimidines, thiouracil, aquemous media, multicomponent reaction

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Diamondoids: Ranging from Nature's Bounty to Pharmaceutical Applications

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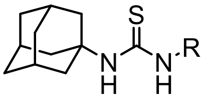
Diamondoids are cage and hydrogen-terminated hydrocarbon molecules that are superimposable on the diamond lattice.[1] Thus, diamondoids as nanometer-sized diamond-like molecules, nanodiamonds, are likely to share some of the unique properties of macroscopic diamond that are very attractive for a number of applications, ranging from material science to medicinal chemistry. Adamantane, the simplest member of the diamondoids, was primarily discovered and isolated from crude oil (natural abundance ~0.0004% petroleum content) in 1933 and became widely available through Schleyer's synthesis in 1957. Thereafter, synthesis of adamantane derivatives started fueling pharmaceutical studies thereof, and drugs incorporating the adamantane motif were quickly introduced to the market.[2] On the other hand, nowadays, adamantane scaffold is viewed as a "lipophilic bullet" for the modification of known drugs in order to enhancing lipophilicity and stability of them, thereby improving their pharmacokinetics and pharmacodynamics.[3] There are many diverse drug candidates based on adamantane-modification of known drugs.[3,5] Hence, the present study will outline the synthesis of privileged structures incorporating an adamantane scaffold, including, thioureas **1**, 1,4-dihydropyridines **2**, pyrimidines **3**, propranolol derivative **4**, and Schiff bases **5**, that are pursued in the group of the author.



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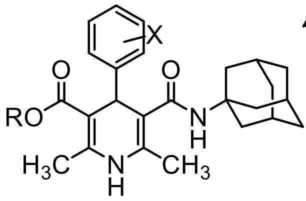

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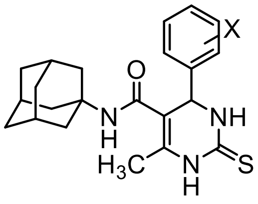

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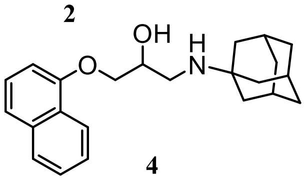

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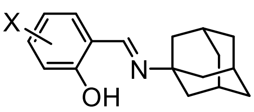

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Keywords: Diamondoid, Nanodiamond, Adamantane motif

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Development of electrospun PCL/SESM/AgNPs hybrid nanofibrous scaffold for application as cutaneous substitutes

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Since, there is grand trend towards using nanofibrous scaffolds in regeneration of cutaneous tissue, therefore, protection of bacterial attack must be considered [1]. In this study electrospun PCL/SESM/AgNPs were prepared for application of regeneration of damaged skin tissue. Present of silver nanoparticle in produced scaffold by XRD, TEM and UV-visible was evaluated. Mechanical features, hydrophilicity, composition and morphology of nanofibers were tests by tensile, contact angle, FT-IR (Fourier transforms infrared spectroscopy) and SEM (scanning electron microscopy) tests. SEM and MTT analysis applied for showing cell adhesion, proliferation. In addition antibacterial activities of scaffolds against E. coli and S. aureus, were examined. This study exhibit modulation of nanofibers with appropriate nanoparticle could enable us to fabricate structures appropriate for skin regeneration [2, 3].

Keywords: Nanofibers; Antibacterial; AgNPs; Tissue engineering

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Pd/Fe_3O_4 Nanoparticles as Catalysts for Synthesize of Amine by *N*-arylation of *p*-toluenesulfonamide

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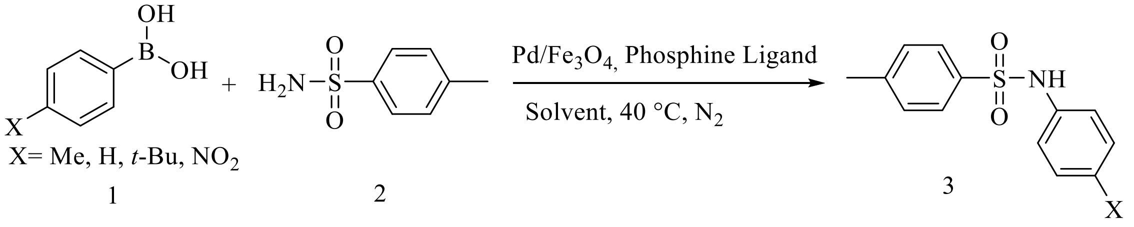
Amines are found in the structure of important pharmacologically active compounds, as well as biologically active for example neurotransmitters. Due to the high importance of amines, several methods have been developed for their synthesis such as the addition reaction of solfunamide compounds [1]. Nowadays, numerous organic compounds such as amines were synthesized through the reaction between amide derivatives and boron reagents. The use of immobilized catalysts on the magnetic supports with the advantage of catalyst separability and recyclability, is one of the suitable developed strategies in recent years. Among the different types of used supports in heterogeneous catalysis, Pd on Fe_3O_4 has been employed as useful and versatile nanomagnetic catalyst [2]. The use of boron reagents **1** as a source of aryl through the exchange of aryl groups between boron and metal is one of the most commonly used methods for the arylation of solfunamide [3]. In this work, amine derivatives were synthesized by *N*-arylation of *p*-toluene sulfonamide **2** in the presence of a hetrogenouse catalyst Pd/Fe_3O_4 and phosphine ligand on the optimum condition in excellent yields and short reaction time (Scheme 1). The structure of the catalyst was characterized *via* SEM, EDAX, TGA and FT-IR techniques, and the prepared products were identified by melting point and IR, ^{1}H NMR, and ^{13}C NMR spectral analysis.



Scheme 1: Synthesize of amine by *N*-arylation of *p*-toluenesulfonamide

Keywords: Amine, Magnetic Nanoparticle, Phosphine Ligand, Boron Reagents

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Green synthesis of substituted triazole hybrids using an efficient: γ-Fe_2O_3@FAp@Cr

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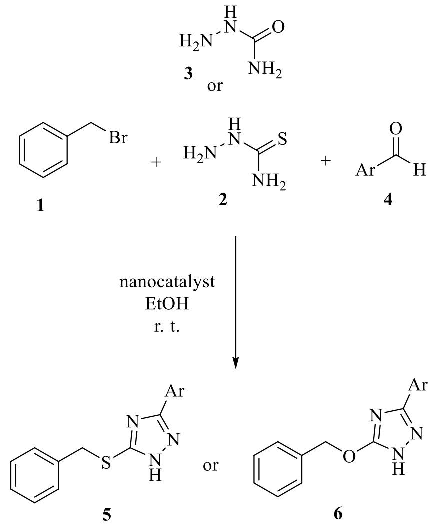
In this work, an efficient cobalt incorporated fluorapatite encapsulated iron oxide nanocatalyst was prepared [1-3] and used in the synthesis of novel derivatives of triazoles by the reaction of various aldehydes, benzylbromide and thiosemicarbazide in ethanol at room temperature. The catalyst was easily removed from the reaction mixture using an external magnet and was used several times without appreciable decreased catalytic properties. This method provided a novel approach for the green synthesis of bis-triazoles in excellent yield (88–95%) and reasonable reaction time (10–30 min). The structures of prepared compounds were confirmed by spectroscopic methods.

Keywords: γ-Fe_2O_3@FAp@Cr, γ-Fe_2O_3, Triazole, Nanocatalyst, Green synthesis



Ar: 4-ClC_4H_4, 4-HOC_4H_4, 4-$MeOC_4H_4$, 2-BrC_4H_4, 2-HOC_4H_4, C_4H_5, 4-$_2ONC_4H_4$, 4-$CH_3C_4H_5$, 2,4-ClC_4H_3,

Scheme 1. Synthesis of substituted triazole derivatives (**5a-i** & **6a-e**).

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Palladium Nanoparticles Supported on Highly Ordered Mesoporous Carbon as an Efficient Catalyst for Formylation of Amines

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Due to their attractive properties such as high surface area, large pore volume, uniform and adjustable mesostructure and pore size and thermal stability, ordered mesoporus carbon (OMC) materials have found an excessive applications in several fields such as adsorption and separation, drug delivery, catalysis and energy storage. Recently, various precursors are utilized for the construction of the heteroatom doped OMC materials through soft or hard templating approaches. In this study, highly ordered mesoporous carbon (OMC) with hexagonal structure was synthesized using carbon precursor derived from egg biomass. Biomass-derived carbon materials have advantages over other carbon materials in terms of low cost and availability. The process of regular mesoporous carbon synthesis was performed by nanocasting using SBA-15 as a hard template and carbonization under nitrogen atmosphere at different temperatures. Palladium nanoparticles were prepared and stabilized on OMC by chemical reduction of Pd^{2+} in the ppresence of ordered mesoporous carbon. The synthesized catalyst was characterized by SEM, EDX, TEM, XRD and FT-IR teqniques. Prepared palladium nanoparticles supported on ordered mesoporous carbon exhibited high catalytic activity in the formylation reaction of amines using DMF.

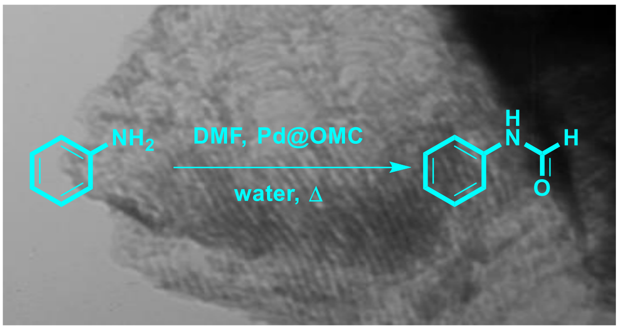

Figure 1. Schematic representation of Pd@OMC catalyzed formylation of amines (Background shows TEM image of the synthesized Pd NPs supported on highly ordered mesoporous carbon)

Keywords: Pd nanoparticles, Ordered mesoporous carbon, SBA-15, Amine, Formylation

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Colorimetric detection of primary aliphatic amines by tetrachloroperylene tetracarboxy dianhydride

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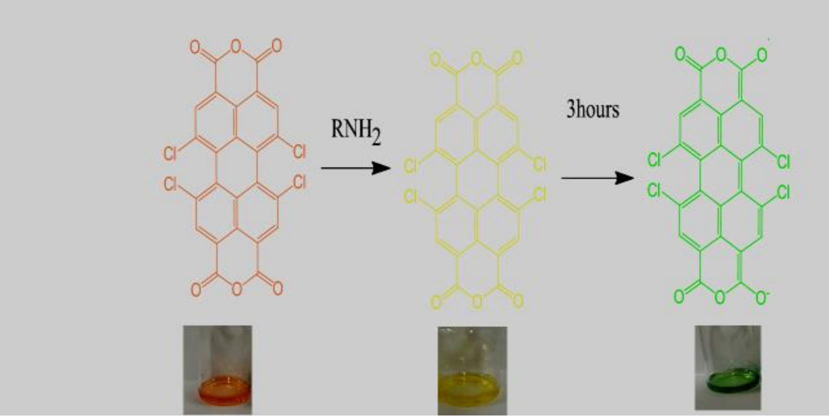
Chemical sensors detecting reliably small amounts of amines are required for a wide range of different applications [1]. Colorimetric sensing with a strong visual response is particularly useful because of quick point-of-care tests [2]. Aromatic dianhydrides and diimides are a class of electron deficient compounds could indicating a distinguished colorimetric change in interaction donor molecules [3]. Herein, tetrachloroperylene dianhydride (TCP) and diimide derivatives were utilized in interacting with different aromatic and aliphatic amines in the organic medium. Experimental and computational methods were used together to investigate the reaction process. TCP was showed a clear color change in interaction with only primery aliphatic amines. Interestingly, a charge transfer complex was formed at first followed by electron transfer with different colors. This feature of TCP can be used as a selective sensor for aliphatic amines type I.

Keywords:, Amine , Charge transfer, Electron transfer, Selective sensor



Scheme1: detection ability of tetrachloroperylene tetracarboxy dianhydride for RNH_2.

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Al-Based Metal-Organic Framework as an Efficient Heterogeneous Catalyst for the Synthesis of Benzimidazole Derivatives

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Metal-organic frameworks (MOFs), also known as porous coordination polymers (PCPs), are a unique class of porous crystalline materials that are constructed by metal ions/clusters and organic ligands [1]. MOFs can act as hosts to include guests exhibiting catalytic properties [2]. Several features make MOFs, at least on paper, excellent candidates as heterogeneous catalysts: (i) an unprecedented structural diversity, (ii) the intrinsic hybrid organic−inorganic nature, (iii) the presence of uncoordinated metal sites and readily accessible organic struts, (iv) the potential for rational design and last but not least(v) a well defined porosity [3]. Metal–organic frameworks (MOFs) containing light and environmentally benign metals have attracted researchers from industry and academia since they are believed to be well suited for applications especially in the field of gas storage. Aluminum is one element of choice for the synthesis of such MOFs since it leads to stable and highly porous materials that can also be formed in water as a green solvent. The potential application of the Al-based MOFs is well documented in various patents [4]. Heterocyclic compounds are playing their key role as templates for a number of antiviral drugs. Benzimidazole ring system is well known for its potential for various biological activities. Benzimidazole consists of a heterocyclic imidazole ring fused with benzene. This ring system is one of the most prosperous heterocycles which is found in many clinically important drugs [5]. Herein, we reported a novel approach to reach such scaffolds by using Al-based metal organic frameworks.

Keywords: Metal-organic frameworks, Heterogeneous catalysis, Al-based MOFs, benzimidazoles, heterocyclic compounds.

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Layered double hydroxides tribological behaviour with different morphologies as oil additives

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Recently, a kind of layered natural mineral called layered double hydroxide (LDH), which can also be prepared by chemical synthesis means, was reported to exhibit excellent tribological properties when utilized as additives in both oil- and water-based lubricants [1]. The chemical formula can be expressed as: $[M^{2+}{}_{1-x}M^{3+}{}_{x}(OH)_2]^{x+}(A^{n-})_{x/n}\cdot mH_2O$. M^{2+} and M^{3+} are divalent and trivalent metal cations, respectively; A^{n-} is the interlayer anion for charge balance. Metal cations are located at the center of the hexagonal crystal of the laminates, while the hydroxide ions occupy the apexes of the hexagonal crystal. Most of metal cations, such as Mg^{2+}, Al^{3+}, Fe^{3+}, Co^{2+}, Ni^{2+}, Cu^{2+}, Zn^{2+}, etc., can achieve atomic-level dispersion in the laminates of LDHs. LDH materials and their composite products have been widely reported in the field of energy storage, ion exchange, drug delivery, and flame retardant additives, etc. [2]. As lubricant additives, LDH nanoplatelets may facilitate the formation of a protective tribofilm with good mechanical properties during sliding process; besides, ultrathin LDH nanosheets were utilized to enable the sliding solid surfaces to be polished and protected because of their relatively weak interlayer interaction [3]. In this paper, as-prepared LDH products were controlled in many aspects including size, morphology (flower-like, spherical and plate-like) and chemical composition (Co^{2+}, Mg^{2}+, Zn^{2+}, and Ni^{2+}) by selecting different preparation methods and adjusting reaction process. The morphology of LDHs can be controlled by adjusting the pH of solution in the crystallization state. Then, they were mechanically dispersed into base oil and their tribological properties were evaluated by a ball-on-disk tester under the same experimental conditions. As comparing different features of LDH additives and observing the wear condition after friction test, the chemical composition and microstructure in contact area were analyzed. Finally, lubrication mechanism of LDHs in base oil was proposed.

Keywords: Layered double hydroxide, Lubricant additive, Tribological property, Friction

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Efficient Synthesis of Primary Amides *via* C-H Functionalization of Aldehydes

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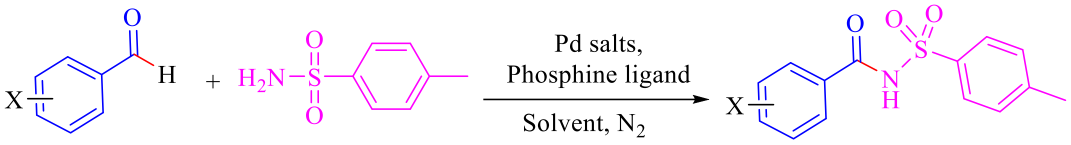
Amides play an crucial role in structure of building blocks such as natural, organic, pharmaceutical, biological and agricultural productts. They are very important intermediates in the synthesis of some drugs and chemicals they also act as ligands for heterogeneous and homogeneous catalysts in the synthesis of other compounds also [1]. Due to the high importance of amides, several methods have been developed for their synthesis such as the C-H functionalization of aldehyde with amines using homogenous catalysts [2].

Palladium in homogenous form, provided many sites to activate many organic functional groups and its ability converted desired compounds to excellent catalysts for chemical reactions involving and is one of the prominent features of this reaction because of its stabilitiy, availability and selectivity [3].

In this work, in order to develop an innovative approach toward for C-N bond formation reactions, C-H bond from aldehyde is broked on surface of palladium and then amine inserted to Pd-C bond. In general *p*-chloro-*N*-tosylbenzamide synthesized by addition of *p*-toluene sulfonamide **2** to aromatic aldehyde **1** in the presence of a organometalic catalyst Pd salts and phosphine ligand in the optimum condition in excellent yields and short reaction time (Scheme 1).

The structure of products is characterized by melting point and IR, ^{1}H NMR, and ^{13}C NMR spectroscopies.



X= Cl, Br, Me, H
1
2
3

Scheme 1: Synthesis of *p*-chloro-*N*-tosylbenzamide derivatives

Keywords: Amide, Homogenous Catalyst, Phosphine Ligand, Boron Reagent

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Tribological behaviour of layered lipophilic graphene quantum dot synthesized over Fe@MgO catalyst

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Friction and wear are two reasons that cause energy losses in mechanical activities. Lubrication is the main subject for improving energy efficiency and mechanical durability. Regardless of the completion of each metal surface, it contains ridges, valleys, asperities and depressions [1]. Adding nanomaterials as additives in lubricating base oil, is a rapidly developing research field, because of the different nature of the nanomaterials from traditional bulk materials due to their very small size and their specific surface area [2]. Graphene and Graphene quantum dots (GQDs) have been known as one of the most important and attractive lubricating nanomaterials and have dominant application in tribological field [3]. Current research focuses on exploring synthetic routes in a more economical synthesis approach by utilizing green chemistry and diversifying possible starting precursors. Covering material was selected based on its ecofriendly nature which later will stand as a better tool in applications that require low toxicity tolerance. Therefore, we tried to synthesize functionalized GQD using the catalyst with high fluorescence at low temperature. The design in GQD synthesis is based on the following considerations: well surface passivation of GQDs plays a key role in quantum dots fabrication. In our research, we chose citric acid as the carbon source due to its well-known low carbonization temperature (<200 °C), and used octyl amine as the capping and functionalizing reagent because of functionalized and passivation surface states with carboxyl groups having a good photo-induced electron transfer property.

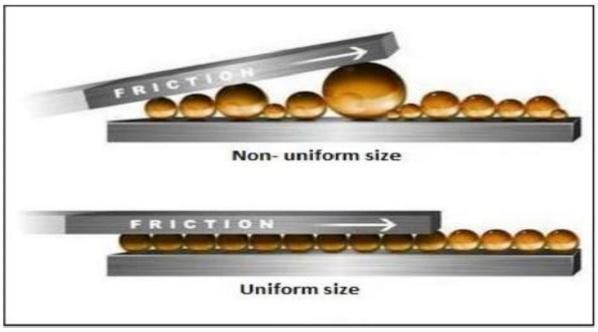

Fig. 1. Lubricant size effect on anti-friction performance.

Keywords: Lipophilic material, Oil additive, Graphene quantum dot, Friction

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Pd (II) supported on magnetically retrievable modified reduced graphene oxide as a highly efficient catalyst for imidazole-aryl coupling reaction via C-H bond activation in deep eutectic solvent

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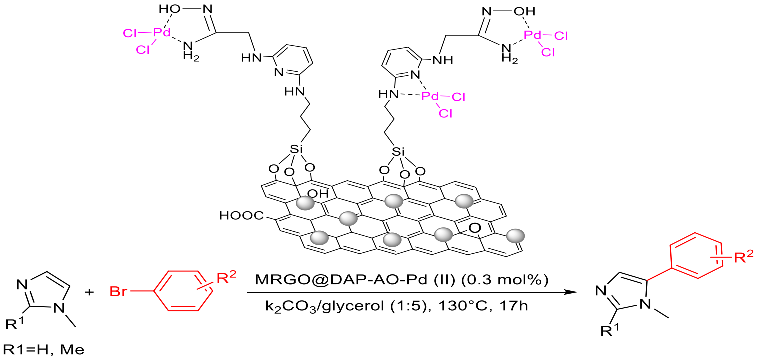
An extremely powerful method for the synthesis of aryl-heteroaryl products has been established via palladium-catalyzed direct C-H arylation reactions of heteroarenes with aryl halides. Among the imidazole derivatives, 5-arylimidazoles have been known as physiologically and pharmacologically active compounds [1]. Ohta and co-workers introduced the regioselective synthesis of C5-arylated imidazoles using $Pd(PPh_3)_4$ as catalyst [2]. Since then, a variety of palladium/ligand catalytic systems have been used for the direct 5-arylation of imidazoles. Recently, graphene oxide has attracted tremendous attention as solid support for C-H activation due to high chemical and mechanical stability, large surface area and excellent dispersibility [3]. In continuation of our interest in developing environmentally benign approach, herein, we have developed a highly efficient palladium-incorporated nanocatalyst for C−H arylation reaction of imidazole with aryl bromide by supporting of palladium (II) species on modified magnetic reduced graphene oxide ($MRGO@DAP-AO-Pd^{ll}$). We also employed K_2CO_3/Glycerol deep eutectic solvent (DES) as a green and sustainable reaction medium.

Keywords: Magnetic reduced graphene oxide, Palladium complex, C-H Arylation, Imidazole, Deep eutectic solvent



Scheme 1. C-H arylation reaction of imidazoles in presence of MRGO@DAP-AO-Pd (II) catalyst

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Copper Nanoparticles Immobilized on Ionic Liquid-Functionalized Halloysite Nanotubes; Synthesis and Application in the Click Synthesis of 1,2,3-Triazole Derivatives

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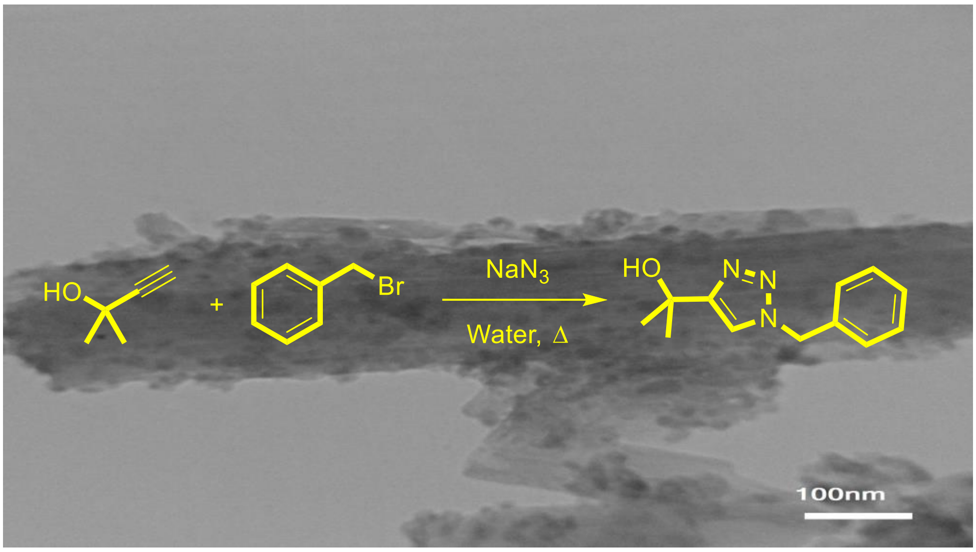
A heterogeneous nanocatalyst, copper nanoparticles supported on ionic liquid modified halloysite nanotubes, named Cu@HNTs-ILs, was prepared by modification of pristine halloysite nanotubes (HNTs) with 3-aminopropyltriethoxysilane (APTES) to give HNTs-APTES, followed by reacting with 1-methyl-3-(oxiran-2-yl-methyl)-1*H*-imidazol-3-ium chloride (ILs) to obtain the desired ionic liquid-functionalized holloysite nanotubes [1]. Finally, Cu@HNTs-ILs was prepared by immobilization of Cu nanoparticles by chemical reduction of Cu^{2+} in the presence of HNTs-ILs using $NaBH_4$. Obtained Cu@HNTs-ILs was characterized by means of FT-IR, SEM, EDX, TEM and XRD. Click reaction is one of the most useful approach for the construction of 1,2,3-triazole moiety [2]. So, the catalytic activity of prepared nanocatalyst was evaluated for the synthesis of 1,2,3-triazole derivatives via click reaction between alkyl halides, alkynes and azide anion.



Keywords: Cu nanoparticles, Halloysite nanotubes, Click reaction, Triazole

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An Efficient Hetregeneouse System from the C-C Bond Formation of Aryl-bromide and Phenylboronic acid

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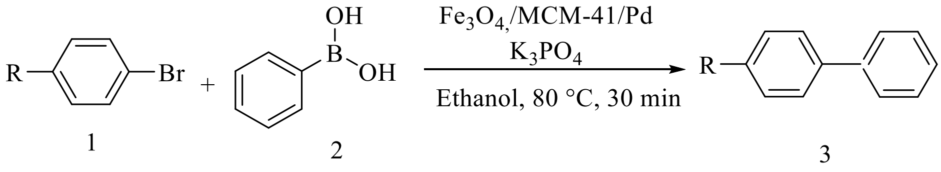
Suzuki cross-coupling reactions, are among the most widely used method for the formation of carbon–carbon bonds to synthesis of biaryl compounds, which constitute a wide range of agriculcural, natural products and pharmaceuticals [1]. These reactions are generally catalysed by soluble palladium (Pd) with mesoporous MCM-41 silica used ordered as a support for synthesising highly dispersed palladium nanoparticles with narrow size distributions inside their pores [2]. In other hand The value of magnetic nanoparticles is one of the discoveries that has recently been developed to an extent that scientists could have never imagined a century ago, and these particles are rising steadily in significance in the field of catalysis because of its advantage of catalyst separation, recyclization and stablization [3].
Due to high stability, excellent performance and low toxicity of boron reagents **1** use as a source of aryl through the exchange of aryl groups between boron and catalyst is one of the most commonly used methods for the C-C formation [4].
In this work, biaryl derivatives **3** were synthesized by arylation **2** of arylhalides **1** in the presence of a hetrogenouse catalyst Fe_3O_4/MCM-41/Pd the optimum condition in excellent yields and short reaction time (Scheme 1).
The prepared biaryls were characterized by melting point and IR, ^{1}HNMR, and ^{13}CNMR spectral analysis and structure of the catalyst was identified *with* SEM, EDAX, TGA, DTA and, FT-IR techniques



Scheme 1: Suzuki cross-coupling by arylation of arylhalid

Keywords:Biaryls, Magnetic Nanoparticle, Suzuki cross-coupling, Mesoporous MCM-41

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Synthesis and characterization of novel micro-sized tetrazole-based high energetic nitrogen-rich polymers

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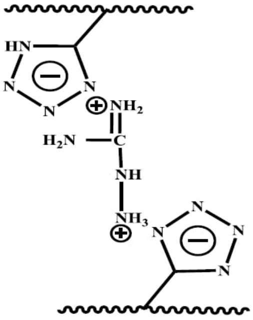
High energetic materials can be classified as three types of nuclear, physical and chemical explosives. The decomposition of compounds with production of heat and gases is the deduction of detonation process of explosives. The important groups of energetic compounds are related to the primary and secondary explosives, propellants and pyrotechnics [1-2]. From a structural point of view, the explosives can be classified as nitro compounds, nitric esters, nitramines, chloric and perchloric acid derivatives, azides [3-4] and various molecules capable of preparing a detonation (acetylides, fulminates, ozonides, peroxides and polynitrogenated compounds (PNCs) such as tetrazole-, triazole-, triazine- and tetrazine-based compounds). Nitrogen-rich polymers point to the polymer structures including a high content of nitrogen atoms, frequently over 50 percent [5-6]. Energetic materials are a class of material with high amount of stored chemical energy that can be released. Typical classes of energetic materials are e.g. explosives, pyrotechnic compositions, propellants (e.g. smokeless gun powders and rocket fuels), and fuels (e.g. diesel fuel and gasoline). The novel functionality of aromatic tetrazole derivatives with high nitrogen content predetermines a great interest to tetrazole-containing polymers. The tetrazole-based nitrogen-rich polymers were well investigated. The tetrazole rings play an important role in development of energetic polymers. The high thermal stability of these rings causes the polymers as good candidates as energetic applications. The aim of the present work is to synthesize novel nano-sized high energy density polymers based on tetrazole rings. The resulted polymer was characterized by SEM, ^{1}H NMR and ^{13}C NMR.



Schem 1. Structure of aminoguanidinium salt of PVT

Keywords: Nano-size, Tetrazole, Nitrogen-rich polymers, Explosives, Energetic materials

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Study of structural properties and photocatalytic activity of nanostructures Synthesized molybdenum disulfide

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In this research, a hydrothermal method has been employed for synthesis of nanostructured MoS_2 particles via the synthesis of MoO_3 [1]. The structure of MoS_2 samples was investigated by using a different precursor, such as Disodium Thiourea and Thioacetamide. Several investigation tools including FTIR, XRD, SEM, TEM, Raman and UV-Vis spectroscopy were used in order to characterize MoS_2 nanostructures. XRD studies confirmed the hexagonal crystalline structure of samples. The FTIR spectra indicated the well-bonded MoS_2 nanostructures [2]. The size and the nearly uniform distribution of particles was detected by SEM and TEM. Photocatalytic activity of the MoS_2 particles was checked by degration of Methylene Blue. Results showed the enhanced photocatalytic activity for the synthesized MoS_2 with the molar ratio of 1:3 under UV irradiation.

Keywords: Nanostructure, Molybdenum Disulfide, Hydrothermal, Photocatalytic activity

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Cellulose-PMAA/layered double hydroxide hybrid as a promising adsorbent for simultaneous removal of auramine O and rhodamine-B

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In recent years, the treatment of dye-containing wastewater has become very significant, because these dyes are a serious environmental problem owing to high toxicity and accumulation in the sea [1-6]. In this study, NiCo-layered double hydroxide (LDH) was synthesized in situ on the surface of cellulose beads-poly(methacrylic acid) (CB-PMAA) to form CB-PMAA/LDH nanocomposite. CB-PMAA was fabricated via the radical polymerization of methacrylic acid (MAA) monomer onto the surface CB molecules. CB-PMAA/LDH was characterized by FT-IR, XRD, SEM, EDX, and STA analyses and applied as a robust adsorbent for the quick removal auramine O (AO) and rhodamine B (RB) as cationic dyes from aqueous media. The effective parameters on dye removal, including pH, adsorbent dosage, contact time, and dyes concentration were investigated and optimized. The optimum conditions were pH = 6, adsorbent dosage of 15 mg, contact time of 10 min and dyes concentration of 10 mg/L. UV-vis spectrophotometer was used to determine the amount of residual dyes in solution. To determine the type of adsorption isotherm, the Langmuir, Freundlich, Tempkin, and Dubinin-Radushkevich adsorption isotherm equations were applied. Pseudo-first-order, pseudo-second-order, intraparticle diffusion, and Elovich models were used to determine the kinetics of adsorption and the results exhibited an appropriate fit for Langmuir adsorption isotherm and the pseudo-second-order kinetics model with an adsorption capacity of 79.70 (AO) and 108.27 mg/g (RB), respectively. Regarding the obtained values of thermodynamic parameters such as enthalpy and Gibbs free energy, removal of AO and RB dyes by CB-PMAA/LDH was exothermic and spontaneous.

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A green method for confirming the Sonogashira reaction with magnetic nanoparticles

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Today, many catalysts are designed and synthesized to perform chemical reactions, which is very efficient in the chemical and medical industries [1]. Therefore, the first step in the synthesis of a magnetic nanocatalyst with a magnetic property called magnetite nanocatalyst is to form a nuclear / shell structure and its nanoparticles are confirmed by SEM, TEM analysis. The Fe_3O_4 magnetic nanocatalyst, obtained by combining two metal salts, iron 2 and iron 3, in a ratio of 1: 2 in distilled water, at room temperature and weighing 0.005 g, is surrounded by a silica coating (SiO_2, to prevent Excess oxidation of its surface). In the next step, the trimethoxyl-isylpropyl chloride linker is first bonded to the silica cores, and along it, the morpholine linker is covalently bonded to the previous linker, and the overall structure of the nanocatalyst becomes regular and integrated. Finally, to increase the efficiency of the catalyst in many reactions such as carbon-carbon triple coupling reaction (sonogashira coupling reaction), 2 acetate nanoparticles are coated on the surface of the catalyst with connected linkers and prepare the nanocatalyst surface for this reaction. The reaction conditions were as follows: from a solvent of ethanol used (as green solvent) and triethylamine base to bind two triple bonds together at 75° C, completely green products with efficiencies above 98% were obtained. The efficiency of this magnetic nanocatalyst is very high and its features include synthesis using inexpensive materials, physico-chemical connection between aqueous and organic phases, creation of high efficiency products and easy extraction by external field. By comparing the results of this reaction with the research reactions of other researchers [2-4], the efficiency and high power of 96% of this catalyst in performing Sonogashira reaction several times during ten periods showed.

Keywords: Magnetic nanoparticles, Copper nanoparticles, Sonogashira reaction

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CuO nanorod decorated on graphitic carbon nitride ($CuO_{NR}/g\text{-}C_3N_4$) as a green and water-soluble catalyst for selective oxidation of alcohols

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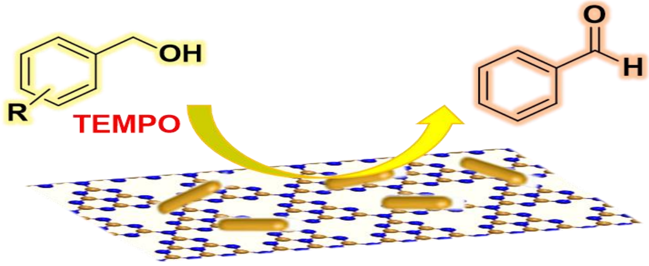
Oxidation of organic compounds in water-based systems is in demand in the chemical industry due to its environmental and economic advantages [1]. In particular, the oxidation of alcohol is one of the key reactions in the synthesis of complex organic molecules and fine chemicals [2]. Most oxidation reactions in organic chemistry are inconsistent with the principles of green chemistry and sustainable developments owing to the lack of selectivity, the use of toxic metal reagents or catalysts that are continuous pollutants, or the use of halogenated solvents [3]. In this study, we design a sustainable substrate to support CuO nanorods (Scheme 1). This catalyst exhibited excellent catalytic activity in the oxidation of various aromatic alcohols to the corresponding aldehyde in the presence of TEMPO under mild conditions and short-time reaction. $CuO_{NR}/g\text{-}C_3N_4$ displayed good stability in the water after 8 recoveries and reuse.

***Keywords*: CuO nanorods, Graphitic carbon nitride, Green catalyst, Selective oxidation**



Scheme 1. $CuO_{NR}/g\text{-}C_3N_4$ catalyzed oxidation of various alcohols.

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Doped-boron nitride nanostructures as a potential removal of rimantadine from environment: A DFT study

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When a drug is released in large quantities into the environment and nature, it is dangerous and requires removal where the drug accumulates, for example in water and soil. Therefore, design of a device to removal the accumulated drugs in environmental is very important. The rimantadine drug (Rd) can be one of those drugs that needs to removal the amount in environment [1]. The purpose of this computational study is to measure and evaluate the interaction of rimantadine drug with boron nitride and its doped nanostructures. The BN nanoparticles have a wide range of attractive properties such as stability, high temperature strength, low dielectric constant, high thermal conductivity and oxidation resistance, which leads to a number of potential applications as electronic materials [2].

In this work, we studied that replacing the Al, Si and Ga atoms instead of a boron atom in boron nitride nanosheet (BNNSh) is a useful way to removal of Rd from environment. We studied the interaction between Ge-, Si- and Ga-doped-BNNSh and the Rd drug to determine which one of the doped nanostructure is better to removal of Rd using the B3LYP method with a basis set of 6-31G(d) by Gaussian software 09. A poor energy interaction between the Rd drug and the boron nitride nanoparticle was observed. The results show that the Ga-doped BNNSh is the best nanostructure for removal of Rd drug.

Keywords: Boron nitride nanostructures-Removal-Rimantadine-Environment,DFT

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Enantioselective Synthesis of Chiral Amine Using a Green Nano-organocatalyst

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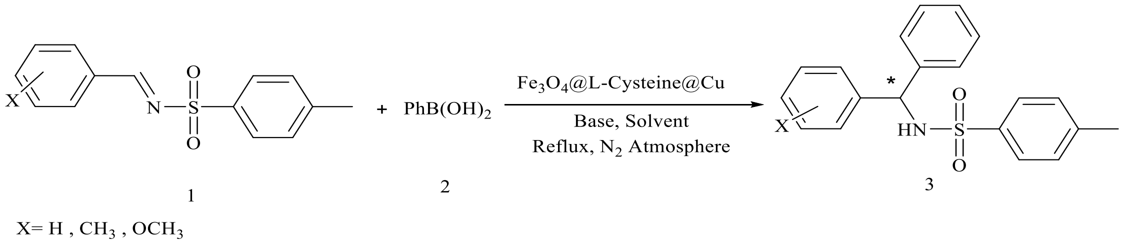
Chiral amines and their derivates are essential building blocks for the preparation of many pharmaceutical and biologically active molecules [1]. They are used directly as resolving agents, building blocks, or chiral auxiliaries [2]. The discovery and development of new catalytic reactions that lead to C-C bond formation by the addition of organometallic reagents to C=N of imine are important developments in efficient processes for chemical synthesis [3]. Asymmetric catalysis has emerged as one of the most effective synthetic methods for the preparation of enantiopure compounds [4]. Lots of Methods for preparing chiral aromatic amines have been developed using a suitable chiral catalyst. A large number of catalytic systems using transition metal complexes have been developed for the direct carbon-carbon bond formation of aromatic amines [5].In this work, to develop a new method of chiral amine formation using a chiral catalyst that can be easily recycled and reused, we have investigated the catalytic activity of nanomagnetic L-Cysteine coated by copper metal catalyst on arylation of imines **1** by Phenyl boronic acid **2** (Scheme 1). The structure and morphology of prepared nanomagnetic catalysts were characterized by EDAX, SEM, and FT-IR. The structure of chiral products is identified by IR, ^{1}H NMR, and ^{13}C NMR spectroscopies. The enantiomeric excess (ee) of chiral products is also detected by the polarimeter.



Scheme 1: Synthesis of chiral amins using a green nanomagnetic organocatalyst

Keywords: Asymmetric synthesis, Chiral amine, Chiral nanomagnetic catalyst

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One-Pot Synthesis of quinoxaline derivatives via the of 1, 2-Phenylenediamines, ethyl bromopyruvate and alkoxides

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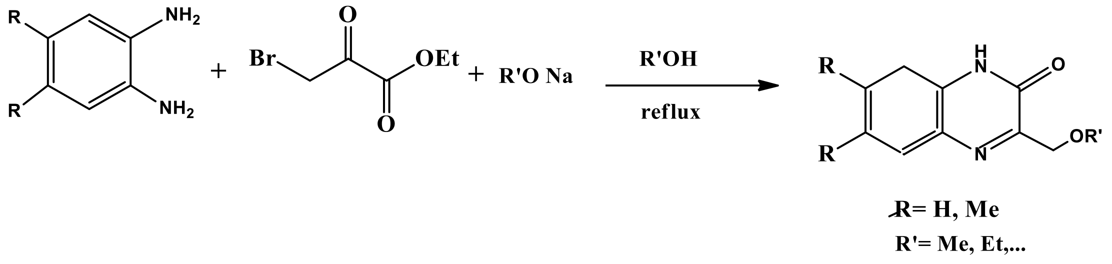
Using of novel chemical reactions and strategy, can review and discussion in production of product with higher added value in synthesis of organic chemistry [1]. Preparation of basic material and doing this kind of reactions is one of the most basic challenges in chemistry to synthesis intended compound. Merging of two or more chemical reactions without isolating previous materials for synthesis of new compound, is one of the best way to solving this challenge [2]. Today used of multi-component reactions as powerful tools for synthesis lots of heterocyclic compound, usage of heterocyclic compound can be referred to pharmaceutical properties, agriculture, optical brightener and corrosion inhibitor material [3].in our previous studies, In this work were synthesized quinoxaline derivatives with high efficiency from the reaction of 1,2-phenylenediamines and ethyl boromopyruvate in the presence of alkoxides (Scheme 1).



Scheme 1. Reaction of 1,2-phenylenediamines and ethyl bromopirovate in the presence of alkoxides

Keywords: Diamines, Ethyl boromopyruvate, Quinoxaline, Alkoxides.

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Synthesis of two-dimensional polymers based on triazine structures with nucleophilic monomers

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Two-dimensional polymers (2DPs) with unique physicochemical properties have emerged as a new class of materials in the last decade. The harsh synthetic conditions and associated limited structural diversity together with unknown mechanisms hamper further development and large-scale synthesis of defined two-dimensional triazine structures. The efficient synthesis of two-dimensional polymers (2DPs) with tailorable structures and properties is highly desired but has remained as a long standing challenge [1],[2]. Herein, we report on new strategies for the synthesis of two-dimensional triazine polymers from cyanuric chloride and commercially available nucleophilic monomers at mild conditions. We have studied the mechanism of reactions in detail to find the correlation between the strcture and properties of materials through which the desired compounds for special applications can be constructed. We have used aromaticity of the growing sheets as the main factor to drive polymerization in certain topologies and orientations [3],[4]. Taking advantage of such new strategies many new nanomaterials with defined structures can be synthesized. The synthesized polymer was characterized by FT-IR, SEM, XRD and TGA. SEM images show surface morphology with a medium-sized layer structure in the micrometer range.

Keywords: Two-dimensional polymers, Triazine, Nucleophiles

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synthesis of new thiazoles using one-pot reaction

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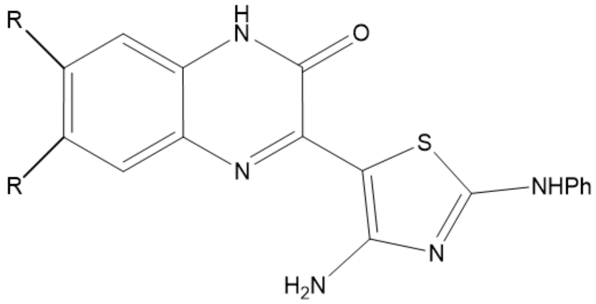
Heterocycles containing the thiazole ring have different pharmacological and biological activities and is used as antibacterial, anti-tumor, anti-oxidant and anti-inflammatory drugs [1]. Previous research has reported several therapeutic properties of thiazole derivatives, but its antibacterial properties have received more attention than any other effect [2].

In this study, derivatives of thiazole were synthesized using a one-pot reaction and the structure of the synthesized compounds was confirmed by HNMR and ^{13}CNMR spectral data. Mild conditions, high efficiency and cost-effectiveness are among the features of this method (Scheme 1).



Scheme 1: synthesis of new thiazoles

Keywords: Thiazole, Heterocycles, One-pot reaction.

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Synthesis and characterization of bimetallic heterogeneous catalyst supported on natural asphalt sulfonic acid and its application in organic reactions

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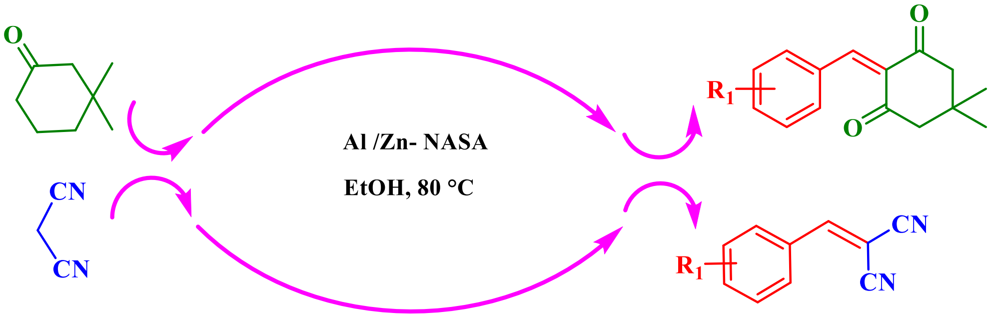
In recent years, carbon substrates have been widely developed and used due to the large surface that they produced and different factor of the groups on their surface [1-3]. In this research, aluminum and zinc grafted natural asphalt sulfonate (Al/Zn-NASA) as a new and efficient nanocatalyst was identified, synthesized and introduced, and its catalytic activity was investigated in the knoevenagel condensation (Scheme 1). Al/Zn-NASA was identified using Transmission Electron Microscopy (TEM), Energy Dispersive Spectroscopy (EDS), Scanning Electron Microscopy (SEM), N_2 sorption isotherms, Inductively Coupled Plasma (ICP), X-Ray Diffraction (XRD), Thermogravimetric Analysis (TGA) and Fourier-transform infrared spectroscopy (FT-IR). The advantages of this nano-catalyst including have high-carbon, cost-effective and synthesis simplicity given the availability of natural materials.



(Scheme 1)

Keywords: Heterogeneous catalyst , Sulfonic acid , Natural asphalt, Organic reactions

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Nanocatalyst Zr@NASA: synthesis, characterization and application as a recyclable heterogeneous catalyst in some organic reduction reactions

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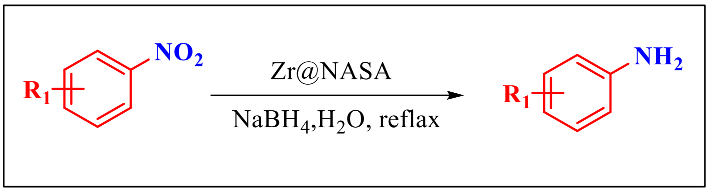
Most chemical reactions in industry and biology are catalytic. Some chemists and chemical engineers seek to understand and apply catalyzing processes [1-3]. In this research, zirconium grafted natural asphalt sulfonate (Zr-NASA) as a recyclable and carbonaceous heterogeneous nano-catalyst was synthesized and introduced, and its catalytic activity was investigated in the direct reduction of nitrobenzene derivatives to aniline via sodium borohydride ($NaBH_4$) reagent (Scheme 1). The prepared catalyst was characterized by FT-IR, XRD, EDS, ICP, SEM, EDX and BET analysis. The advantages of this reaction including have low cost, simple of application, mild nature, and satisfactory yields.



(Scheme 1)

Keywords: Heterogeneous catalyst, Reduction reactions, Nanocatalyst

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synthesis and characterization some new derivative polymers pyrazine carboxylic acids

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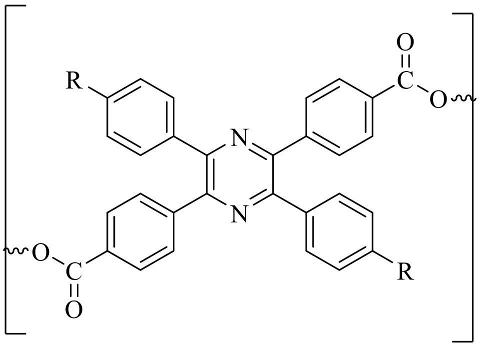
Pyrazine is a kind of natural product which can be found in plants, animals, insects, marine organisms and microorganisms. The main function of pyrazine in living organisms is used as flavor of the raw foods. Pyrazine and its derivatives were also produced in industries mainly for fragrance, flavor and pharmaceutical applications. [1,2]. This research includes some new polymers derivatives from pyrazine carboxylic acids that these products were characterized using FT-IR, C-NMR, H-NMR, TGA and CHN (Scheme 1). These polymers were obtained from reaction of benzil with α-amino acid D-alanine.



(Scheme 1)

***Keywords**:* Derivative polymers, Pyrazine, Carboxylic acids

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Synthesis and characterization of catalyst $ZrCl_4$-supported on natural asphalt sulfonic acid and its application in Claisen -Schmidt condensation reaction

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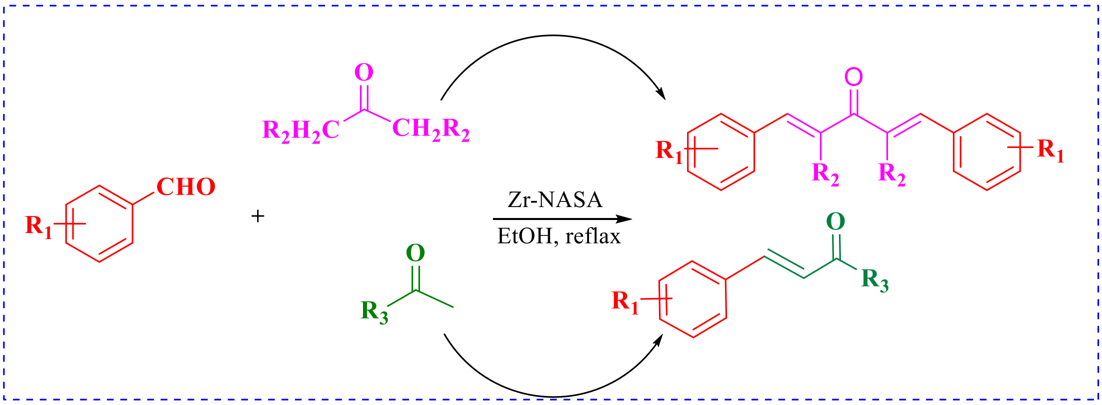
Recently, the development of nanocatalysts formed on various supports can be an effective strategy to increase the efficiency of chemical reactions [1-2]. In this study, taking into account the principles of green chemistry and extension of economical and industrials catalysts (as the heart of the chemical processes), Zirconium-grafted natural asphalt sulfonate (Zr-NASA) was synthesized, identified and introduced as a new efficient heterogeneous nanocatalyst for the synthesis of α،β- unsaturated compounds. This nanocatalyst has advantages such as simple preparation from commercially available materials, high catalytic activity, simple operation, high yields.



(Scheme 1)

Keywords: Heterogeneous catalyst , α،β – unsaturated compounds , Aldehydes, Ketones

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Stabilization of $CuCl_2$ on the NASA substrate and study of its catalytic activity in Knoevenagel condensation reactions as a recyclable heterogeneous catalyst

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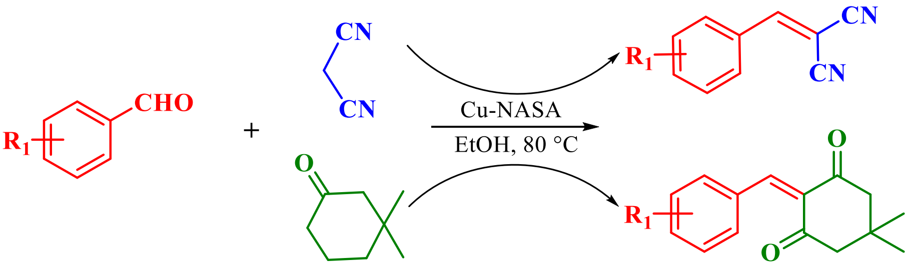
In recent years, nano-catalysts with carbon substrates, including carbon black, carbon nanofibers, graphene and nanotubes have been investigated as a useful and sustainable alternative catalyst substrate. [1-3]. In this work, the heterogeneous nanocatalyst, Cu- natural asphalt sulfonate (Cu-NASA) was synthesized using sulfonated natural asphalt. For the characterization of the synthesized catalyst used of different techniques such as FT-IR, TGA, XRD, ICP, BET, EDS and SEM. Then the activity of the catalyst successfully examined in the formation of C-C bond through knoevenagel condensation (scheme 1). The obtained products were identified using FT-IR, ^{1}H-NMR and ^{13}C-NMR techniques.



(Scheme 1)

Keywords: Heterogeneous catalyst , Knoevenagel condensation reactions , Recyclable

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Synthesis and characterization of recyclable heterogeneous Zn@NASA nanocatalyst by supporting $ZnCl_4$ on the NASA substrate and its application in reduction reactions

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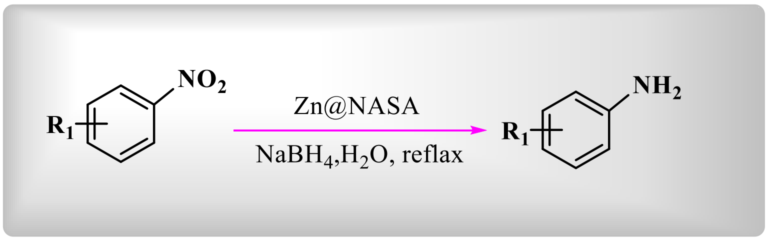
Nowadays, nanotechnology has attracted attention in different field such as therapeutics, food and nutraceuticals, biology and medicine, biotechnology, fabrics, textiles and environmental applications and so on [1,2]. In the present study, a novel heterogeneous nano-catalyst was synthesized by sulfonating natural asphalt as a high-carbon, cost-effective and accessible substrate using a high-concentration sulfuric acid. Ultimately, the nanocatalyst was synthesized through a reaction of natural asphalt sulfonate with $ZnCl_2$. Catalytic activity of this catalyst was investigated in the synthesis of aniline derivatives. The series of nitroarenes containing a variety of functional groups were reduced to their corresponding products. (Scheme 1). The prepared catalyst was characterized by FT-IR, XRD, EDS, ICP, SEM, EDX and BET analysis.



(Scheme 1)

Keywords: Heterogeneous catalyst, Recyclability, Reduction reactions, Nanocatalyst

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Synthesis of α‹β – unsaturated compounds through the reaction of aldehydes with ketones (Claisen -Schmidt reaction) in the presence of a heterogeneous nanocatalyst Zn/Al@NASA

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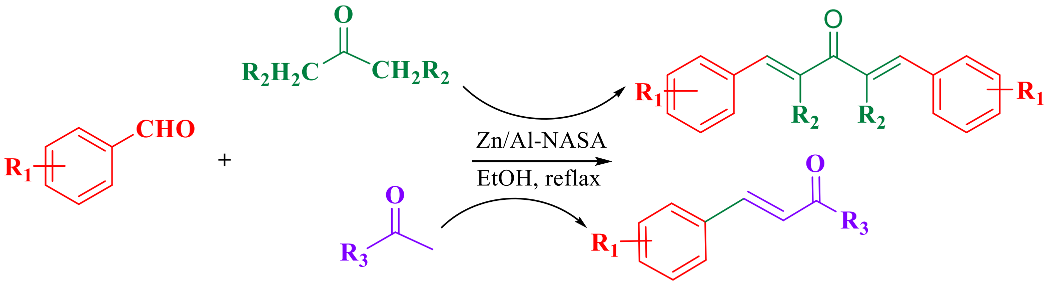
Research on the different areas of chemistry is mainly focused on synthesizing and introducing new and efficient catalysts, including heterogeneous nano-catalysts, as the most appealing. [1-3]. Herein, we report aluminum and zinc grafted natural asphalt sulfonate (Al/Zn-NASA) an efficient nanocatalyst for the formation of α‹β – unsaturated compounds. This nanocatalyst was characterized by FT-IR, XRD, EDS, AAS, SEM, WDX and BET analysis. The advantages of this nano-catalyst including being environmentally friendly and economically sound and simple purification and separation from the reaction mixture.



(Scheme 1)

Keywords: Heterogeneous catalyst , α‹β – unsaturated compounds , Aldehydes, Ketones

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[3]A. Singhania, S. Gupta, *Catal. Lett*, **2018**,1, 946.

Synthesis and characterization of heterogeneous catalyst Ni@NASA and study of catalytic activity and its recyclability in some reduction reactions

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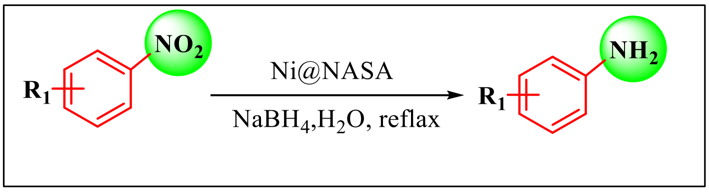
Nanocatalysis is swiftly mounting in various catalyzed organic reactions. A wide variety of nano sized species such as nanoparticles or nanocomposites are effectively employed as catalyst [1,2]. In this research, nickel grafted natural asphalt sulfonate (Ni-NASA) as a novel and recyclable heterogeneous nano-catalyst was synthesized and its catalytic activity was investigated in the synthesis of aniline derivatives via sodium borohydride ($NaBH_4$) reagent (Scheme 1). The prepared catalyst was characterized by FT-IR, XRD, EDS, ICP, SEM, EDX and BET analysis. This nano-catalyst was recycled several times without any significant changes in its catalytic properties.



(Scheme 1)

Keywords: Heterogeneous catalyst, Recyclability, Reduction reactions, Nanocatalyst

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Stabilization of Oxalic acid on the NASA substrate and study of its catalytic activity in the multicomponent organic reactions

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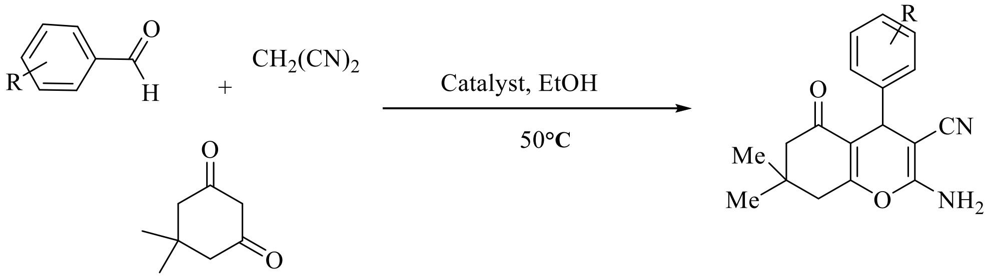
In recent years, Carbon-based-materials due to their unique properties such as different shapes with tunable sizes, high surface area, low cost and availability, have been wildly used for a diversity of applications and have shown good potential for producing heterogeneous catalysis [1-3]. In this work, the heterogeneous nanocatalyst, oxalic acid- natural asphalt sulfonate was synthesized using sulfonated natural asphalt. For the characterization of the synthesized catalyst used of different techniques such as FT-IR, TGA, XRD, ICP, BET, EDS and SEM. Then the activity of the catalyst successfully examined in the for the synthesis of 2-amino-4-H-pyran derivatives (scheme 1). The obtained products were identified using FT-IR, ^{1}H-NMR and ^{13}C-NMR techniques.



(Scheme 1)

Keywords: Heterogeneous catalyst , 2-amino-4-H-pyran, Carbon-based-materials

References

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[2]P.Latos, A. Szelwicka, S. Boncel, S. Jurczyk, M. Swadzba-Kwasny, A. Chrobok, *Aces. Sustain. Chem Eng*, **2019**, 8, 5184.
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Preparation of oxazoles by reaction of benzoin with α- amino and D-alanine

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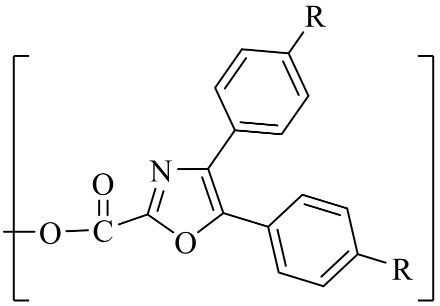
Oxazoles represent an important class of five-membered heterocyclic aroamtic compounds. The increasing interest in the exploitation of oxazole ring system is due to its widespread prevalence in numerous complex natural products as well as in a number of organic building blocks. A significant number of oxazole-enriched natural products have been isolated from several marine invertebrates and microorganisms. [1,2]. This research includes some new polymers derivatives from oxazole carboxylic acids that these products were characterized using FT-IR, C-NMR, H-NMR, TGA and CHN (Scheme 1). These polymers were obtained from reaction of benzoin with α-amino acid D-alanine.



(Scheme 1)

***Keywords**:* Derivative polymers, Pyrazine, Carboxylic acids

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Syntheses of new derivatives of 3-(2,4-dichlorophenoxy)-1,4-diphenylazetidin-2-one and study of biological activity

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Aztidine-2 -ones also known as β-lactam, are a broad group of antibiotics that have a beta-lactam ring in their molecular structure. Given the important role of beta-lactams in the pharmaceutical industry, designing economical and cost-effective methods for beta-lactam synthesis can be a great help in this industry [1,2].The use of nano catalysts in the synthesis of beta-lactam from schiff base and acetic acid derivatives has attracted the attention of researchers as an efficient method. Among the various compounds, the use of nanocellulose as a catalyst will have good potential due to the low cost of raw materials and high efficiency. Therefore, in this research, using magnetic nanocomposite Fe_3O_4 α- Cellulose-NH_2-CuI, as a catalyst in the process of synthesis of beta-lactam from imine and carboxylic acid and its effect on efficiency and reaction rate was investigated. In the first phase of the study, imine compounds with different derivatives of the reaction of aniline and aromatic aldehydes were synthesized in the presence of acetic acid. In the second step, the imine derivatives obtained with acetic acid derivatives were reacted using the Fe_3O_4 α- Cellulose-NH_2-CuI catalyst to produce aztidine-2-ones.

Keywords: Aztidine-2- one, Nanocomposite, Biological activity

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Asymmetric Arylation of Imines in the Presence of Mgnetically Nano Liagnds and Pd Metal

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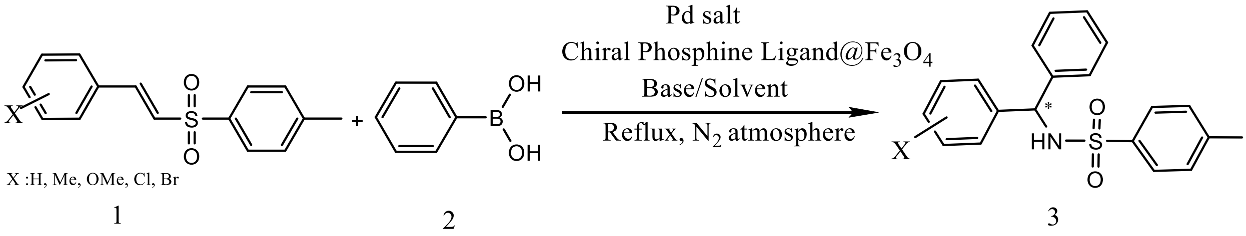
Nowadays, chiral nanoligands act a great role in the synthesis of optically active compounds that are used in the production of pharmaceutical precursors [1]. For the preparation of these nanomagnetic ligands, magnetic nanoparticles Fe_3O_4 (MNPs) were widely used as support owing to facile separation, non-toxically effects, and highly recyclable and reusable properties [2].As well as, chiral amines play an important role in biological activities and agricultural, natural, and pharmaceutical products. They are important intermediates in the synthesis of some drugs and chemicals and act as important ligands in the synthesis of chiral compounds. Therefore, the development of chiral amines synthesis methods such as the addition reactions on imines has attracted the attention of chemists [3].

In this work, in order to develop an innovative approach, we synthesize chiral amines **3** *via* C-C bond formation by addition of boron reagent **2** to aldimines **1** in the presence of recoverable and reusable chiral phosphine nanoligands supported on MNPs that complexed with Pd metal (scheme1). The structure of the catalyst was characterized *via* SEM, EDAX, TGA and FT-IR techniques, and the prepared products were identified by melting point and IR, ^{1}H NMR and ^{13}C NMR spectral analysis.



Scheme1. Synthesis of chiral amines by arylation of imines

Keywords: Asymmetric Synthesis, Chiral Amines, Phosphine Ligands, Magnetic Nanoparticles

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Design and synthesis of a new type dibenzosuberenone-dihydropyridazine based fluorescent dyes for heavy metal ion and multi-analyte sensing applications

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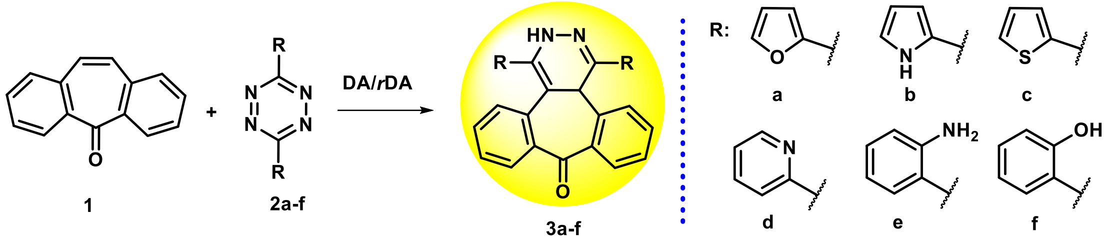
The widespread use of heavy metal ions in the industry results in serious environmental pollutions and human health problems, negatively affects agriculture, and destroys natural life [1]. Therefore, the development of fluorescence chemosensors for the determination of heavy and transition metal ions has attracted much attention in recent decades [2]. Dibenzosuberenone and polyconjugated derivatives exhibit photophysical properties such as photosensitizatione, fluorescence, and aggregation-indduced emission (AIE) [3]. Recently, our research group discovered a new class of dibenzosuberenone derived fluorescent dyes, and their photophysical and/or anion sensor properties were investigated [4,5]. In this study, various analogues of a new family of fluorophores based on derivatives dihydropyridazine-dibenzosuberenone were synthesized by inverse electron-demand Diels-Alder cycloaddition reactions between a dibenzosuberenone and derivatives tetrazine that bear various substituents (Scheme1). Then, the photophysical, heavy metal and multi-analyte sensor properties of these compounds will be investigated.



Scheme1. Derivatives dihydropyridazine-dibenzosuberenone.

***Keywords*:** Fluorescence chemosensor, Heavy metal ion, Multi-analyte sensor, Dibenzosuberenone, pyridazine.

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Synthesis of nickel metal-organic framework with 4,6-diamino-2-mercaptopyrimidine as reusable and efficient catalyst in the synthesis of pyranopyrazoles and selective oxidation of sulfides

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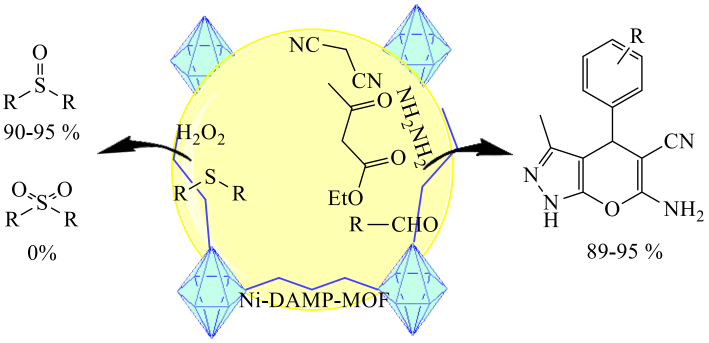
In this work, 4,6-diamino-2-mercaptopyrimidine was applied as an outstanding chelating agent for the synthesis of a new nickel metal-organic framework (Ni-DAMP-MOF) as a reusable, selective and efficient catalyst. The obtained Ni-DAMP-MOF was characterized by BET, SEM, WDX, EDS, FT-IR, XRD, and AAS techniques. Then, this metal-organic framework was applied as a novel catalyst in the selective oxidation of sulfides to sulfoxides and synthesis of pyranopyrazole derivatives. All products were obtained with high yields and good purity based on ^1H NMR spectroscopy of the products, which indicate the practical activity of Ni-DAMP-MOF as catalyst. Pyranopyrazoles exhibit significant biological properties [1,2] and sulfoxide derivatives are an important material in organic chemistry which have some biological activities [3]. Also, Ni-DAMP-MOF was shown a excellent selectivity in the oxidation of sulfides to sulfoxides. Finally, the recoverability and reusability of this catalyst were investigated as an important principle in green chemistry.

Keywords: Ni-DAMP-MOF;; multicomponent reactions; selective oxidation of sulfides; pyranopyrazoles.



Scheme 1. Catalytic application of Ni-DAMP-MOF in the selective oxidation of sulfides and synthesis of pyranopyrazoles

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A copper complex stabilized on boehmite nanoparticles as an efficient nanocatalyst for the selective synthesis of diaryl ethers

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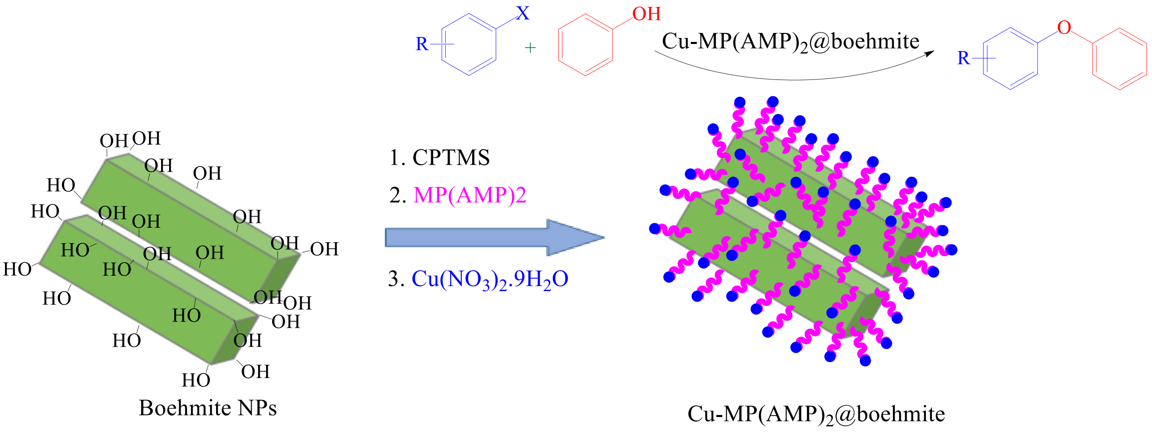
In this work boehmite nanoparticles (NPs) were synthesized from NaOH and $Al(NO_3)_3.9H_2O$ solutions. Then, the surface of boehmite NPs was modified by (3-chloropropyl)trimethoxysilane and further Schiff-base ligand (MP-bis(AMP)) was immobilized on its surface. At final step, a copper complex was stabilized on the surface of modified boehmite NPs (Cu(II)-MP-bis(AMP)@boehmite). These obtained nanoparticles were characterized using SEM, EDS, WDX, AAS, TGA, BET, FT-IR, and XRD techniques. In continue, the catalytic activity of Cu(II)-MP-bis(AMP)@boehmite has been investigated in the synthesis of biphenyl ether derivatives through C-O coupling reaction. C-O coupling reaction is a powerful tool for the synthesis of ether derivatives [1-4]. Cu(II)-MP-bis(AMP)@boehmite catalyst has been reused for several times in the synthesis of ether derivatives.

Keywords: Boehmite nanoparticles; ether derivatives; coupling reaction; C-O coupling reactions; copper complex.



Scheme 1. Catalytic application of Cu(II)-MP-bis(AMP)@boehmite in the synthesis of ether derivatives

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Homoselective synthesis of tetrazoles in the presence of Schiff base complex of lanthanum on modified MCM-41 as a reusable nanocatalyst

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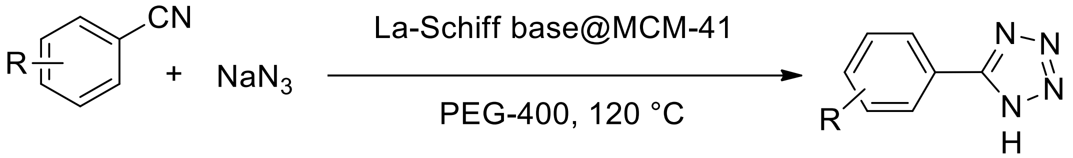
Mesoporous MCM-41 has unique properties such as large specific surface area homogeneous hexagonal pore, ease of functionalization, high thermal stability, relatively hydrophobic nature, simple preparation and easy separation from the reaction mixture [1]. Therefore, in this work, hexagonal arrangement mesoporous MCM-41 was synthesized and functionalized with a new Schiff base ligand. Then, a lanthanum complex was stabilized on the surface of modified mesoporous MCM-41 (La-Schiff base@MCM-41). The prepared La-Schiff base@MCM-41 was characterized by BET, SEM, WDX, EDS, XRD, and AAS techniques. Then, La-Schiff base@MCM-41 was used as a new catalyst in the homoselective synthesis of tetrazole derivatives. Because, tetrazoles were used in drugs and they are used as analgesics, herbicides, antimicrobial, anti-proliferative, anti-inflammatory, and anticancer agents [2-4]. For example, Valsartan, Losartan and TAK-456 are several pharmacologically important of tetrazoles [5]. Finally, the recyclability and reusability of this catalyst were investigated as an important principle in green chemistry.

Keywords: Mesoporous MCM-41; Schiff base complex; Homoselective catalyst; Tetrazoles, Reusable nanocatalyst.



Scheme 1. Catalytic application of La-Schiff base@MCM-41 in the homoselective synthesis of tetrazole derivatives

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Synthesis the Boehmite-SSA nanoparticles as an additive to enhance the electrochemical properties of the heterogeneous cation exchange membrane

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Ion exchange membranes have an important role in efficiency of electrodialysis process which is a well-known water treatment technology. The synthesis and modification of these membranes can be so effective in developing electrodialysis process in different applications [1, 2]. Incorporation of nanoparticles is one of the modification methods for enhancing electrochemical properties of the cation exchange membranes (CEM) [3]. So, in the current study the synthesis of Boehmite silica sulfuric acid (Boehmite- SSA) was carried out with the aim of its apply as an additive to enhance the electrochemical properties of a heterogeneous CEM. The effects of Boehmite- SSA concentration on the electrochemical properties and hydrophilicity of the membrane were investigated. The FTIR and SEM analyzes verified the functionalization of nanoparticle and their size in nanometer scale, respectively. The results showed that the presence of Boehmite- SSA functional groups significantly improved the electrochemical properties of the membrane [4]. At a concentration of 2 wt.% nanoparticles, membrane potential, Ion exchange capacity, permselectivity and conductivity were enhanced by 8%, 7% and 50%, respectively.

Keywords: Cation exchange membrane, Boehmite- SSA nanoparticles, Membrane potential, Ion exchange capacity

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A new complex of neodymium on biochar magnetic nanoparticles as a reusable nanocatalyst in the selective synthesis of tetrazole derivatives

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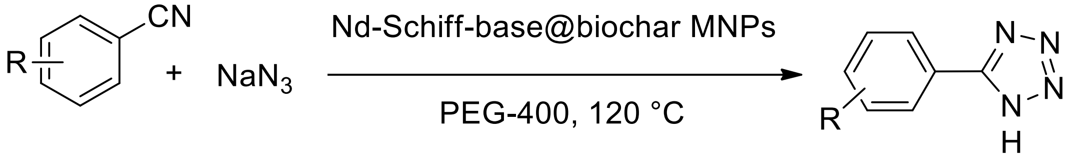
Catalyst species and waste recycling are important factors in chemistry, industrial, medicinal, green chemistry and economic efficiency. Therefore, in order to waste recycling, biochar nanoparticles were synthesized from chicken manure as a novel catalyst support. Biochar nanoparticles are an inexpensive heterogeneous solid with high density of hydroxyl, carbonyl, and carboxylic acid functional groups for immobilization of various ligands [1-3]. In the other hand, magnetic biochar nanoparticles have advantages of both biomaterials (such as large specific surface area, stability and inexpensively) and magnetic nanoparticles (such as feasible separation by an external magnet). Therefore, biochar nanoparticles were magnetized using nickel magnetic nanoparticles and then modified by 3-chloropropyltrimethoxysilane. Finally, a Schiff-base complex of neodymium was immobilized on modified biochar magnetic nanoparticles (Nd-Schiff-base@biochar MNPs) as reusable and efficient catalyst in the homoselective synthesis of tetrazole derivatives. Because, tetrazoles are used for herbicidal, anti-HIV drug candidate, analgesic, antimicrobial, anti-proliferative, anti-inflammatory, and anticancer agents [4-6]. This catalyst can be reused for several times without significant loss of its catalytic efficiency.

Keywords: Biochar nanoparticles; magnetic nanoparticles; neodymium; Schiff-base complex, tetrazoles.



Scheme 1. Synthesis of tetrazole derivatives in the presence of Schiff-base complex of neodymium on modified biochar magnetic nanoparticles

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A green method for confirming the Sonogashira reaction with magnetic nanoparticles

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Among the common chemical reactions in the research world, one of the most interesting reactions is the Sonogashira coupling reaction. The reaction involves carbon-carbon coupling between two triple bonds by a magnetic nanocatalyst with a silicate coating, a morpholine linker, and copper-coated copper. The greenness of the reaction is due to the reaction in ethanol solvent at a temperature of 75 degrees Celsius, where the resulting products are above 98% and the efficiency of the catalyst is above 90% of its power. The efficiency of nanocatalysts is comparable to other research works [2-4], which is more than 25% more efficient than them in performing Sonogashira reaction. Other applications of this nanocatalyst in the medical industry [1] include the adsorption of drug biomolecules that have been presented in previous research.

Keywords*:* Magnetic nanoparticles, Copper nanoparticles, Sonogashira reaction

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Approaches Towards First Total Synthesis of Onosmone and Analogues

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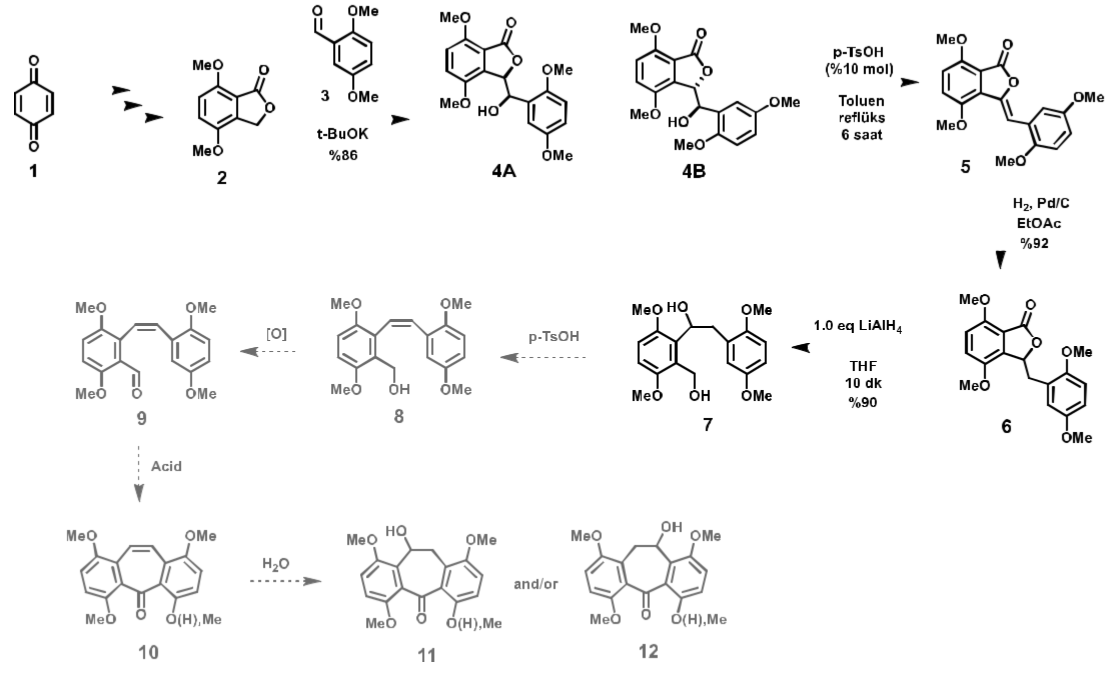
Onosma plant is used as tonic, demulcent, diuretic and refrigerant. Onosmone is isolated from *Onosma Limutaneum* plant in trace amounts and is a dibenzosuberone derived compound [1]. The total synthesis of this molecule has not been done yet. In this study, the first total synthesis of onosmon is aimed. For this purpose, lactone **2** was synthesized from *p*-benzoquinone **1** according to the methods in the literature[2-4]. So far, the synthesis steps from lactone **2** to diol **7** have been carried out successfully (Scheme1). Our work continues intensively for the synthesis of **8-12** compounds.



Scheme 1. Total Synthesis of Onosmone and Analogues

Keywords: Onosmone, *Onosma Limutaneum,* Dibenzosuberone, Natural product synthesis, Total synthesis

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Synthesis of Fe_3O_4/polyaniline nanoparticles as an MRI contrast agent

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Magnetic resonance imaging (MRI) is one of the most powerful imaging techniques, being noninvasive, with good spatial resolution [1] and Fe_3O_4 magnetic nanoparticles (MNPs) are suitable for MRI contrast since the MNPs can enhance the alterations of proton relaxation in the tissue microenvironment, and thus provide better MRimaging and longer life times in the bloodstream. However, relatively high toxicity of magnetic nanoparticles restricts the use of these materials to human beings. Therefore, many approaches have been focused on surface modification of magnetic nanoparticles with biocompatible materials, because these materials have biocompatible and biodegradable properties as well as low toxicity [2]. In this work polyaniline have been onto NPs via chemical polymerization of the corresponding monomers and may have been modified [3]. First, Fe_3O_4 were synthesized by co-precipitation of Fe^{2+} and Fe^{3+} ions [4]. Then Fe_3O_4 NPs surface was modified by polymerization of aniline [5] and Fe_3O_4/PANI NPs were synthesized. Synthesized Fe_3O_4/PANI NPs by FTIR, SEM, VSM and MRI techniques were studied. The surface chemical structure of NPs was characterized by FTIR which confirmed the correctness of synthesis and showed that polymerization was well performed by aniline. Images from the SEM showed that the NPs were synthesized as core-shell with an average diameter of 23/4nm. The magnetic properties of NPs were characterized by VSM that show the saturation magnetization of NPs is 58emu/g. Images from the MRI, which show an increase in the magnetic resonance signal of NPs in water as a function of the increase in the concentration of synthesized NPs, indicate that as the concentration increases, the measured weight T_2 contrast gradually increases. According to studies and the non-toxic NPs and that NPs are relatively easy to synthesize and are well dispersed, the NPs obtained as contrast material are suitable for use in magnetic resonance imaging and cancer cell detection.

Keywords: Contrast agent, Core-shell structure, MRI, Polyaniline

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Synthesis of Fe_3O_4/MIL-100(Fe) nanoparticles as an MRI contrast agent

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Magnetic resonance imaging (MRI) is one of the most powerful non-invasive imaging modalities utilized in clinical medicine today. Fe_3O_4 nanoparticles (NPs) have been widely used for MRI in diagnostic applications. With proper surface coating, Fe_3O_4 NPs can be well dispersed into suitable solvents, forming homogeneous suspensions, called magnetic fluids [1]. The MIL-100(Fe) due to non-toxic and medical applications in MRI was used for surface modification and due to its iron content, it strengthens its magnetic properties [2]. In this work, MIL-100(Fe) shell be specifically formed on the surface of Fe_3O_4 by self-assembly of Fe^{3+} ions and carboxylic acid. First, Fe_3O_4 were synthesized by co-precipitation of Fe^{2+} and Fe^{3+} ions [3]. Then layer-by-layer method was utilized to fabricate the porous Fe_3O_4/MIL-100(Fe) core-shell NPs [4]. Synthesized Fe_3O_4/MIL-100(Fe) NPs by FTIR, SEM, VSM and MRI techniques were studied. The surface chemical structure of NPs was characterized by FTIR and the resulting peaks show that the NPs synthesis is done correctly. Images from the SEM showed that the NPs were synthesized as core-shell with an average diameter of 28nm. The magnetic properties of NPs were characterized by VSM that show the saturation magnetization of NPs is 57emu/g. Images from the MRI, which show an increase in the magnetic resonance signal of NPs in water as a function of the increase in the concentration of synthesized NPs, indicate that as the concentration increases, the measured weight T_2 contrast gradually increases. Fe_3O_4/MIL-100(Fe) demonstrated excellent MRI property and could potentially be used as MRI contrast agent for magnetic resonance imaging.

Keywords: Contrast agent, Fe_3O_4, Magnetic resonance imaging, MIL-100(Fe)

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A New Approach to Calibration Methodology of WD_XRF Applied in Elemental Analysis of Zeolite Compounds with High Accuracy and Precision

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X-ray Fluorescence spectrometry (XRF) is offered in terms of quantitative, fast, and reliable analysis in a wide range of mineral compounds. The intensity of the fluorescence X-ray radiation emitted from the analyte is used for the quantitative analysis of elements in the sample. [1] However, there is no simple proportion between the intensity of X-ray fluorescence and concentration of each element, due to the interaction between the emission of secondary fluorescent radiation and the sample matrix, especially when the matrix contains heavy elements. While matrix effects cannot be reduced or omitted during sample pretreatment, perfect matching between standards and samples, and adjusting of the calibration based on standard reference materials (CRMs) with a matrix quite similar to the test sample are required for better estimates. [2] The present paper describes an innovative XRF calibration method using validated samples and an inert binder, to make some matrix-matched standard samples. The uncertainty-weighted least-square linear regression (UWLR) model was applied for the authentic quantitative multi-elemental analysis. [3] Moreover, the effect of the parameters such as particle size, spectral line interferences, and moisture content of the samples on the accuracy of XRF was assessed. This evaluated method was adapted to determine five major elements, including Al, K, Na, Si, and La in the most common type of synthetic zeolites like A, Y, and ZMS-5. Variations represented that the limits of detection were 0.20%, 0.12%, 0.31%, 0.18%, and 0.10%, respectively which computed from statistical analyses of duplicate sample aliquots, with RSD <2% for most elements mentioned above, and RSD < 5% for Na. Analytical accuracies were verified by Inductively Coupled Plasma Spectroscopy (ICP) measurements and classical analysis with reliable ASTM test methods.

Keywords: WD-XRF analysis, Calibration method, Zeolite sample, UWLR model.

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Stimuli responsive nano-composite co-delivery of Doxorubicin and ciprofloxacin using HPLC-UV combined spectroscopy methods

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This work has been done to present a kind of stimuli-responsive drug nano-carrier for embedding and consequently delivering combinational pharmaceutical agents including Doxorubicin (DOX, anticancer) and Ciprofloxacin (Cipro, antibiotic) into or in close vicinity of ailment for enhancing therapeutic effects of drugs and reducing their side effects. Applied biocompatible magnetics drug carriers were synthesized through in-situ polymerization techniques. [1][2] Characterization techniques reveal that the suggested nano-carrier had a well-defined spherical shape with the pore size of 10–30 nm and typical super paramagnetic features. Synthesized nano-carriers were used for loading drugs with the percentage of 53.90% and 82.32% for DOX and Cipro, respectively. On the other hand, nano-carriers were demonstrated as a kind of promising drug delivery system for in-vitro breast cancer investigations. [3] Cumulative release profile of drugs was obtained at different pH values using methods of Ion-mobility spectrometry (IMS) and HPLC-UV to navigate magnetic polyurethane nano-composite kinetic mechanisms through different mathematical models. The results showed that the nano-carrier exhibited a smart controlled release profile following Higuchi model with the highest correlation coefficient. In-vitro Cytotoxicity of nano-composite was tracked on MCF-7 cell lines using methyl thiazoletetrazolium (MTT) viability assay which shows nano-carriers have no toxicity for intelligent targeted drug delivery.

Keywords: Magnetic nano particles, Polyurethane, Drug delivery, Kinetic investigation, Polymerization.

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A novel and facile synthesis of TiO_2/PANI/Au NPs as a new substrate for high sensitive and selective Hydrazine sensor

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Hydrazine is a toxic substance and its measurement is very important due to its widespread use in agriculture, industry, and rocket fuel [1]. In the present study, a new electrochemical sensor for the oxidation of hydrazine is presented that modifies the glassy carbon electrode surface layer by layer. Metal oxide nanoparticles are widely used in energy applications due to their relatively high catalytic activity, low cost, high chemical stability, and non-toxicity [2]. PANI is a substance used as a converter to transform a chemical signal into an electrical signal [3]. Our aim in the present work is to develop a fast and sensitive electrochemical sensor for the measurement of hydrazine. For this aim, synthesized TiO_2 sample, and polyaniline and gold, which are electrochemically synthesized on glassy carbon electrodes, are used as electrochemical modifiers to produce the hydrazine sensor. XRD, SEM, EDX were used to investigate the structural, morphological and compositional details of these synthesized materials. The behavior of hydrazine on glassy carbon modified with TiO_2/PANI/Au NPs and on unmodified glassy carbon electrodes was studied. The modifier used in this work dramatically increases the hydrazine response and reduces the potential for oxidation, due to the excellent conductivity and high adsorption and high surface area of TiO_2/PANI/Au NPs/GCE. The proposed sensor display high electrocatalytic activity to hydrazine oxidation. The electrochemical behavior of hydrazine on various modified electrodes was investigated by cyclic voltammetry technique. DPV technique was used to construct the calibration graph for hydrazine under optimized conditions. The linear range and limit of detection for hydrazine were calculated with this proposed sensor. It was compared with other electrodes used in sources. The results also showed that TiO_2/PANI/Au NPs/GCE, as a sensor, has good stability, repeatability and repeatability in hydrazine measurement. The modified electrode was also successfully used for the determination of hydrazine in different water samples.

Keywords: Hydrazine, Electrochemical sensor, Differential pulse voltammetry, Glassy carbon electrode, TiO_2/PANI/Au NPs

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Potentiometric Ferric measurement by using solid-state sensor based on carbon nano tube and N- ((bis (dimethyl amino) methylene) carbamothiol) benzamide

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Although iron is the fourth most abundant element in the earth's cortex, however it is only present in trace amounts in the open ocean. Iron is an extremely important bioactive trace metal in the ocean, as it limits phytoplankton production and is also effective in regulating carbon dioxide concentrations in the atmosphere[1]. Therefore, tracing of ferric ions is of great importance in environmental samples. Various common methods are used to determine iron such as complexometric, spectrophotometry, flame and atomic absorption spectrometry (AAS), inductively coupled plasma (ICP), fluorimetry, voltammetry, and potentiometry[2]. Some methods such as complexometric has high detection limit and the available methods for low-level determination of Fe (III) in solutions include flameless AAS and ICP, involve expensive instrumentation and sample pretreatment, which is time consuming and inconvenient. Potentiometric methods offer great advantages such as easy preparation and procedures, short response time, high selectivity, low-energy consumption, wide linear working range at low cost compared to the other analytical methods [3]. There are different types of potentiometric ion selective electrodes including PVC membrane electrodes (PME), coated wire electrodes (CWE), carbon paste electrodes (CPE), solid state electrodes (SSE) and field effective transistors (FET) [4]. PVC membrane electrodes have low mechanical stability and high detection limit [5].In this research, solid-state potentiometric PVC membrane sensor for rapid recognition and measurement of Fe^{3+} is fabricated. The best composition for membrane was achieved with PVC (30%), sodium tetraphenylborate (NaTPB) as ionic additive (2%), N-((bis (dimethyl amino) methylene) carbamothiol) benzamide (10%) and dibutyl phthalate (DBP) as plasticizer (58%). Conductive compound of solid-state electrode was made from graphite, carbon nano tube, epoxy resin and hardener on a Copper wire. The coated wire was soaked in membrane composite and a thin layer PVC membrane was coated on surface the conducting transducer. The Nernstian slop of 20.286 mV/decade obtained for Fe^{3+} in concentration range 1×10^{-1} to 1×10^{-8} mol/L with low detection limit 3×10^{-9} mol/L at PH range of 5 to 10. The sensor response time was approximately 5s. The sensors were applied as indicator electrode in potentiometric titration of $Fe^{3+}$with EDTA.

Keywords: Sensor, Solid state, Potentiometry, Carbon nano tube, Ferric

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Electrocatalytic performance of nanostructured MgFe-LDH for determination of vitamin B6

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Vitamin B includes various water-soluble vitamins and a bunch of considerably bioavailable 3-hydroxy-2-methylpyridine derivatives, mainly attend together within the form of non-phosphorylated and phosphorylated in food samples and the whole of them are essential for natural growth and metabolism, however, humans do not synthesize any of them in sufficient amounts. Pyridoxine hydrochloride is a white crystal and is soluble in water. Pyridoxine is commonly considered vital for human nutrition and by revealing a deficiency in other elements of the B vitamin family, also vitamin B_6 is considered to be deficient in-patient body[1-4] In this research work, an electrochemical sensing assay has been developed by using MgFe-LDH for the highly sensitive and selective determination of vitamin B_6 in various samples. At first, MgFe-LDH has been synthesized via hydrothermal-assisted ultrasonic method as an eco-friendly method. Afterward, the obtained MgFe-LDH was dispersed in water and deposited on a glassy carbon electrode (GCE) by the dropping method. Then electrochemical methods differential pulse voltammetry and cyclic voltammetry (DPV and CV) have been applied for sensitive determination and characterization of the mentioned target. Moreover, electrochemical impedance spectroscopy (EIS) has been also used for approving the obtained cyclic voltammetry consequences. For confirming the successful synthesis of the MgFe-LDH, various characterization methods including FE-SEM, EDS, XRD, FTIR, and BET have been utilized. After the plotted the calibration diagram with the DPV technique, the detection limit, and the linear range were calculated for vitamin B_6 oxidation. Therefore, the method is sensitive, simple, and specific with a short analysis time, and the main advantages of this sensor are an easy synthesis route, low detection limit, excellent stability, repeatability, and good selectivity in vitamin B_6. One of the successes of this sensor is in determining vitamin B_6 in tablets, human plasma, and rice flour samples.

Keywords: Differential pulse voltammetry, Glassy carbon electrode, Vitamin B_6, Electrochemical sensor, MgFe-LDH

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Genetic algorithm coupled with using back-propagation artificial neural network (BP-ANN) pattern recognition method and infrared spectrometry to classification of Listeria samples

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Nutrition-caused listeriosis is one of the most serious and most severe nutrition-transferable diseases that can be considered a threat to human health. Owing to the high resistance of listeria monocytogenes against environmental conditions, existence of this bacterium in raw or processed foods is also possible and the appropriate evaluation and monitoring is necessary actions and regulations from the beginning of the production cycle to the consumption of the nutrients. The diagnosis of pathogens in food safety is essential [1,2].
This study investigated the classification of Listeria samples using IR spectroscopy. The Mid-FTIR spectra were pretreated by baseline corrected, multiplicative scatter correction (MSC) transformation to eliminate the baseline shift deletion and multiplicative effect of scattering and orthogonal signal correction (OSC) which removes unrelated or orthogonal systematic variation from the spectral data. In the next step, from 792 wavelengths, 202 wavelengths were selected by the genetic algorithm (GA) algorithm as a feature selection procedure for back-propagation artificial neural network (BP-ANN). The dataset of 1717 samples was split into two subsets as calibration and validation sets through randomly. 1288 samples were used to construct the calibration model and 429 samples were used for the validation. The results are summarized in Table1. As seen in Table1, the results presented BP-ANN with OSC preprocessing providing better results by providing 93.00% ACC, 99.00% non-error rate, and 1.00% error rate in the test set, respectively. Therefore, the aim of this research is to introduce an easy, fast, and low cost method to identify listeria based on spectroscopy studies and using chemometrics method.

Table1. The efficiency parameters for training, Cross validation and test sets by BP-NN chemometric

Method		Training set				Cross validation				Test set			
	Preprocessing	Error rate	Non-error rate	Accuracy	Not assigned	Error rate	Non-error rate	Accuracy	Not assigned	Error rate	Non-error rate	Accuracy (ACC)	Not assigned
BP-ANN	OSC	0.0	100.0	100.0	2.0	1.0	99.0	99.0	4.0	1.0	99.0	99.0	3.0
	MSC	6.0	94.0	96.0	24.0	8.0	92.0	95.0	23.0	13.0	87.0	88.0	24.0

Keywords: Listeria samples, Pattern recognition method, Genetic algorithm, Back-propagation artificial neural network (BP-ANN)

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Paraquat herbicide removal in aqueous solution using some advanced oxidation processes

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Paraquat is a nonselective contact herbicide to control or suppress a broad spectrum of emerged weeds. It is used as the third most widely herbicide in the world [1,2]. The United States Environmental Protection Agency (USEPA), classified paraquat dichloride as a restricted use pesticide due to high acute toxicity to animals and people with the acute oral toxicity of 4,4-bipyridyl with an LD_{50} value of 40-200 mg/kg body weight [3]. Nowadays, advanced oxidation processes (AOPs) intensively studied as the most environmentally friendly and promising techniques for the degradation of recalcitrant organic pollutants in water by powerful oxidants especially hydroxyl radicals or superoxide radicals [4]. Heterogeneous photocatalytic degradation in presence of nanostructure catalysts attained good efficiencies in degradation of organic compounds among the various AOPs the photocatalytic activity of TiO_2 consists in the production of photo-generated electrons, leading to the formation of highly oxidative holes in the valence band where a reaction occurs with the adsorbed water (i.e., surface hydroxyl) to form the highly reactive hydroxyl radicals [5]. Inorganic oxidants such as H_2O_2, $S_2O_8^{2-}$ and IO_4^{-} have been considered by researchers and used for removal and mineralization of various organic pollutants from aqueous solutions [6-8]. In this study, the performance of UV-C irradiation, TiO_2 nanophotocalysise (TiO_2NP), UV/KPS (potasium persulfate), UV/KPI (potasium periodate), UV/TiO_2NP/KPI and UV/TiO_2NP/KPS as advanced oxidation processes (AOPs) in removal of paraquat (PQ) herbicide aqueous solution have been comparaded. Removal studies were carried out by measuring the absorbance at λ_{max}=258 nm with the help of a UV–visible spectrophotometer. Results shown that in constant conditions (400 mL of 30 mgL^{-1} PQ solution, pH=6, tempratuer=25 ˚C and time=20 min), [TiO_2]= 100 mgL^{-1}, initial PS concentration of 200 mgL^{-1} and initial PI concentration of 100 mgL^{-1}, the removal efficiency for UV/TiO_2NP/KPI process has been the most amount (about 70%).

Keywords*:* Paraquat herbicide, Advanced oxidation processes, Removal efficiency.

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Pirimicarb insecticide removal using advanced oxidation processes

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Pirimicarb is a selective systemic insecticide that is widely employed against aphids with a contact action. The United States Environmental Protection Agency (USEPA), classified it as a highly toxic substance and carcinogenic to humans and animals due to LD50 = 100-200 mg/kg body weight (or LC50 = 22-26 mgL^{-1}) and toxic stimulant effects on lung cell culture in humans and carcinogenic potential high [1]. Advanced oxidation processes (AOPs) intensively studied as the most environmentally friendly and promising techniques for the degradation of recalcitrant organic pollutants such as insecticides in water by powerful oxidants especially hydroxyl radicals or superoxide radicals [2]. Heterogeneous photocatalytic degradation in presence of nanostructure catalysts such as TiO_2, as one of the AOP, attained good efficiencies in degradation them. Photocatalysts act by production of photo-generated electrons in the conduction band of the catalysts, leading to the formation of highly oxidative holes in the valence band where a reaction occurs with the adsorbed water (i.e., surface hydroxyl) to form the highly reactive hydroxyl radicals [3]. Inorganic oxidants such as ClO_3^-, BrO_3^-, H_2O_2, $S_2O_8^{2-}$, and IO_4^- have been considered by researchers and used for removal and mineralization of various organic pollutants from aqueous solutions [4-6]. In this study, the performance of UV-C irradiation, TiO_2 nanophotocalysise (TiO_2NP), UV/KPS (potasium persulfate), UV/KPI (potasium periodate), UV/TiO_2NP/KPS and UV/TiO_2NP/KPS as processes of advanced oxidation (AOPs) in removal of pirimicarb (PC) insecticide aqueous solution has been comparaded. Resuls of uv-vis spectroscopy shown that in constant conditions (400 mL of 30 mgL^{-1} PC solution, pH= 6, tempratuer = 25 ˚C and time=10 min), $[TiO_2]$= 30 mgL^{-1}, initial PS concentration of 30 mgL^{-1} and initial PI concentration of 30 mgL^{-1}, the removal efficiency for UV/TiO_2NP/KPS process and and for UV/TiO_2NP/KPI process were about 50% and 75%, respectively.

Keywords: Pirimicarb insecticide, Advanced oxidation processes, Removal efficiency.

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Efficiency of powder activated carbon magnetized by iron magnetic nanoparticles coated with lignin for ofloxacin antibiotic removal from hospital wastewater

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Emerging contaminants in the environment have caused enormous concern in the last few decades, and among them, antibiotics have received special attention. On the other hand, adsorption has shown to be a useful, low-cost, and eco-friendly method for the removal of this type of contaminants from water. An understanding of the interaction mechanisms of antibiotics with environmentally relevant sorbents is important to determine the environmental fate of antibiotics and to develop wastewater treatment strategies. Ofloxacin (OFX) is a broad spectrum fluoroquinolone that has been linked to serious side effects which include ruptured tendons and neurological damage resulting from seizures. As micro-contaminants, antibiotics in the aquatic environment may persist and be transported to reservoirs, surface and groundwater sources which supply raw water to treatment plants [1]. Activated carbon has been widely used to remove organic contaminants from water and wastewater in industrial scale application. It has high adsorption capacity as well as removal efficiency for certain organic substances. In some application, the removal efficiency can reach 100% [2]. Lignin is the second most abundant natural polymer with cellulose being number one, making up to 10–25% of lignocellulosic biomass. Lignin is a three-dimensional, highly cross-linked macromolecule composed of three types of substituted phenols, which include: coniferyl, sinapyl and p-coumaryl alcohols [3]. Iron magnetic nanoparticles (Fe_3O_4) are used because of their high magnetic properties for separation and biological applications. Fe_3O_4 nanoparticles could easily aggregate due to the nanoscale effect and magnetic gravitational effect [4,5]. In this work powder activated carbon magnetized by iron magnetic nanoparticles coated with lignin were used for ofloxacin adsorption from aqueous solution. powder activated carbon magnetized by iron magnetic nanoparticles coated with lignin were prepared and subsequently characterized using FTIR, XRD, TEM, SEM and VSM methods. This type of adsorbent is low cost, high efficient and reusable. Also, the parameters of the adsorbent dose, the pH, contact time and adsorption isotherms in the antibiotic removal process were investigated. The maximum removal percentage was obtained 91.5% for adsorption of ofloxacin.

Keywords: Lignin, Fe_3O_4, Activated Carbon, Antibiotic, Ofloxacin

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Photo-assisted removal of CR and BR46 dye contaminated wastewater via a new MT-COF/Cu-MOF nanohybrid

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The application and expansion of porous compounds have a long history. In the meantime, covalent-organic frameworks (COFs) and metal-organic frameworks (MOFs) materials have attracted extensive attention because of their great application potential in the fields of adsorption, photocatalysis, drug delivery, luminescence, sensor, separation analysis, energy storage, and others [1]. Current research results show these hybrid materials have ingenious obvious structural characteristics and superior performance. COFs/MOFs hybrid materials incorporate the COFs and MOFs advantages. Among the reasons for preference to hybridize MOF and COF compounds are improving the framework strength in harsh conditions: i.e., organic, acidic, and alkali environments, and enhancing the special surface area and the active sites. In general, the hybridization of COFs and MOFs covers their inherent defects through the synergistic effect and improves the properties of the final composition [2, 3]. In this study, by hybridization of copper-based metal-organic framework (Cu-MOF) and melamine-terephthaldehyde-based π-conjugated covalent organic framework (MT-COF), a novel MT-COF/Cu-MOF hybrid material prepared and characterized by Fourier transform infrared, field-emission scanning electron microscopy, X-ray diffraction, transmission electron microscopy, and Brunauer-Emmett-Teller (BET) surface area analysis. As-synthesized MT-COF/Cu-MOF applied as a practical adsorbent for rapid and high-efficient photo-assisted removal of anionic Congo red (CR) and cationic Basic red 46 (BR46) dyes via electrostatic interactions, H-bonding, and π–π stacking from aqueous solution. The hybrid substrate yielded a removal capacity of 63.9 and 81.03 % for CR and BR46 dyes, respectively, at neutral pH. The adsorption study of CR and BR46 dyes by prior MT-COF comprises kinetic studies, which found follow a pseudo-second-order model. These results reveal the potentiality of the MT-COF/Cu-MOF hybrid as an excellent organic-contaminants removal agent.

Keywords: Covalent organic framework, Metal organic framework, Hybridization, Photo-assisted removal

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A facile method for synthesis of Ag/Ni(OH)$_2$ composites and its application for electrocatalytic determination of Nitrofurantoin

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Antibiotics, also called antibacterials, are drugs that stop or slow down the growth of bacteria. Nitrofurans are a common part of antibiotics and one of the most important derivatives of nitrofuran is Nitrofurantoin (NFT), driven from antibiotic drugs and is recognized and believed to be one of the most important antibacterial agents for urinary tract infection curement in animals and humans. Noble metallic nanoparticles such as Pt, Ag, and Au NPs with high stability and simple chemical synthesis have been utilized in different fields such as energy, biotechnology, catalysis, and electronics. Compared to other noble metal nanoparticles, silver nanoparticles exhibit more advantages. Ni(OH)$_2$ was utilized as a catalyst for the degradation of dyes and hydrogen production. Furthermore, Ni(OH)$_2$ by having a wide surface and indicating great synergistic effects is suitable for producing noble metal nanoparticles. Ni(OH)$_2$ has been utilized as a support and an adsorbent [1-3]. The aim of this study was to present a successful synthesis of Ag/Ni(OH)$_2$ composites by mixing Ni(OH)$_2$ and ethanol solution of AgNO$_3$ via magnetic stirring at room temperature, without the addition of any strong reductant or surfactant. The structure and morphological details of Ag/Ni(OH)$_2$ composites were investigated by Transmission Electron Microscopy (TEM), field emission scanning electron microscopy (FESEM), X-ray diffraction (XRD), energy-dispersive X-ray spectroscopy (EDX), and element map techniques. In the present research work, this synthesized sample has been used to measure nitrofurantoin by the DPV technique. By preparing the suspension, a synthesized sample was used to modify the surface of the glassy carbon electrode. The linear range of concentration was 0.11-13 µM and 13-212 µM and the limit detection (LOD) was calculated to be 0.079 µM. The advantages of this method include high sensitivity of the method and wide linear range, low detection limit, high repeatability and long-term stability, easy synthesis method, low cost, and short analysis time. This sensor was successfully used to determine nitrofurantoin in tablet and serum blood samples.

Keywords: Electrochemical detection, Ag/Ni(OH)$_2$ composites, Antibiotics, Glassy carbon electrode, Differential pulse voltammetry

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Bi_2Te_3 decorated on graphitic carbon nitride nanosheets as a electrochemical sensor for determination of epinephrine in biological and pharmaceutical samples

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Adrenaline, also known as epinephrine, is a neurotransmitter hormone and class of endocrine catecholamines. It increases heart rate, constricts arteries, dilates the airways, and is effective in triggering a sympathetic nervous system warfare response. Therefore, it is important to measure this hormone. Bi_2Te_3 is a good electrocatalytic material which known as nanoplate catalyst material that can be used for optoelectronic and electrochemical applications. In the present work, Bi_2Te_3 sheets were deposited on graphitic carbon nitride (GCN) nanosheets to obtain a Bi_2Te_3/GCN nanocomposite [1-3]. Bi_2Te_3/GCN was synthesized by two-step synthesis techniques (solvothermal and hydrothermal) method and after preparing the suspension of this synthesized sample, about 5µl were dropped on the electrode, and then the modified electrode was placed at room temperature for drying. The synthesized nanocomposite was characterized using Transmission Electron Microscopy (TEM), field emission scanning electron microscopy (FESEM), X-ray diffraction (XRD), energy-dispersive X-ray spectroscopy (EDX), and element map techniques. To determine epinephrine, glassy carbon electrode (GCE) modified with Bi_2Te_3/GCN nanocomposite was used. The proposed sensor was used for rapid determination of epinephrine with high sensitivity by differential pulse voltammetry (DPV) technique. The DPV technique was used under optimal conditions to plot an epinephrine oxidation calibration graph. The linear response was observed over the epinephrine concentration range of 40–200 µM for DPV and the lowest detection limit of 0.42×10^{-6} M for epinephrine oxidation. The results indicated that the fabricated sensor can easily be measured epinephrine, and this is due to its good repeatability, and excellent stability in determining epinephrine. One of the successes of this sensor is in determining epinephrine in pharmaceutical and biological samples.

Keywords: Bi_2Te_3/GCN sensor, Electrochemical sensor, Glassy Carbon Electrode, Epinephrine

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Electrodeposited histidine-layered double hydroxide nanosheets composed with carbon dot as coating for in-tube solid phase microextraction of chlorophenols from waters, juices, and honey samples

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Present work reports the synthesis of amino acids intercalated CuCr-layered double hydroxide nanosheets and composition of the nanosheets with carbon dot (C-dot). The prepared nanocomposite was employed as sorbent in an on-line in-tube solid phase microextraction (IT-SPME) method. The prepared coating was fabricated successfully on the inner surface of a copper tube by a facile two-electrode electrodeposition method. The prepared nanocomposites were characterized by X-ray diffraction (XRD), scanning electron microscope (SEM), transmission electron microscope (TEM), and Fourier transform infrared spectroscopy (FT-IR). The IT-SPME method followed by HPLC-UV was used for extraction, preconcentration, and determination of some chlorophenols (CPs). Important parameters affecting on the extraction efficiency of the CPs such as solution pH, salt concentration, and extraction and desorption conditions were investigated and optimized. Under optimal conditions, the response for CPs was linear with coefficients of determination at 0.9918 at the concentration range of 0.5 to 1000 µg L^{-1}. The detection limits (at S/N = 3) were obtained in the range of 0.1 to 1.0 µg L^{-1}. The inter- and intra-assay precisions (RSD%, n = 3) were obtained in the range of 4.0-6.5% and 4.5-8.4%, respectively. Considerable extraction results were achieved for determination of six chlorophenols in the real solutions (four water samples, two juices, and one honey).

Keywords: Carbon dot, Chlorophenols, Electrodeposition, In-tube solid phase microextraction, Layered double hydroxide.

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Electrochemical Determination of Paracetamol Using Carbon Paste Modified Electrode With MoO_3 nanobelt-graphene composite

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Paracetamol (PA) is a common analgesic and antipyretic medication that is widely used to reduce pain and fever [1]. Various analytical techniques have been reported for the determination of paracetamol (PA) in pharmaceuticals and biological samples, including chemiluminescence, fluorescence, HPLC, UV-Vis spectrometry, mass spectrometry, and electrochemical methods [2,3]. In the present work, MoO_3 nanobelt-graphene composite was synthesized by a hydrothermal method and characterized by SEM (Fig. 1.) and XRD analysis. Afterward, the prepared MoO_3 nanobelt-graphene composite was used to modify carbon paste electrode for the determination of paracetamol. The electrochemical characteristics of the sensor were evaluated using cyclic voltammetry (CV) (Fig. 2.), differential pulse voltammetry (DPV), and electrochemical impedance spectroscopy (EIS). To achieve the best electrochemical performance, important parameters such as pH, the amount of the modifier, deposition time, supporting electrolyte, pulse amplitude, pulse width, and step increment were investigated and optimized. Under optimal conditions, the obtained calibration curve using DPV was linear in the range of 1.0–20.0 μM with a detection limit of 3.2×10^{-8} M. High sensitivity, good reproducibility, and repeatability with RSD values of 3.7% and 2.2%, respectively and also good stability with a simple fabrication process are all features of this sensor.

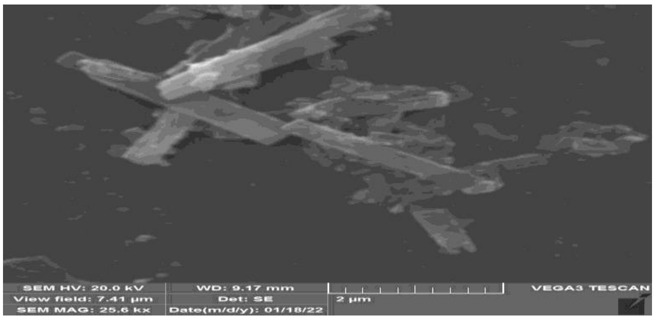

Fig. 1. SEM image of the prepared MoO_3 nanobelt-graphene composite.

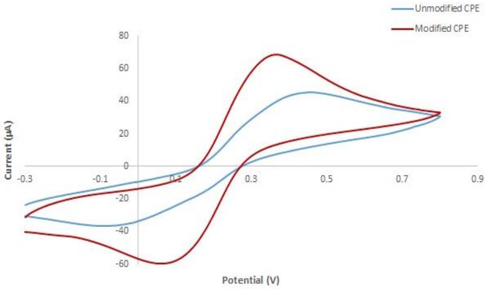

Fig. 2. CV for $[Fe(CN)_6]^{3-/4-}$ at BCPE (blue line) and MCPE (red line) at scan rate of 50 $mV.S^{-1}$

Keywords: Paracetamol, Nanobelt, Electrochemical sensor, Carbon paste electrode

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Preparation and Application of a Nano-composite Based on Clinoptilolite Zeolite in Magnetic Solid-phase Extraction of Triptorelin from Biological Samples

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Prostate cancer is the most commonly diagnosed cancer among men after the lung cancer, therefore finding the ways to cure and control of these disease is very important [1]. Triptorelin acetate is the long acting agonist that has the FDA approval in curing prostate cancer. This drug effect on pituitary gland and results in an initial increase in circulating levels of gonadotropins. Continuous administration of triptorelin acetate cause pituitary desensitization and down-regulation, leading to suppressed circulating levels of gonadotropins and sex hormones [2]. Therefore, development of rapid and reliable selective or multi-component methods is necessary for extraction and detection of this drug in different matrices. Zeolite nano-composite have found a wide range of applications in different sample preparation technologies because of their unique properties [3]. This dissertation aims to develop simple, rapid, sensitive and environment-friendly magnetic solid phase extraction (MSPE) methods based on zeolites as adsorbents. In this work, a magnetic zeolite was synthesized, characterized and then applied as an effective adsorbent for MSPE of triptorelin prior to HPLC analysis. Various experimental parameters affecting the extraction recovery including the amounts of sorbent, volume of desorption solvent, extraction and desorption time, pH, temperature, washing solvent type were optimized. The method was then validated by figures of merit under the optimal conditions. The applicability of the “MSPE” was evaluated by detecting of triptorelin in biological samples.

Keywords: Magnetic solid-phase extraction, Clinoptilolite zeolite, Magnetite nano-particles, Nano-composite, Triptorelin

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Application of copper chloride modified copper electrode for electrocatalytic oxidation of ethylene glycol

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In these studies, the copper chloride modified copper (CCMC) electrode was prepared and used for electrocatalytic oxidation of ethylene glycol. For the preparation of the modified electrode, the polished copper electrode was placed in 0.1 M $CuCl_2$ solution for 20 s. In this step, a layer of copper (I) chloride was formed at the surface of copper electrode. Then, the electrode was placed in 0.1 M NaOH and the electrode potential was cycled between -1 and 0/8 V (vs. Ag, AgCl) at a scan rate of 50 mVs^{-1} for 5 cycles in a cyclic voltammetry regime until a stable voltammogram was obtained. Electrocatalytic activity of the modified electrode was used for the oxidation of ethylene glycol, in aqueous alkaline solution. Electrochemical behavior of ethylene glycol greatly improved at copper chloride modified copper electrode, indicating that the anodic oxidation of ethylene glycol could be catalyzed at copper chloride modified copper electrode. This proves that the copper chloride layer formed on the surface of the copper electrode bears the main role in electrocatalytic oxidation of ethylene glycol on the surface of CCMC electrode. The modified electrode shows a stable and linear responses in the concentration range of 5 to 100 mM. Kinetic parameters such as the electron transfer coefficient (α = 0/62) and the number of electrons involved in the rate determining step ($n\alpha$ = 1~ 1.2) for the oxidation of ethylene glycol were determined utilizing cyclic voltammetry (CV).

Keywords: Ethylene glycol, Copper chloride, Modified copper electrode, Electrocatalytic oxidation

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Application of Cyclic voltammetry based artificial neural network as chemometric approach and genetic algorithm for the simultaneous determination of five drugs

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The new simple, cost effective and well performing cyclic voltammetry method for the simultaneous determination of antibiotics such as Aspirin, Atrovastatin, Iboprofen, Metronidazol and Metformin in Britton–Robinson buffer (pH 7.96) developed [1]. The voltammograms of these five compounds overlap strongly, and show non-linear character. Thus, it is difficult to analyse the compounds individually in their mixtures. In this work, back-propagation artificial neural network chemometrics method were applied. Before implementing the ANN technique, the genetic algorithm (GA) algorithm was performed for wavelength selecting for the simultaneous determination of these compounds. Table 1 is shown results prediction of Aspirin, Atrovastatin, Iboprofen, Metronidazol and Metformin by cyclic voltammetry using artificial neural network as chemometric approach.

Table 1- Summary of the basic features of the models.

Analyte		Number of spectra	R	Correlation coefficient (R^2)	Root mean squares (RMSE)	R_{total}
Aspirin	Training	216	0.9984	0.9997	0.0287	-
	Validation	47	0.9647	0.9287	0.8551	-
	Testing	47	0.9730	0.9468	0.7186	-
	Total					0.9914
Atrovastatin	Training	216	0.9962	0.9991	0.0363	-
	Validation	47	0.9637	0.9611	0.3315	-
	Testing	47	0.9267	0.9478	0.3478	
	Total					0.9893
Iboprofen	Training	216	0.9991	0.9982	0.3070	-
	Validation	47	0.9726	0.9521	3.4880	
	Testing	47	0.9743	0.9492	3.5332	-
	Total					0.9907
Metronidazol	Training	216	0.9999	0.9841	1.0839	-
	Validation	47	0.9558	0.9127	5.5773	-
	Testing	47	0.9042	0.9400	5.0110	
	Total					0.98071
Metformin	Training	216	0.9955	0.9986	0.6415	-
	Validation	47	0.9825	0.9653	6.9578	-
	Testing	47	0.9763	0.9548	7.8349	
	Total					0.9933

Keywords: Cyclic voltammetry, Back-propagation artificial neural network (BP-ANN), Genetic algorithm, Drugs

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An accurate simple fluorimetric method for determination of asparaginase enzyme concentration

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L-asparaginase (L-ASNase) is an enzyme that is of crucial importance as an effective antitumor agent for acute lymphoblastic leukemia (ALL) through the depletion of L-asparagine (L-Asn) resulting in cytotoxicity to leukemic cells [1]. L-asparaginase is also important in the food industry, preventing acrylamide formation in processed foods [2]. In order to monitor the activity of L-asparaginase in plasma, we design a rapid and sensitive method by using a photoluminescent hollow carbon dot as a probe. When L-asparaginase was exposed to the nanosensor, fluorescence quenching occurred quickly at the emission peak of 430 nm. The developed nanosensor exhibited a wide linear response within the range of 50–350 IU and a reproducible detection limit at the level down to 6.59 IU. By virtue of the high selectivity and sensitivity of the nanosensor, L-asparaginase can be detected at trace levels in complicated human serum samples.

Keywords: Hollow carbon dots, Fluorescence detection, L-asparaginase

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Microfluidic-based analysis of organophosphate insecticides by miniaturized electrochemical detection system; Instrumentation and trace analyze

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Recently miniaturized analytical devices were appeared and are used in our daily life. In fact, since the introduction of the micro-total analysis system (µ-TAS) concept [1], various researcher introduced new analytical devices. Among these, microchip capillary electrophoresis coupled to a miniaturized electrochemical detection system (MCE-EC) [2, 3] introduced a new area in the separation and trace analysis of compounds. In the current research, we have developed a new concept for trace analysis of organophosphate compounds. In the new analytical system, microextraction technique (e.g. AALLME) [4] was coupled to MCE and after the separation of the analytes in the microchannel, the electrochemical signals were evaluated and the analytical system was validated. In the first step, the microchip capillary electrophoresis technique was used to serve as a separation and detection system. Analytes were injected and separated by applying a direct electrical field (+1800V) between reservoirs. The electrochemical detection was performed using three Pt microelectrodes with the width of working, counter, and reference electrodes 50, 250, and 250 µm, respectively in the out channel approach. In the second step, air-assisted liquid-liquid microextraction technique (AALLME) was used for the extraction and preconcentration of analytes from human blood plasma. 1, 2 di-bromoethan was used as extractant solvent, The extraction recoveries were about 91% and 87%, and detection limits were 240 and 360 ppb for FT and PA, respectively.

Keywords: Microfluidics, Microchip capillary electrophoresis, Organophosphate, Microextraction

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Synthesis of NiS nanoparticles and their application for determination of amoxicillin and cefazolin by using a chemiluminescence method

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Chemiluminescence (CL) reactions are chemical reactions releasing energy as electromagnetic emission. Analytical approaches based on CL reactions are usually convenient, economical, and exhibit good figures of merits such as wide linear concentration range and high sensitivity [1]. NiS nanoparticles (NPs) have many utilizations in diverse fields of advanced research like catalysts, cathodes of rechargeable lithium batteries, solar cells, and supercapacitors [2]. In this work, a new and sensitive CL method was proposed for determination of amoxicillin (AMX) and cefazolin (CFZ) in pharmaceutical preparations. The CL method is based on enhancing effect of AMX and quenching effect of CFZ on the NiS NPs-luminol-O_2 chemiluminescence (CL) reaction in a strongly alkaline medium. NiS synthesized by hydrothermal synthesis method by X-ray diffraction (XRD), scanning electron microscopy (SEM), and Fourier-transform infrared spectroscopy (FTIR) methods. The effects of various chemical reagents, involved in the CL reaction, on the CL emission intensity were also investigated and optimized. Under the optimum conditions, a linear relationship was obtained between the CL intensity and the concentration of CFZ and AMX in the range of 1.00×10^{-5}- 1.00×10^{-3} mol L^{-1} and 1.00×10^{-6} – 8.00×10^{-4} mol $L^{-1}$with limit of detections of 4.5×10^{-6} and 2.5×10^{-7} mol L^{-1}, respectively. The mechanism of CL system was also discussed, briefly.

Keywords: Amoxicillin, Cefazolin, Luminol, NiS nanoparticles

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Facile Synthesis of $Ni(OH)_2$ Nanorods through Electrodeposition Method for Supercapacitor Electrode Application

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1D nanorods due to unique architecture and easy electron access, facile ion transport, are considered as desirable nanostructure. Here in, we report a new method for synthesis of $Ni(OH)_2$ nanorods through a ZnO nanorod scaffold.

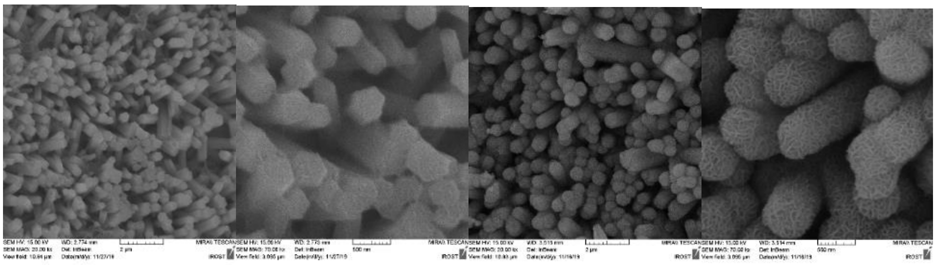

Fig.1 SEM images of (a,b) ZnO and (c,d) $Ni(OH)_2$ nano-rods arrays at different magnifications.

Fig 1. Illustrates SEM images of as prepared nanorods. Fig.2 illustrates CV voltamogram of $Ni(OH)_2$ nanorods. Two strong peak at 0. 2 and 0.4 v corresponding to cathodic and anodic peak represents that the mechanism of the charge storage is pseudo-capacitance [1]. Charge-discharge behavior is shown in Fig 2. (b) at different current densities of 1,2,5,10,15 and 20 mA/cm^2. Specific capacitance calculated from the charge-discharge voltamogram is then 848 mFcm^2. High specific capacitance and low diffusion resistance results from nano rod array which provides multiple channels and enables fast ion transport [2].

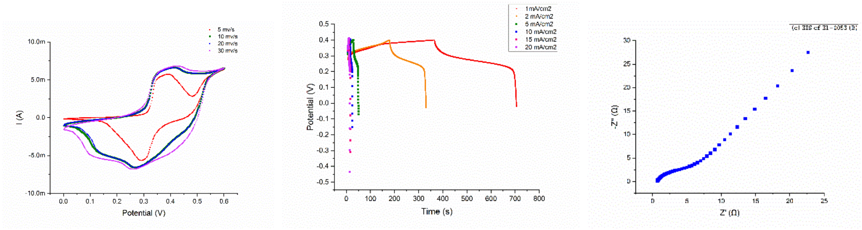

Fig.2 (a) CV, (b) Charge-discharge and (c) EIS behavior of $Ni(OH)_2$ nanorods

These results indicate that $Ni(OH)_2$ nanorods can be considered as promising electrode material for application in high performance supercapacitors.

Keywords: Supercapacitor, Pseudo-capacitance, $Ni(OH)_2$, Nano-rod.

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$NiCo_2O_4$ Nanosheets through a Facile Electrodeposition Method for Application in Supercapacitor Electrode Material

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With increasing demand in electrical energy storage for electrical vehicles and mobile electronics, supercapacitors have attracted great research interest both in industry and academia. Supercapacitors or ultra -capacitors are energy storage devices which store charges on highly porous electrode materials [1]. Designing a highly porous nanostructure is a critical point in developing supercapacitors. A nanosheet which is a two-dimensional nanostructure with thickness in a scale ranging from 1 to 100 nm and arranged as a single- or multiple-layer two-dimensional array of atoms or molecules is considered as desirable nanostructure [2].
Herein we report a facile electrochemical deposition method for synthesizing of the $NiCo_2O_4$ nanosheets arrays as a supercapacitor electrode material. The $NiCo_2O_4$ nanosheet arrays were in situ grown on Ni foams by a facile one-step electrodeposition method. The morphology of prepared nanorods have been evaluated by field-emission scanning electron microscopy (FESEM). Electrochemical properties of fabricated electrode for application as a supercapacitor electrode material were characterized by cyclic voltammetry (CV), galvanostatic charge/discharge (GCD) measurements, and electrochemical impedance spectroscopy (EIS). The outstanding supercapacitive performance of $NiCo_2O_4$ nanosheet arrays can be attributed to nanosheet structure with good mechanical and electrical contact, low crystallinity and good wettability, rich redox reactions as well as high conductivity and transport rate for both electrolyte ions and electrons.

Keywords: Supercapacitor, Pseudo-capacitance, $NiCo_2O_4$, Nano-sheet.

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pH-switchable hydrophobic deep eutectic solvent-based liquid phase microextraction for the extraction of phosalone and chloropyrifos in water samples

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Organophosphorous pesticides (OPPs) are widely used for agricultural activities due to their relatively low price and effective ability to control pests, weeds and diseases [1]. They are very important to obtain productions with high-yield, sustainable agriculture. Pesticides and herbicides residues are widely presented in our environment, including water, soils, agriculture products and food [2]. So, it is necessary to develop effective methods for determination of OPPs in water, foods and environmental matrices. A pH-switchable hydrophobic deep eutectic solvent-based liquid phase microextraction (DES-LPME) technique [3, 4] was established and combined with high performance liquid-liquid chromatography-ultraviolet detector (HPLC–UV) for the extraction and determination of phosalone and chloropyrifos in water samples. A DES was synthesized using *l*-menthol as HBA and (1S)-(+)-camphor-10-sulfonic acid (CSA) as HBD, and used as a green extraction solvent. By adjusting the pH of the solution, the unique behavior of the DES in the phase transition and extraction of the desired analytes was investigated. The homogenization process of the mixture is done only by manual shaking in less than 30 seconds and the phase separation is done only by changing the pH and without centrifugation. Some effective parameters on the extraction and derivatization, such as molar ratio of DES components, DES volume, KOH concentration, HCl volume, salt addition and extraction time were studied and optimized. Under the optimum conditions, recoveries for different water samples are in the range of 78-85%. The calibration graphs are linear in the range of 2–300 μg L^{-1} and limit of detections (LODs) are in the range of 0.7–5 μg L^{-1}. The repeatability (intra-day) and reproducibility (inter-day) for 50 μg L^{-1} of phosalone and 100 μg L^{-1} of chloropyrifos in water samples are in the range of 3.5–6.6% and 5.3-8.4%, respectively (n=5).

Keywords: Organophosphorous pesticides, pH-switchable, Hydrophobic deep eutectic solvent

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Synthesis and application of heteroatom doped graphite as the electrode material: The influences of defect density and heteroatom on heterogeneous electron transfer rate

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Thermal method was applied for the synthesis of O-doped and N-doped graphite materials using melamine and glucose as the sources of O and N, respectively [1,2]. Graphite paste electrodes were prepared with the synthesized O-doped and N-doped graphite materials. The route of synthesis was explored by cyclic voltammetry using the fabricated paste electrodes and $[Fe(CN)_6]^{3-/4-}$ as a simple outer sphere redox probe [3]. The results of structural and electrochemical investigations clearly showed that doping of O and N as heteroatom in the synthesized materials not only increased the defect density, the ratio of edge versus basal plane sites, of graphite materials but also enhanced the rate of heterogeneous electron transfer at their corresponding paste electrodes. The heterogeneous electron transfer rate constant (k^o) for $[Fe(CN)_6]^{3-/4-}$ at the fabricated O-doped and N-doped graphite paste electrodes (1.39×10^{-2} and 1.24×10^{-2} cm s^{-1}) were about 51 and 46 times of that observed for graphite paste electrode, respectively. The values of electroactive surface area calculated for both O-doped and N-doped (0.166 cm^2) were about 5 times of that obtained for graphite paste electrode (0.033 cm^2). Thereafter, electrochemical behaviors of isoniazid, ascorbic acid, dopamine, and uric acid in the concentration range between 10 to 100 μM as the models of biologically relevant molecules were investigated at the prepared heteroatom-doped graphite paste electrodes and the obtained results were revealed that the sensitivity of the measurements using O-doped and N-doped graphite paste electrodes is two times of that of using graphite paste electrode.

Keywords: N and O-doped graphite, Defect density, Heteroatom doped graphite, Heterogeneous electron transfer rate.

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Removal of nalidixic acid antibiotic by iron magnetic nanoparticles coated with lignin from hospital wastewater

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Emerging contaminants in the environment have caused enormous concern in the last few decades, and among them, antibiotics have received special attention. On the other hand, adsorption has shown to be a useful, low-cost, and eco-friendly method for the removal of this type of contaminants from water. An understanding of the interaction mechanisms of antibiotics with environmentally relevant sorbents is important to determine the environmental fate of antibiotics and to develop wastewater treatment strategies. One of the widely used antibiotics is nalidixic acid, which has been identified among the top 10 of high priority pharmaceuticals relevant for the water cycle in general. [1,2]. Lignin is the second most abundant natural polymer with cellulose being number one, making up to 10–25% of lignocellulosic biomass. Lignin is a three-dimensional, highly cross-linked macromolecule composed of three types of substituted phenols, which include: coniferyl, sinapyl and p-coumaryl alcohols [3]. Iron magnetic nanoparticles (Fe_3O_4) are used because of their high magnetic properties for separation and biological applications. Fe_3O_4 nanoparticles could easily aggregate due to the nanoscale effect and magnetic gravitational effect [4,5]. In this work, lignin coated magnetic Fe_3O_4 nanoparticles were used for nalidixic acid adsorption from aqueous solution Fe_3O_4@Lignin nanoparticles were prepared and subsequently characterized using FTIR,XRD,SEM,VSM methods. This type of adsorbent is low cost, high efficient and reusable. Also, the parameters of the adsorbent dose, the pH, contact time and adsorption isotherms in the antibiotic removal process were investigated. The maximum removal percentage was obtained 74.5% for adsorption of nalidixic acid.

Keywords: Lignin, Fe_3O_4, Antibiotic, Nalidixic acid

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Electroanalytical Determination of Malathion in Grapes Juice Samples using Molecularly Imprinted Polymer based on GQDs Modified Carbon Paste Electrode

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Malantione (S-1,2-bis(ethoxy carbonyl) ethyl O,O-dimethyl phosphorodithionate) is a non-systemic Pesticides that has been classified by the EPA as a Class III substance for carcinogenicity [1]. Carbon paste electrodes have same advantages such as high electrochemical reactivity, commercial availability, good mechanical rigidity, disposable, low cost, low technology and easy of modification. Molecularly imprinted polymers (MIPs) was prepared by polymerizing functional monomers, crosslinkers, and other essential components (primers) in the presence of a target analyte called a "template". After removing the target analyte, cavities are created that preserve the size and chemical shape of the target analyte, allowing the specific analyte to be specifically identified [2]. Graphene quantum dots (GQDs) are as novel carbon-based quantum dots with graphene sheets of less than 100 nm. They have merits of low toxicity, good biocompatibility, resistance to photobleaching, stable luminescence, high specific surface area, and abundant surface functional groups. GQDs have been shown to be potential candidates in the sensors [3]. In this work, firstly MIPs was synthesized, then GQDs, MIP, graphite powder and mineral oil was mixed and electrode was prepared. The DPV data showed that the obtained anodic peak currents were linearly dependent on the MAL concentrations in the range of 0.2–100.0 µM, with the detection limit of 0.05 nM. Finally, the obtained MAL-imprinted electrochemical sensor was applied to the selective detection of MAL in vegetable samples.

Keywords: Malatione, Carbon paste electrode, Molecularly imprinted polymers.

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A dual-template imprinted polymer electrochemical sensor based on GQDs for simultaneous determination of carbendazim and malantione

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Carbendazim is a carbamate ester-amine used against various fungal diseases, preventing loss in agricultural crop yield and quality. This benzimidazole fungicide is entered through roots, leaves, or seeds and then spreads out in all plant parts [1]. Malantione (S-1,2-bis(ethoxy carbonyl) ethyl O,O-dimethyl phosphorodithionate) is a non-systemic Pesticides that has been classified by the EPA as a Class III substance for carcinogenicity [2]. Carbon paste electrodes (CPEs) have interesting advantages such as adsorption capacity, selectivity, sensitivity, and renewability of the surface which makes them one of the most attractive materials as working electrodes [3]. The formation process of MIPs mainly includes template, functional monomer, and cross-linking agent polymerization in an aqueous solution through electrostatic interaction. After elution, the shape of the template is retained in the recognition sites of the complementary functional monomer [4]. Graphene quantum dots (GQDs) are a kind of graphene. GQDs have large surface area, high electron transfer rate, and excellent electrical conductivity, In addition, GQDs are highly electroactive by which can reduce the overpotential of analyte. Thus, they are used in sensors [5]. Modification of carbon paste electrodes with GQDs and MIPs increase sensitivity and selective recognition, respectively. In this study, firstly MIPs was synthesized, then MIP, graphite powder, GQDs, and mineral oil was mixed and electrode was prepared. The DPV data showed that the obtained anodic peak currents were linearly dependent on the malathion and carbendazim concentrations in the range of 0.2–9.0 μM and 0.02-0.9, with the detection limit of 0.01 and 0.04 nM for malatione and carbendazim, respectively. Finally, the obtained MAL-imprinted electrochemical sensor was applied to the selective detection of MAL in vegetable samples.

Keywords: Malatione, Carbendazim, Carbon paste electrode, Molecularly imprinted polymers.

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Determination of Micro Quantities of Iron in Fruits After Preliminary Concentration by Chelate-forming Sorbent

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A technique has been developed for the sorption-spectrophotometric determination of trace amounts of iron (III) in needles using 3-((2-hydroxyphenyl)diazenyl)pentadione-2,4 (R) and 1,10-phenanthroline (Phen). Iron (III) forms with the reagent a colored complex compound in the medium at pH 1.0-8.0 with maximum light absorption at $\lambda = 434$ nm, and the reagent itself absorbs at $\lambda = 382$ nm. The maximum yield of the complex is observed at pH 4.5-5.0. In the presence of 1,10-phenanthroline, a multi-ligand complex Fe(III)-R-Phen is formed, and a bathochromic shift and a hyperchromic effect are observed in the absorption spectrum. The light absorption of the Fe(III)-R-Phen complex is maximum at 506 nm. To determine the optimal conditions, the influence of the concentration of reacting substances, temperature, and time on the formation of binary and mixed-ligand iron (III) complexes was studied. The ratio of the components in the composition of the formed colored iron (III) complexes was determined by the method of isomolar series, the relative yield of the Starik-Barbanel and the shift in equilibrium. All methods showed that the ratio of the components in the binary complex is 1:2, and in the mix-ligand complexes it is 1:2:2. The composition and stability constant of the Fe(III)-R complex were determined by the method of intersecting the curves, and the stability constant of the Fe(III)-R complex was calculated Fe(III)-R-Phen, taking into account the ratio of components in its composition: $\log\beta$ (Fe-R- Phen) = 5.76 ± 0.10; $\log\beta$ (Fe-R-Phen) = 14.38 ± 0.24. The molar absorption coefficients of the Fe (III) -R and Fe (III) -R-Phen complexes at λ_{opt} are respectively $(3.10 \pm 0.06)\cdot 10^3$ and $(1.16 \pm 0.01)\cdot 10^4$. The linearity of calibration graphs for the determination of iron (III) is established and their mathematical equations are compared. A new chelating sorbent synthesized by modification of a copolymer of maleic anhydride-styrene with m-aminophenol. The sorption of iron (III) ions with a synthesized sorbent under static and dynamic conditions was studied. It was found that the sorbent quantitatively extracts iron (III) at pH of 3.8-4.2 and the sorption capacity of the sorbent is 280 mg/g. Ionic strength up to 0.8 M does not affect sorption, and its subsequent increase leads to a significant decrease in sorption. Complete sorption of iron (III) ions is observed after 2 hours under static conditions. The effect of the concentration of HNO_3, $HClO_4$, H_2SO_4, and HCl solutions on desorption was studied and it was found that Fe (III) ions are maximally extracted from the sorbent using 1.5 M H_2SO_4. The degree of desorption is 96%. The developed technique was applied to determine the microquantities of iron (III) in fruits: in white and red cherries, in strawberries and in quince.

Keywords: Iron (III), 3-((2-hydroxyphenyl)diazenyl)pentadione-2,4, Chelating sorbent, Fruits

Mixed-Ligand Complexes of some Metals with 2,2',3,4-tetrahydroxy-3'-sulfo-5'-nitroazobenzene and Hydrophobic Amines

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The complex formation of some metals with pyrogallol-based azo compound 2,2',3,4-tetrahydroxy-3'-sulfo-5'-nitroazobenzene (R) in the presence and absence of hydrophobic amines (Amine) - 1,10-phenanthroline (Phen), bathophenanthroline [4,7-diphenyl-1,10-phenanthroline] (Bphene), diphenylguanidine (DPG), and triphenylguanidine (TPG) was studied. It has been established that Al(III), Ga(III), Ti(IV), Zr(IV) and Hf(IV) in an acidic medium at pH 0–7.0 form colored complex compounds with the reagent. In the presence of hydrophobic amines, mixed-ligand complexes Al(III)-R-DPG, Ga(III)-R-Phen, Ti(IV)-R-Phen, Zr(IV)-R-TPG and Hf(IV)-R-Bphene are formed, with the formation of which bathochromic shifts are observed in the absorption spectra in comparison with the spectra of the corresponding homogeneous-ligand complexes, and the maximum yield of the complexes is shifted to a more acidic medium. It has been established that all complexes are formed immediately after mixing the solutions of the components and are stable. The ratio of components in the composition of the formed colored complexes was determined by the methods of Asmus, shift of equilibrium, relative yield of Starik-Barbanel and isomolar series. The results of all methods showed that the ratios of Me:R in the composition of homogeneous ligand complexes are 1:2, and in the composition of mixed-ligand complexes Me:R:Amine - 1:2:2. The number of protons displaced during complex formation was determined by Astakhov's method, and the indicated ratio of components in the complexes was confirmed. The stability constants of the complexes were determined by the method of intersection curves and it was found that in the presence of hydrophobic amines, the stability constant of the complexes increases by about 7-14 orders of magnitude. Conductometric titration was used to determine the electrical conductivity of the complexes, and it was found that with an increase in the stability constant, their electrical conductivity decreases. The molar coefficients of light absorption of homogeneous-ligand and mixed-ligand at λ_{max} were calculated, the linearity of the calibration curves was established, and their mathematical equations were compiled. It has been established that with the formation of mixed-ligand complexes, the molar coefficient of light absorption significantly increases and the lower limit of detection decreases. The effect of accompanying ions on the determination of Al(III), Ga(III), Ti(IV), Zr(IV) and Hf(IV) ions has been studied. It has been shown that the reaction selectivity increases significantly in the presence of hydrophobic amines. The developed methods were tested in the analysis of drinking water, soil, clay and standard samples on various basis.

Keywords: 2,2',3,4-tetrahydroxy-3'-sulfo-5'-nitroazobenzene, hydrophobic amine, mixed-ligand complex, metal ions

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Dairy industry wastewater treatment by amine Functionalized magnetite iron oxide nanoparticles by photo-degradation method

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Dairy products such as milk, butter, cheese, yogurt, and by-products including buttermilk, whey, and their derivatives are produced using pasteurization or homogenization methods. These products have a high nutrient concentration (such as dissolved sugars, proteins, and fats), biological oxygen demand (BOD), chemical oxygen demand (COD), and organic and inorganic contents. The effluent of dairy industrials must be reduced before being discharged to municipal treatment plants [1].Functionalized iron oxide nanoparticles (IONPs) are of great interest due to wide range applications, especially in wastewater treatment. However, they face challenges preventing their further applications such as rapid agglomeration, oxidation, etc. Appropriate surface modification of IONPs can conquer these barriers with improved physicochemical properties. [2-3] The aim of this study is to investigate the efficiency of photo-degradation and adsorption process for removal of organic contaminant by using of IONPs from dairy wastewater. In this work firstly IONPs were synthesized by Co-precipitation method, secondly the surface of prepared IONPs were modified by 3-aminopropyltriethyloxysilane. Photo catalytic degradation of organic dairy wastewater was performed in the presences of amine modified IONPs. the optimum pH and catalyst loading for the solar photochemical oxidation was found to be 5 and 300 mg/L, respectively. The solar photocatalytic oxidation using IONPs removed 85% of the COD from dairy wastewater. The findings suggest that IONPs solar photo-degradation would be a promising alternative for the treatment of dairy wastewater.

Keywords: Wastewater treatment, Iron oxide nanoparticle, Photdegradetion, Dairy industry.

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Preconcentration of Pb(II) by magnetic MOF prior to graphite furnace atomic absorption spectrometry determination

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Lead is a very stable and non-biodegrade that accumulates in the environment [1]. It is considered as one of the toxic heavy metals, which can cause damage to the human health, even at the low concentrations. Numerous techniques have been used for the determination of lead such as electrochemical method [2], electrothermal atomic absorption spectrometry (ETAAS) [3], inductively coupled plasma-atomic emission spectroscopy (ICP-AES) [4] and flame atomic absorption spectroscopy (FAAS) [5]. However, their selectivity and sensitivity are not sufficient for direct determination of lead in real samples at very low concentrations. In this study, a magnetic metal-organic frameworks (MOFs) is synthesized based on magnetic Fe_3O_4 and Cu-BTC as a sorbent for solid phase extraction (SPE) of trace amounts of Pb(II) in water and lettuce samples. Pb(II) ion was adsorbed on magnetic MOFs and easily separated by a magnet; so, no filtration or centrifugation was necessary. The analyte ions were eluted using HCl 0.5 M and analyzed via graphite furnace atomic absorption spectroscopy. Under optimal experimental conditions, the method has a linear range of 0.1–50 ppb and detection limit (LOD) of 0.08 ppb. The results showed that the prepared sorbent has high selectivity for Pb^{2+} even in the presence of other interfering metal ions.

Keywords: Magnetic MOF, Pb(II), Preconcentration, Graphite furnace atomic absorption spectrometry

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Convergent paired electrocatalytic strategy to improve degradation of nitroaromatic compounds by engineered mixed metal oxide anodes

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One of the most challenging problems in environmental science nowadays is the presence of numerous forms of persistent organic pollutants (POPs) and hazardous in water wastewater. Nitroaromatic compounds are non-biodegradable chemicals that have negative human health and environmental consequences and are among the most POPs in the environment. In this research, a new and creative idea for the mineralization and electrocatalytic degradation of the 2,4-dinitrotoluene (DNT) as a POPs in aqueous solutions uses the G/β-PbO_2-ZrO_2 electrode, and by the convergent paired electrocatalytic degradation method is presented. This modified anode for electrocatalytic degradation of POPs has significant properties and characteristics, including a long service lifetime, excellent electrocatalytic degradation efficiency and high oxygen evolution overvoltage. Effect of effective operating parameters such as initial concentration of DNT pollutant (180, 90, 45 mg/L), applied current density (2, 3,5 mA/cm^2), initial pH value (1.0-10.0), the kinetics of degradation process, electrochemical current efficiency and electrochemical energy consumption in the process of convergent paired electrocatalytic degradation of DNT have been thoroughly investigated. The results of these studies showed that after 90 minutes of electrolysis at an initial concentration of 90 mg/L, the current density of 5 mA/cm^2 and pH=6.0, the rate of DNT degradation reached 95% and COD removal reached 83%, while the electrochemical energy consumption is 6.42 kWh/kg COD. Kinetic studies of the degradation process showed that the electrocatalytic degradation of DNT on the G/β-PbO_2-ZrO_2 electrode followed pseudo-first-order kinetic. Also, the electrochemical behavior of DNT at different pHs (1.0-10.0) was completely investigated using the cyclic voltammetry method on a glass-carbon electrode, and all possible paths for the electrocatalytic degradation mechanism of the DNT contaminate are also predicted. As a significant finding, it was established that during the breakdown of DNT, the compound is first reduced to its amino form (diamino-toluene) on the cathode surface, and subsequently the amino form on the anode surface is attacked by hydroxyl radicals. The attack of hydroxyl radicals leads to the opening and breaking of the aromatic ring of the molecule and the formation of a series of carboxylic acids, and these compounds are also finally mineralized to CO_2 and H_2O by hydroxyl radicals.

Keywords: Electrocatalytic degradation, Nitroaromatic compounds, G/β-PbO_2-ZrO_2 anode.

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Preconcentration of trace amount of As (III) ions with magnetic metal-organic frameworks (MOFs) and determination by Graphite furnace atomic absorption spectrometry

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Arsenic is one of the toxic heavy metals, which is found in soil, air and water resources [1]. Arsenic contamination can cause serious health problems, including skin damage, heart, liver, bladder cancer and death [2]. The World Health Organization's (WHO) have set maximum contaminant level for arsenic as 10 ppb in drinking water [3]. Various instrumental techniques have been introduced for the determination of As (III). Since the arsenic concentration level in real samples is very low and matrix complexity is the main problem; thus separation and preconcentration methods are often required. In this work, Cu-BTC@Fe_3O_4 nanocomposites have been prepared by growing H_3BTC thin layers onto Fe_3O_4 nanoparticles that are grafted with carboxylic functional groups. These Cu-BTC@Fe_3O_4 nanocomposites have large pores and cavities that can increase the large surface area and strong affinity for As (III), which provides excellent adsorption. The superparamagnetic of Cu-BTC@Fe_3O_4 contributes to the rapid separation of the adsorbent from the matrix solution. The As (III) ions adsorbed on surface of magnetic MOFs and oxidized to As(V) and preconcentrated in acetate buffer by applying potential in an electrochemical cell equipped by two electrodes. Under the optimum condition, the proposed method displayed a linear range of 1.0–25 ppb and detection limit (LOD) of 0.25 ppb. The proposed method showed high selectivity for As(III) measuring in the presence of other interfering metal ions and it was applied for determination of As(III) in water and rice sample.

Keywords: Magnetic metal-organic frameworks (MOFs), As(III), Preconcentration, Graphite furnace atomic absorption spectrometry

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Green dispersive solid-phase microextraction of melamine using crosslinked ß-cyclodextrin with citric acid followed by HPLC-UV

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Melamine (MEL) is a polar triazine-based organic compound containing high nitrogen levels which commonly is added to dairy products to increase the fake protein content of them [1]. However, MEL is an important material in chemical industries to produce kitchen wares. The migration of MEL at high temperatures or acidic conditions from the kitchen wares into foods is known as a source of MEL contamination [2]. MEL can cause serious health problems such as kidney failure, kidney stone, bladder cancer, etc [2]. In this research, a green approach of dispersive solid-phase microextraction (d-SPME) was introduced for the extraction and determination of MEL. In this way, a natural and polar polymer named ß-cyclodextrin was cross-linked with citric acid to create a water-insoluble absorbent [3]. The extraction was carried out by dispersing the sorbent in the sample solution. The effective parameters on the extraction efficiency, including ionic strength, extraction time, sample volume, absorbent value, pH, type of desorption solvent, desorption type, and desorption solvent volume were optimized by one variable at a time approach. Under the optimal conditions, the method showed good dynamic linearity for MEL in the range of 1.0-1000 µg L^{-1} and the limit of detection of 0.3 µg L^{-1} with the coefficient of determination of 0.9985. The intra-day and inter-day RSDs (n = 3) were 3.1% and 3.2% respectively. Finally, this technique was applied for extraction and determination of MEL in melamine dish and infant formula with acceptable and satisfactory results.

Keywords: ß-cyclodextrin, Dispersive solid-phase microextraction, Melamine.

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Designing chemical sensors using silica inverse opal photonic crystals

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Inverse opals (IOs) are porous materials that contain a close-packed array of spherical voids in the face-centered-cube (FCC) crystal, fabricated by infiltration of the artificial opals with a silica precursor and the elimination of the spheres as a template by chemical etching or calcination. The special optical characteristics of IOs make them useful for sensing applications. They can absorb the input light at particular wavelengths that depends on the refractive index of IOs [1]. Altering the refractive index by changing the material within the pores will produce a shift in the photonic bandgap (PBG) or stopband of the IOs structure [2]. In this work, silica inverse opals (Si-IOs) were fabricated by the co-assembly method. Factors affecting the growth conditions of the Si-IOs are the final concentration of the polymethylmethacrylate (PMMA) suspension in a mixed solution, the amount of silica precursor relative to the final concentration of PMMA suspension, and the calcination's temperature. Also, the proper time for calcination to remove the spheres is important [3]. Here, the conditions required for the fabrication of Si-IOs were optimized, and finally, inverse opals were used as chemical sensors to detect solutions of various salts. To evaluate and compare the sensory performance of inverse opals for different salts, solutions containing zinc chloride, mercury (I) nitrate, mercury (II) nitrate, lead (II) nitrate, cobalt nitrate, ammonium chromate, tin (II) chloride, cadmium chloride and iron (II) sulfate with the concentration of 0.002 molars (M) were injected into inverse opals. By examining the absorption spectrum of the structure of inverse opals containing salts solutions, at the maximum absorption wavelength (λ_{max}) of the inverse opals relative to the pre-injection state, a redshift was observed. The maximum redshift of 17 nm for inverse opal containing zinc chloride and the minimum redshift of 4 nm for inverse opal containing iron (II) sulfate were observed indicating the sensitivity of 8.5 and 2 nanometers per unit concentration (nm/mM) in the experiment performed, respectively. The results showed that due to the injection of these salts solutions with a higher refractive index and different from the refractive index of air cavities of inverse opal structure, the effective refractive index of the inverse opals structure changes, which causes a shift in the photonic bandgap and the amount of shift for different salts with the same concentration is different and depends on the type of the salts. Also, with increasing salt concentration, a higher amount of PBG shift has been observed.

Keywords: Silica inverse opals, Artificial opals, Co-assembly method, Chemical sensors

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Electrocatalytic determination of Uric Acid by CdS-$CoFe_3O_4$ magnetic nanocomposite modified GCE

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Uric acid is one of the components of non-protein nitrogen (NPN) and the end product of purine metabolism. Uric acid is formed by the enzyme xanthine oxidase from intermediate metabolites such as hypoxanthine and xanthine. Like vitamin C, uric acid is considered an antioxidant and can be said to contain about half of the antioxidant capacity of human plasma. Uric acid can be produced in the body from both endogenous and exogenous sources. The source of exogenous uric acid production in the body is urate from purines in the diet, especially animal foods such as red meat and legumes [1,2]. Determination of uric acid in blood serum and urine is of great importance. In the present research, CdS-$CoFe_3O_4$ magnetic nanocomposite have been chemically synthesized and used as a modifier in the preparation of modified glass carbon electrodes for electrochemical measurement of uric acid [3]. The synthesized nanocomposites were characterized by conventional surface study techniques including scanning electron microscopy (SEM), X-ray scattering analysis (XRD) and radiation energy diffraction (EDS). Cyclic voltammetry (CV) and electrochemical impedance spectroscopy (EIS) was used to investigate the electrochemical behavior of the modified electrode. The proposed modified electrode was used for as a sensor in electrocatalytic determination of Uric Acid (UA). Influence of some effective parameters was investigated in the determination of UA. Construction of the calibration plot for UA oxidation was performed using Differential pulse voltammetry (DPV) method. Two linearity ranges were obtained from 0.2 to 20.2 µM and 20.2 µM to 125.1 µM. The detection limit was obtained as 1.1 µM. Finally, the reliability of the nanosensor was confirmed with real sample analysis in human urine and serum samples.

Keywords: Differential pulse voltammetry, Glassy carbon electrode, Uric acid, Electrochemical sensor, CdS-$CoFe_3O_4$

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Synthesis and application of nanofiber yarns of MXene composite in packed in-tube solid phase microextraction of beta-blockers residue from biofluids

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β-Blocker drugs are commonly used in the treatment of cardiovascular diseases because they can improve the heart's ability and decrease anxiety [1]. Owing to these effects, they have been also used in sports competitions to enhance the potency and steadiness of athletes. So they are prohibited substances and their measurement is important both in controlling of their side effects and in the field of doping control [2]. Determination of trace concentrations of β-blockers in complex matrices requires powerful sample pretreatment methods capable of matrix removal and analyte enrichment. In-tube solid phase microextraction (IT-SPME) with the use of a suitable sorbent and its several advantages, becomes the same powerful method in question [3]. Electrospinning can be use in the production of nanofibers web with multiple priority. Direct electrospinning of nanofibers yarn can turn them to woven fabrics, which leads to improve nanofiber endues possibilities and applications [4]. In this work a successful nanofiber yarn spinning system was used with the help of a rotating funnel. Yarn formation by composited PAN/MXene polymer solution ejected from two nozzles with opposite charges was analyzed and their application for packed IT-SPME of β-blocker drugs form biofluids was shown. Separation and determination of analytes were performed by HPLC-UV analysis. The 3D yarn PAN/MXene sorbent exhibited high flexibility, mechanical stability and reusability. Its characterization was carried out utilizing FT-IR spectroscopy, FE-SEM, EDS mapping and XRD analysis. Important factors affecting extraction efficiency such as extraction time, pH, ionic strength and flow rate of sample solution, and type, volume and flow rate of eluent were optimized. Under the optimal conditions, LODs and linearity with $R^2 \geq 0.990$ were obtained in the range of 1.5–3.0 $\mu g\ L^{-1}$ and 5.0–1000.0 $\mu g\ L^{-1}$, respectively. The inter- and intra-assay RSDs ($n = 3$) are in the range of 2.5–3.5%, and 4.5–5.2%, respectively. Finally, the validated method was applied for the analysis of the atenolol, propranolol and betaxolol in human urine and saliva samples.

Keywords: In-tube solid phase microextraction, Electrospinning, MXene, Yarn nanofibers, β-Blockers drugs.

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An easy spectrophotometric method for simultaneous determination of nitroglycerin and nitrocellulose in solid rocket propellants

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Solid rocket propellants as double-base propellants (DB propellants) are best known as smokeless propellants and are used in guns and rockets [1]. DB propellants consist mainly of nitroglycerine (NG) and nitrocellulose (NC) that used in rocket and gun applications as energetic base materials [2-3]. Due to high application and consumption of NG and NC in DB propellants, as well as needing to development of high-safely methods, there are always challenges for determination of these two compounds. So, an accurate, simple and safe method was developed for simultaneous determination of NG and nitrocellulose NC in DB solid propellants. The proposed method is based on alkaline hydrolysis of NG and NC, and followed by colored reaction of released nitrite ion with p-nitroaniline in the presence of diphenylamine in acidic media and produce azo dye. The absorbance of the azo dye was measured at 534 nm. Two sets of reaction conditions and calibration curves were developed. In the first set, at room temperature, only NG was hydrolyzed and calibration curve obtained. In the second set, at 60 °C, NG and NC were hydrolyzed simultaneously. Based on obtained amount for the NG at room temperature, and total amount of NG and NC at 60 °C, the amount of NC was determined by using stoichiometric equations. The calibration curve was linear over the concentration ranges of 0.2-5.0, 0.5-10 μg mL^{-1} for NG and NC, respectively. The limits of detection (S/N=3) were 0.1 μg mL^{-1} and 0.25 μg mL^{-1} respectively for NG and NC. The proposed method was successfully applied for the determination of NG and NC in DB propellants with good recoveries ranged from 99-101 %, and RSD less than 2.0 %. The method statistically compared based on t- and F-tests with those obtained in according to military standard method *(MIL-STD-286)*. The results showed that the proposed method offers an accuracy and reliable approach for the determination of these compounds in DB propellants, and can be suggested as a routine method in military quality control laboratories**.**

Keywords: Nitroglycerine, Nitrocellulose, Simultaneous spectrophotometric determination, Double base solid propellants.

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Electrochemical sensor based on a surface-imprinted polymer- modified electrode for rapid and sensitive detection of *S. aureus*

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According to the latest statistics, Pathogenic bacteria cause a large number of hospitalizations and deaths worldwide each year. Staphylococcus aureus (S. aureus) is one of the most dangerous zoonotic pathogen responsible for serious bloodstream infections. Therefore, the rapid and sensitive detection and measurement of this bacteria is vital [1-2]. S. aureus-imprinted polymer-based sensor was prepared to detect S. aureus by electropolymerizing pyrrole on the Glassy carbon electrode (GCE) surface using the cyclic voltammetry method in the presence of S. aureus as the template and pyrrole as the functional monomer. After removal the bacterial template from the electrode surface, a series of cavities will be formed in the shape of the desired bacteria in the polymer structure. Then polypyrrole was overoxidized using chronoamperometry method in an alkaline medium [3]. To study the morphology of the desired bacterium, SEM images of different polymer films modifed electrodes were used during the process of bacterial imprinting and recognition. CV and EIS techniques were used to characterize the imprinting process and DPV technique was introduced to draw a calibration graph under optimal conditions and for all of the electrochemical measurements. The selectivity of the proposed sensor was investigated by interfering bacteria. The high selectivity of the sensor against the template bacteria could be ascribed to its sensitivity to the chemical conformation of bacterial outer cell structures. The imprinted electrochemical sensor based on a surface-imprinted polymer- modified electrode was successfully applied to detect S.aureus in food real sample.

Keywords: S.aureus, Differential pulse voltammetry, Over-oxided polypyrrole, Glassy carbon electrode, Electrochemical sensor

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A highly sensitive and selective electrochemical determination of anticancer drug 5-flourouracil based on an electrochemically activated disposable graphite rod electrode

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5-Fluorouracil (5-FU) is a cytostatic and anti-cancer agent that is widely used in the treatment of tumors and is considered one of the most active anti-neoplastic agents in advanced colorectal cancer and head and neck malignancies. This compound is one of the most common chemotherapy drugs in cancer that kills cancer cells. Therefore, providing a fast, easy and reliable method for determination of 5-Fluorouracil is very important [1]. In this research electrochemically activated disposable graphite rod electrode was used as electrocatalytic determination of 5-Fluorouracil [2]. The proposed activated electrode exhibited an excellent electrocatalytic activity toward the oxidation of 5-Fluorouracil. Effects of some potentially effective parameters in the preparation of the activated electrode were investigated. At the optimum conditions, calibration curve was obtained using differential pulse voltammetry. Voltammetric response of the electrode toward the 5-FU showed a dynamic calibration curve with linear range between 38.02 µM to 1.92 mM and a detection limit of 32.09 µM. The sensitivity was 0.027 µA/µM. The prepared electrode was used for determination 5-FU in the pharmaceutical and biological samples.

Keywords: Differential pulse voltammetry, Activated disposable graphite rod electrode, Electrochemical sensor, 5-flourouracil

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Size determination of silver nanoparticles based on surface plasmon resonance using smartphones

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One of the basic methods for determination of chemical compounds is colorimetry. Use of digital factors like RGB, Hue, HSB etc. as analytical signals by smartphone camera is a good way for using smartphones as alternative for spectrophotometers [1]. Smartphones as detector convert color values to electrical current signal using CCD or CMOS sensors. Light is received by pixel panels containing electron which absorbs the light and change it to electrical current [2]. Color of metallic nanoparticles is size dependent due to the surface plasmon resonance [3]. Surface Plasmon resonance is the most outstanding optical property of metallic nanostructures. It consists of a collective oscillation of conduction electrons excited by the electromagnetic field of light. In this research we designed a method for determination of silver nanoparticles size based on colorimetry using smartphones. Size controlled synthesis of silver nanoparticles was performed by Shekher Agnihotri and coworkers [4]. Cell holder and imaging box was designed by solid work software and made by FDM 3D printer using poly lactic acid (PLA). Stable conditions for imaging and determination of digital factors needs imaging box and cell holder. Programing codes was used as comparing factors between calibration images color density and unknown sample images. Proposed program selected stable and central point of the sample and compared recorded values with program library.

Keywords: Smartphone, Surface plasmon resonance, Metallic nanoparticle

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Synthesis and chemical modification of magnetic adsorbents from plant sources and their use to remove EDTA from aqueous solution

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According to the United Nations World Water Development Report (UNWWD), the world will face a 40% water shortage by 2030. Domestic wastewater contains large amounts of various chemicals. One of the most important of these is Ethylenediaminetetraacetic acid (EDTA), which is present in significant amounts in detergents, cosmetics, and pharmaceuticals, which penetrates easily into the soil and remains in many aquatic environments due to its low biodegradability. According to the EU Risk Assessment Report, the maximum permissible concentration of EDTA in an aqueous solution is 2ppm [1]. Therefore, using different methods such as adsorption, ion exchange, coagulation and flocculation, distillation, burning, reverse osmosis, advanced oxidation, etc, to purify water is very important. Among these, the adsorption method is one of the most effective methods due to its simplicity, cost-effectiveness, high efficiency, easy absorber design, and, most importantly, the absence of secondary contaminants during the adsorption process, is one of the most suitable methods for wastewater treatment [2, 3]. An ideal adsorbent for wastewater treatment should have criteria such as environmentally friendly, high adsorption capacity and selective action to remove low-concentration contaminants, easy removal of adsorbed contaminants from its surface, and recyclability. Activated carbon(AC) is one of the most common adsorbents in the adsorption process due to its unique properties such as high porosity, specific surface area, very high adsorption capacity, optimal pore size, large internal cavities, and high surface reaction [4, 5]. In this research, magnetically activated carbon synthesized from coffee grounds was used to remove EDTA in an aqueous solution. Coffee waste was prepared from coffee shops in Urmia and used as a precursor in the production of activated carbon (AC) and then modified by $CoFe_2O_4$ magnetic particles for use as an EDTA adsorbent. Both AC / $CoFe_2O_4$ and AC adsorbents were analyzed and characterized by FESEM, XRD, BET, VSM, and FT-IR techniques. Experimental parameters such as adsorbent dose, contaminant concentration, pH, and temperature were investigated in EDTA removal. In this study, a concentration of 30 ppm EDTA, in the presence of 0.05 gr of adsorbent, pH=5.5, and 25°C, 100% removal of EDTA was observed. A comparison of the results obtained with commercial activated carbon in this study showed that the prepared adsorbent had a high potential for removing EDTA from water and could be used for industrial-scale applications.

Keywords: Activated carbon, EDTA, Adsorption, Coffee waste

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3D-QSAR study on the DYRK1A inhibitors by CoMFA and CoMSIA methods and design of new compounds for treatment of diabetes

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Since human drugs are directly related to human health, the production of such drugs is a very costly and time-consuming process and must go through certain steps that, in many cases, the drug fails to meet the standards and a lot of time and money is wasted. In order to prevent this problem, it is better to perform standard simulations before starting the production process, and if the correct answer is given, the production process should start, and if it is not suitable in terms of drug design theory, the production process should be prevented. In this work, the 3D-QSAR on a series of 1,5-naphthyridine derivatives were studied using Comparative Molecular Field Analysis (CoMFA) and Comparative Molecular Similarity Indices Analysis (CoMSIA) [1]. Statistically significant CoMFA (r^2_{cv} =0.554, r^2_{ncv} =0.988) and CoMSIA (r^2_{cv} =0.365, r^2_{ncv} =0.975) models were generated using the training set on the basis of the common substructure-based alignment. Further, the predictive ability of the CoMFA and CoMSIA models was determined using a test set of nine compounds [2]. The information obtained from CoMFA and CoMSIA contour maps can be used for further design of new 1,5 naphthyridines based analogs as anti-diabetes agents. The resulting contour maps, produced by the best CoMFA and CoMSIA models, were used to identify the structural features relevant to the biological activity in this series of analogs[3]. Newly designed molecules in this series of compounds may show stronger anti-diabetic activity.

Keywords: 3D-QSAR, CoMFA, CoMSIA, DYRK1A, Drug design

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Microextraction by packed sorbent of selective and non-selective β-blocker drugs with chitosan@mof-199 bio-composite in human saliva, plasma, and urine samples

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In recent decades, selective (atenolol, and betaxolol) and non-selective (propranolol) beta-blocker drugs have been widely used by patients. The over dosage use of these drugs has several side effects such as shortness of breath, poor heart function, and dry eyes and mouth. On the other hand, the beta-blocker drugs are on the doping agents list of the World Anti-Doping Agency. Therefore, for both clinical and doping testing purposes, introduce an effective method for extraction trace amounts of atenolol, propranolol, and betaxolol drugs in human biological samples is vital [1]. The current study introduces a microextraction by packed sorbent (MEPS) for beta-blocker drugs in biological samples. For this purpose, chitosan@ MOF 199 bio-composite was packed into a metal spinal syringe for selective and non-selective beta-blocker drugs extraction. Compared to conventional SPE formats, MEPS uses the minimum amount of adsorbent (approximately 1-5 mg) and the volume of sample solutions (microliter volumes). Because preparing a large volume of samples from saliva and blood plasma is difficult, MEPS is a practical and effective method for the extraction of drugs in these samples [2]. Chitosan is a biodegradable and abundant natural polymer with surface hydroxyl and amine functional groups. By incorporation of the metal organic frameworks (MOFs) nanoparticles into the chitosan gel, the adsorption capacity of bio-composite can be significantly increase [3]. The effective parameters on the extraction efficiency of the analytes like as sample solution pH, adsorption and desorption flow rate, adsorption and desorption cycle number, type, and volume of eluent solvent as effective parameters were evaluated and optimized. Under optimal conditions, 2 mL of the spike sample solutions were extracted and quantified by HPLC with a UV detector. Linear dynamic ranges (LDRs = 5 -600 ng mL^{-1}), limit of detections (LODs= 0.3 -1.5 ng mL^{-1}), the relative standard deviation (RSD% = 4.7 - 5.3% with three repelicate determinations at concentration of 100 ng mL^{-1}) were obtained. Acceptable relative recovery (RR%) values of 72.4-93.9%, 85.6-92.3%, and 74-98.4% were obtained in plasma, saliva, and urine, respectively. In this study, the drug release profile of propranolol in urine was evaluated. Based on the obtained results, this method was an effective, fast, sensitive, reproducible, environmental, and user-friendly method for beta-blocker drugs extraction in biological samples.

Keywords: MEPS, Beta-blocker drugs, Chitosan, MOF-199, Bio-composite

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3D-QSAR study on CB2 receptors as analgesics and anti-inflammatory compounds

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Three-dimensional quantitative structure- activity method is extensively used in drug design to study the activity of the new designed molecules.[1] The 3D-QSAR relationships was developed for a series of 5-Sulfonyl-benzimidazoles as selective CB2 agonists derivatives as anti-inflammatory agents using the CoMFA and CoMSIA methods[2]. Statistically significant CoMFA($R^2 = 0.989$) and CoMSIA ($R^2 = 0.936$) models were derived based on 45 compounds as training set on the basis of the selected alignment. Further, the predictive ability of the CoMFA and CoMSIA models was determined using a test set of 11 compounds. Based on the information derived from CoMFA and CoMSIA contour maps [3], we have identified some key features for increasing the activity of compounds and the results have been used to design of new anti-inflammatory compound agents. The results obtained from this study will be useful in the design of potent anti-inflammatory agents.

Keywords: 3D-QSAR, CoMFA, CoMSIA, Anti-inflammatory, Drug design

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Synthesis and characterization of $LaNiO_3$ nanoparticles and its application in the hydrogen storage

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In this research, $LaNiO_3$ as a ternary metal oxide was synthesized successfully by the sol-gel method. Then, to optimize the structure, the phase formation, morphology, and extent of particle size of $LaNiO_3$ nanostructures were studied by changing the calcination temperature at range of 600-1100 ˚C. X-ray diffraction (XRD) analysis results in Fig. 1 (a) show that the $LaNiO_3$ powder, obtained at a calcination temperature of 900 ˚C, crystallized as a single phase without any impurities in a rhombohedral structure with the space group R-3m (JCPDS card no. 00-033-0711). Thus, it can be concluded that 900 ˚C is the best calcination temperature for $LaNiO_3$ nanoparticles during 5 h. Also in this study, the hydrogen storage performance (HSP) of the $LaNiO_3$ nanoparticles, calcinated at 900 ˚C, was explored by the charge-discharge chronopotentiometry (CHP) technique that is an effective technique because it is carried out at ambient temperature and pressure [1]. Hence, the electrochemical cell assembled with three different electrodes consists of a calomel electrode (SCE), platinum foil, and $LaNiO_3$/copper plate (1×1 cm^2) as reference, counter, and working electrodes which are placed in the same electrolyte solution (KOH, 6 M), respectively. According to discharge profile in Fig. 1 (b), after 10 cycles, the discharge capacity this sample measured 2000 mAh/g at constant current of 1 mA. Based on our results, the $LaNiO_3$ nanostructures demonstrated suitable capacity as promising active material for hydrogen storage device.

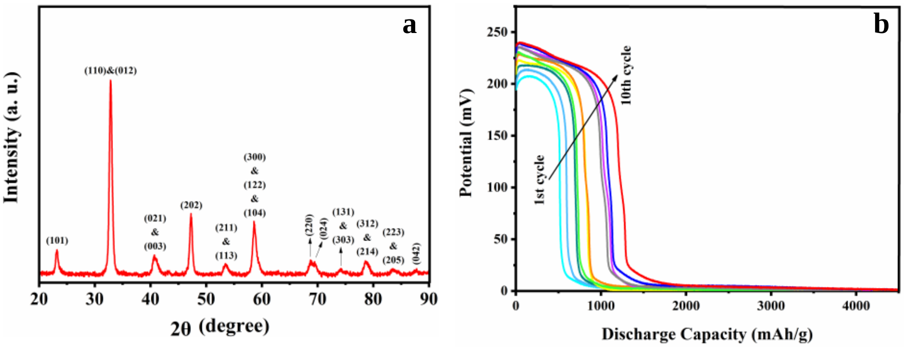

Fig. 1. (a) XRD pattern and (b) Discharge curves of the $LaNiO_3$ nanoparticles at 1 mA.

Keywords: Ternary metal oxide, $LaNiO_3$, Calcination temperature, Electrochemical hydrogen storage, Chronopotentiometry

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New Analytical Methodology based on HPLC-DAD after Magnetic Solid Phase Extraction for Sensitive Analysis Glipizide Molecules, Diabetes Drug

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Determination of drugs in biological samples is very important in therapeutic drug follow-up, pharmaceutical research, analytical and toxicological studies. This type of analysis is very difficult, both due to the very low concentrations of the target species and the complexity of the sample matrix, and necessarily involves a sample preparation process [1]. In this sample preparation process, a carrier surplus is usually made to transfer the target molecules to another environment where there are no enterprising species. In this way, the analysis of target molecules is also facilitated by means of sample preparation technicals [2]. Diabetes is known as one of the most important health problems today. The incidence of diabetes and the number of patients with diabetes are increasing rapidly both around the world and in our country as well. Along with the direct or indirect effects of this disease, it creates negative consequences on health systems and social life[3]. A new magnetic core-shell nanocomposite material was synthesized, characterized and used as magnetic solid-phase extraction material. The usability of material was checked on the separation and pre-concentration of Glipizide molecules in urine samples by magnetic solid-phase extraction and high-performance liquid chromatography with diode array detector system. HPLC analysis was carried out on isocratic elution mode with methonol, acetonitrile and acetic acid (% 0.6, pH:5.0). There was a linear relationship between chromatographic area and concentration of Glipizide in the range of 5.0–800 ng mL^{-1}. The limit of detection and quantification limits were 1.58 and 4.84 ng mL^{-1}, respectively.

Keywords: Glipizide, Magnetic solid phase extraction, HPLC, Analytical method development

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A green ultrasound-assisted emulsification-microextraction based on a low viscous deep eutectic solvent for the enrichment of propranolol

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In the last decades, miniaturized sample preparation methods, including solid-phase microextraction (SPME) and liquid-phase microextraction (LPME), have been developed to solve problems related to conventional methods. These pretreatment methods have the advantages of low consumption of organic solvent, high enrichment factor, high recovery, and simplicity. However, the use of organic solvents, even at a low level, is a problem and should be resolved [1]. A unique kind of solvents so-called deep eutectic solvents (DESs) has emerged recently as a green solvents and they are considered as ionic liquids analogs. Compared with conventional ILs, DESs have many advantages over them such as easy availability of cheap and renewable components, ease of preparation, chemical inertness, and easy storage. They are chemically tailorable solvents in general, composed of two or three inexpensive and safe components, including hydrogen bond donor (HBD) and hydrogen bond acceptor (HBA) molecules in a proper mole ratio [2]. In this study, a new type of ternary deep eutectic solvent has been prepared and used as extraction solvents for ultrasound-assisted emulsification-microextraction (USAEME) for the microextraction and determination of propranolol from human Saliva samples. The propranolol concentration in DES rich phase (extraction phase) was determined by spectrofluorimetry. Different parameters effective on extraction efficiency such as DES volume, pH, ultrasonication time, and salt addition effect were optimized using a multivariate approach by central composite design (CCD) in combination with the desirability function approach. The optimum conditions were found to be: pH=10.33, 117 μL DES volume, 4.25 min ultrasonication time, and 2.75 %w/v salt amount. The performance of the method was evaluated under optimum conditions, and the method exhibited good linearity, low limit of detection and quantitation, good precision, and high extraction recovery. The established method was successfully applied to determine drug in human saliva samples with high relative recoveries.

Keywords: Deep eutectic solvent, Ultrasound-assisted, Propranolol, Drug

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Easy Applicable Solid Phase Extraction and Determination Method for Chloramphenicol Residues in Milk Samples

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Determination of pharmaceutical substances and biological active molecules in biological matrix is crucial in various fields of medicine and pharmacy, e.g., in pharmacokinetic studies, development of new drugs or in therapeutic drug monitoring [1]. Antibiotic molecules are proposed for treating and preventing of bacterial infections since penicillin was discovered in 1928. Like most of synthetic drug, their consumption is gradually growing in all world. As one of the most used group of Pharmaceutical and Personal Care Products (PPCPs), antibiotics are commonly used in veterinary medicine, human therapy and aquaculture. Chloramphenicol(CP) is used for the treatment of bacterial infections and it is one of the first antibiotic synthetically manufactured on a large scale [2,3]. As a broad spectrum antibiotic, it shows activity against both gram-positive, gram-negative bacteria and also other microorganism groups. Fabric solid phase extraction (FPSE) coupled with HPLC-DAD approaches was used for determination of Chloramphenicol anbitiotic residues in milk samples. As a solid phase carrier, fabric phases modified with poly ethylene gylicol was synhezied and used for batchtype solid phase extractions. Experimental variables of FPSEE method for antibiotic molecules was investigated and optimized systematically. The HPLC analysis of CP molecules was performed by using a phonomex C18 column, isocratic elution of triflouro acetic acid (0.1 %), methanol and acetonitrile (17:53:30) with a flow rate of 1.0 mL min^{-1}. After FPSE, the linear range for both molecules ($r^2 > 0.9982$) was obtained in the range of 10.0–600.0 ng mL^{-1}. The limit of detections (LOD) is 3.42 while RSDs % are below than 4.5 %. Finally, the developed method basen on FPSE-HPLC-DAD was applied to milk samples to determine antibiotic residues.

Keywords: Chloramphenicol, Fabric phase extraction, HPLC, Milk samples

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Determination of lead in vegetables and soil samples irrigated with treated sewage using deep eutectic solvent followed by GFAAS

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Despite the useful aspects of using urban wastewater in agriculture as a rich source of nutrients, and the presence of some heavy and toxic metals in it, long-term use of wastewater in agricultural soils will be problematic, resulting in excessive accumulation of these elements in the soil [1]. Soil contamination with heavy and toxic elements causes them to enter the food chain through plant intake and toxicity [2]. In the present study, a new microextraction approach termed as vortex-assisted liquid phase microextraction based on deep eutectic solvent (VALPME–DES) combined with graphite furnace atomic absorption spectrometry (GFAAS) has been developed for the extraction, preconcentration and determination of lead in vegetables and soil samples irrigated with treated sewage from two different regions of Iran. The new DES was prepared by mixing 1:1 molar ratio of choline chloride and citric acid monohydrate [3−5]. The introduced method exhibited good linearity with coefficient of determinatin (r^2) 0.9988 and an acceptable linear range of 0.6–100 μg l^{-1}. Accordingly, the detection limit was 0.2 μg l^{-1} (S/N=3) for Pb ions, and the high enrichment factor was obtained. The proposed method was successfully utilized to determine trace level of the lead in vegetables and soil samples. The results of the sample analysis showed that 25% of the vegetables samples and 32% of the soil samples were much higher than expected level to contaminated lead, and this contamination posed a serious threat to users.

Keywords: Lead, Deep eutectic solvent, Soil, Vegetables

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Utility of Co and Ni incorporated graphitic carbon nitride (Co-Ni@g-C_3N_4) towards high performance supercapacitor application

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Employment of graphitic carbon nitride (g-C_3N_4) as active material in energy storage devices is challenging because of the low number of edge nitrogen atoms and its intrinsic poor electrical conductivity [1]. In this study, the conductivity of g-C_3N_4 is enhanced by doping different ratios of Co and Ni elements in a facile two-step synthesis method. For electrode preparation, the slurry containing an active material, conductive particle, and binder with proper ratios was loaded on it. The investigation of the super capacitive performance of the composite material has been done by cyclic voltammetry (CV), galvanostatic charge-discharge (GCD), and electrochemical impedance spectroscopy (EIS). As prepared electrode showed a high specific capacitance up to 400 F g^{-1} in potassium hydroxide electrolyte in a three-electrode setup at a current density of 1 A/g (fig. a). Also, up to 60% capacitance retention performance (at 8 A/g current density), (fig. b), and well-cycling stability of about 78% capacitance retention after 5000 galvanostatic charge-discharge cycles were attained in potassium hydroxide electrolyte at 3 A/g. This study proposes a new synthesized g-C_3N_4 composite with enhanced electrical conductivity to be used in high-performance energy storage devices.

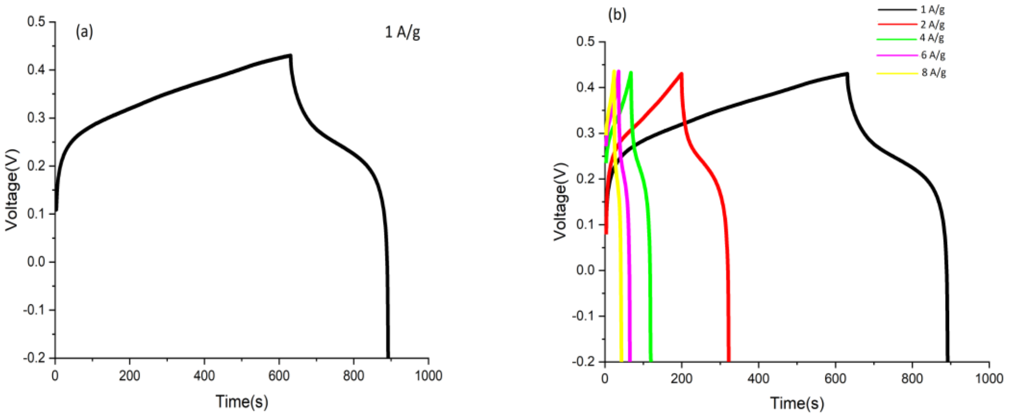

Fig. (a), GCD of the compsite at a current density of 1 A/g in 1 M H_2SO_4; (b), GCD profiles of the composite at different current densities (1–8 A/g).

Keywords: Supercapacitor, Graphitic carbon nitride, Energy storage

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Application of tandem dispersive liquid-liquid microextraction for pre-concentration of naproxen in biological samples using HPLC-UV

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Naproxen (NAP) is a non-steroidal anti-inflammatory drug for mild to moderate pain relief. It works by reducing hormones that cause inflammation and pain in the body [1]. Sample preparation has a key position in modern analytical chemistry. The tendency to measure low concentrations of analytes in complex matrices and the incompatibility of most biological samples with analytical instruments cause the sample preparation step to be an integral part of most analytical methods. Among the various sample preparation methods, dispersive liquid-liquid microextraction (DLLME) has always been considered due to its low extraction time, simplicity, and high preconcentration factor. Despite these considerable advantages, DLLME suffers from a great problem. A low sample clean-up is the main disadvantage of this method. The chromatograms obtained by applying this method for the preparation of samples with complicated matrices, especially biological fluids, are crowded, and this intensifies distinguishing the peaks obtained for the interferences from those obtained for the analytes. To solve this problem, the method of tandem dispersive liquid-liquid microextraction (TDLLME) is proposed. In this method, two stages of consecutive extraction are performed on the sample, which increases the clean-up of the sample [2]. TDLLME was performed in two steps. At first, 8.0 mL of the sample solution containing the analyte (pH 2.5) was put into a 10.0-mL screw cap glass test tube with conic bottom, which was then immersed in an ultrasonic water bath. The optimized extractor organic solvent (150 µL) was slowly injected into the sample solution with a 250 µL syringe. After a 2.0 min sonication, the emulsion formed was centrifuged for 4 min to separate the phases. In the next step, the extractor organic solvent collected was transferred into another glass test tube with conic bottom, and an optimized volume of aqueous extracting solution (pH 10.75) was added to the organic solution. The mixture was repeatedly sucked from the tube and dispensed into it using a 500 µL glass syringe. Then, mixture was centrifuged for 1 min. Finally, 25 µL of the aqueous solution was injected into the HPLC system. In this study, an efficient rapid, and very simple method was introduced for the determination of NAP in complicated matrices. The method provided considerable repeatability (RSD% 4.1), and it exhibited a wide linear range (4.0–1200 ng mL^{-1}). The results obtained show that the combination of two dispersive microextraction methods provides a low-cost and noticeable extraction clean-up in a few minutes.

Keywords: Naproxen, Tandem dispersive liquid-liquid microextraction, Complicated matrices

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Application of a metal nanocomposite in pre-concentration of heavy metals from aqueous samples using flame atomic absorption spectroscopy

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Water contamination by heavy metals is one of the most important challenges involved in human health and the environment protection. Heavy metals can cause severa diseases,like different types of cancers, in humans beings. Due to the low concentration of heavy metals in the aqueous samples, their direct monitoring is not an easy task. Sample preparation procedures such as liquid-liquid extraction (LLE) and solid phase extraction (SPE) are usually used for the extraction and preconcentration of the analytes. Nevertheless, these techniques require large amounts of poisonous organic solvents, a large volume of samples and generate large amounts of pollutants. In recent years, much attention has been paid to the use of the dispersive micro-solid phase extraction (D-µ-SPE) method due to some advantages like reducing the consumption of adsorbent amounts, short extraction time, being eco friendly, and simplicity [1]. Among the various adsorbents used in the D-µ-SPE method, metal nanocomposites have become very important due to their properties such as various chemical interactions, high internal surface area and high extraction capacity [2]. A newly synthesized metal nanocomposite adsorbent was used for preconcentration heavy metals Cu(II) ،Cd(II) and Pb(II) in aqueous samples, utilizing the D-µ-SPE method In order to investigate the effective parameters for the extraction recovery of the mentioned metals, the central composite design (CCD) method was used. As shown in the Scanning Electron Microscopy image [Fig.1], the synthesized metal nanocomposite has a rod and spherical morphology with a particle size of less than 100 nm, so it has a large active surface for pre-concentration of heavy metals. Figure 2 shows the interaction of two parameters pH and the adsorbent dosage, in the extraction recovery of Cu (II) metal. The results show that the synthesized metal nanosorbents have a high ability to pre-concentrate heavy metals from aqueous samples.

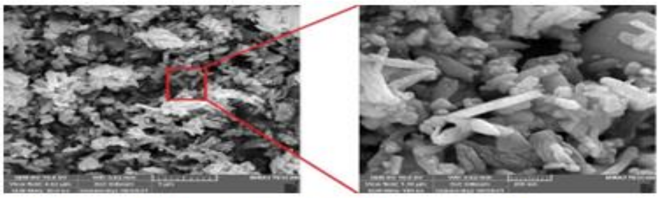

Fig. 1. Scanning electron micrographs for synthesized metal nanocomposite.

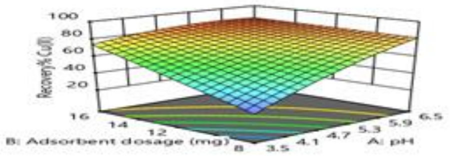

Fig. 2. interaction of two parameters pH and the adsorbent dosage in the extractin recovery of Cu (II) metal.

Keywords: Metal nanocomposite, Dispersive micro-solid phase extraction, Heavy metals.

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Application of a new synthesized eutectic solvent for the extraction of Co^{2+} and Ni^{2+} in aqueous samples using flame atomic absorption spectroscopy

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Industrialization has brought about environmental pollution. Heavy metals such as nickel and cobalt have the highest toxicity among metals. Different techniques such as flame atomic absorption spectroscopy (FAAS), inductively coupled plasma optical emission spectroscopy (ICP-AES), and electro-thermal atomic absorption spectroscopy (ET-AAS) have been used for the determination of elements in aqueous samples. The FAAS has been widely used in the analysis of trace metals because of the low costs, operational facility, and high sample throughput [1]. The determination of heavy metal ions at trace level is possible due to the use of sample preparation and sensitive instrumental techniques. One of the popular sample preparation methods is liquid phase microextraction. This method includes hollow fiber-based liquid phase microextraction, single drop microextraction, and dispersive liquid-liquid microextraction. The deep eutectic solvents, one of the common solvents, was used in the liquid phase microextraction. These solvents are the newest sub-class of ion liquids. The properties of this solvent are simple, novel, and green synthesis. They were used in a wide range of chemical analysis processes [2]. In the present study a simple, low-cost, and green method was used for the determination of trace cobalt and nickel ions in aqueous samples. A new synthesized deep eutectic solvent based on choline chloride and alcoholic ingredient was used as an extraction solvent for the air-assisted dispersive liquid-liquid microextraction procedure coupled with FAAS. The influence of different parameters affecting the dispersive liquid-liquid microextraction including volume of the extraction solvent, sample pH, and several extraction cycles was investigated to optimize extraction efficiency. The method was validated based on linearity ($R^2 > 0.985$), linear dynamic ranges (1.3-250.0 $\mu g\ L^{-1}$), limits of detection (0.1-1.0 $\mu g\ L^{-1}$), enrichment factors (40 and 55), and relative recoveries (90 and 95%) for nickel and cobalt ions, respectively. In this study, extraction based on a new deep eutectic solvent was proposed. This new solvent comprising choline chloride and alcoholic ingredient was simply and cheaply synthesized at room temperature and it was successfully applied as an extraction solvent for the analysis of low levels of copper and lead ions in aqueous samples.

Keywords: Dispersive liquid-liquid microextraction, Deep eutectic, Heavy metals

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Synthesis of pencil graphite electrode modified with molecularly imprinted polymer for detecting vitamin B6 in various aqueous samples

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Vitamin B6 (pyridoxine) is a member of group B vitamins which in the human body is essential for red blood cell metabolism, and plays a major role in the conversion of tryptophan to niacin. Thus, various analytical methods have been developed for the determination of pyridoxine, including flow injections, high-performance liquid chromatography, capillary zone electrophoresis, spectrophotometry, and electrochemical detection. The advantages of the electrochemical technique are the low price of the device and the suitability of its tools, high accuracy, ease of execution, and fast execution speed [1]. Disadvantages of laboratory kits for measurement of pyridoxine include expensiveness, requiring skilled handling, and being time-consuming. Electrochemical sensors modified with molecularly imprinted polymer (MIP) are selective, sensitive and synthetic polymers that, upon the choice of monomers, could have specificity equivalent to antibodies, with much lower cost, high mechanical strength and least maintenance for pyridoxine measurement [2]. First, a pencil graphite electrode (working electrode) with an auxiliary electrode and a reference electrode was placed in a solution containing the materials needed to synthesize the vitamin B6 molecular imprinted polymer. Using cyclic voltammetry (CV) under optimized conditions (scan rate, potential range and the number of cycles), a MIP was synthesized on the surface pencil graphite electrode. CV cycles of MIP preparation on the surface carbon electrode are shown in figure 1A. The electrode modified by the MIP was used to measure vitamin B6 under optimal conditions and using the differential pulse voltammetry method in aqueous samples. Figure 1B shows that the modified electrode has a higher efficiency than the pristine one. By modifying the surface of the pencil graphite electrode with MIP, the sensitivity and selectivity of this electrode for measuring vitamin B6 in different aqueous samples increased significantly.

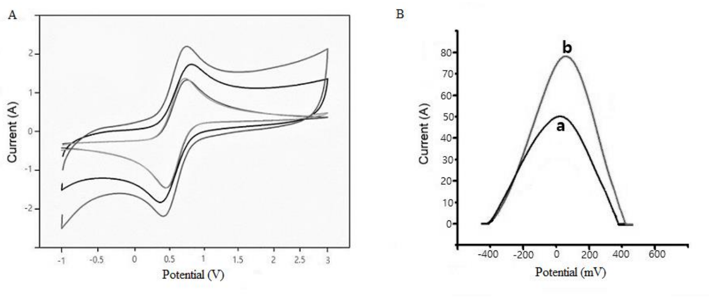

Figure 1 A) Cyclic voltammetry peak related to the synthesis of vitamin B6 MIP on the surface of the PGE.

B) Differential pulse voltammograms of (a) B6 (b) determination of the B6 with modified PGE-MIP as an electrochemical sensor.

Keywords: Molecularly imprinted polymer, Vitamin B6, Electrochemical sensor.

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Determination of venlafaxine drug in aqueous samples using a modified pencil graphite electrode with molecularly imprinted polymer

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Venlafaxine is an antidepressant drug. This group of drugs reduces some of the chemicals in the brain, which are called neurotransmitters and are necessary for a normal functioning of the brain. Antidepressants help depressed patients by making these neurotransmitters (natural chemicals) available to the brain. The various methods for determining venlafaxine include chromatography, spectroscopy and electrochemical methods [1]. Among the available methods for determining venlafaxine, electrochemical sensors are of great importance due to their high sensitivity, simplicity of the system used, and low cost. Molecularly imprinted polymers (MIPs) are tailor-made materials able to selectively bind to a target analyte, under certain experimental conditions, in preference to other closely related compounds [2]. Electrode modification using MIPS increases the efficiency in analyte detection and measurement. The ability to be used in hard conditions (acidic and alkaline pHs, high and low temperatures, etc.), ease of preparation and low cost of preparing MIPS, are other advantages of these supports [3]. Using cyclic voltammetry (CV) under optimized conditions (potential range, scan rate, and the number of cycles), a MIP was synthesized on the surface of a pencil graphite electrode (Fig. 1A). The modified electrode was used to measure venlafaxine in aqueous samples. The parameters affecting the measurement of the drug such as: electrolyte type, sample solution pH and drug concentration were optimized and the differential pulse voltammetry (DPV) method was used (Fig. 1B). By modifying the surface of the pencil graphite electrode with MIP, the selectivity and sensitivity of the method for measuring the venlafaxine drug was significantly increased. Therefore, this electrochemical sensor can be used to measuring trace amounts of the venlafaxine drug in various aqueous samples.

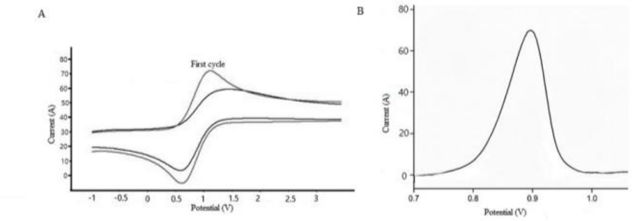

Fig 1 A) The voltammetric peak corresponds to the synthesis of MIP on a CPE.

B) The response DPV of the modified.

Keywords: Molecularly imprinted polymer, Venlafaxine, pencil graphite electrode

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Removal of Congo Red Dye from Aqueous Solutions by GO-CTAB Nanocomposite

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In this work, some studies were conducted for investigate the sorption of congo red on graphene oxide – cetyl trimethyl ammonium bromide (GO-CTAB). The structure of GO-CTAB nanocomposite were investigated by fourier transforms infrared spectroscopy (FT-IR), X - ray diffraction (XRD) and scanning electron microscopy (SEM). The influence of the parameters affecting the adsorption efficiency such as pH of the aqueous solutions, contact time, adsorbent dose and initial concentration of the antibiotics were assessed and discussed. The results showed that the adsorption of congo red on GO-CTAB nanocomposite was highly pH-dependent, and the optimal pH was found to be 6 and for congo red. The adsorption kinetics fitted perfectly pseudo-second-order model. A thermodynamic study showed that the adsorption processes are exothermic with negative entropy changes.

Keywords: Congo red, Graphene oxid, Cationic surfactant, Anionic dye

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Synthesis and application of magnetic cellulose/polyaniline nanocomposite for dye removal

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The purpose of this study was to prepare magnetized cellulose polyaniline nanocomposite for dye removal from aqueous solutions. The cellulose was first magnetized in the presence of Fe(III) chloride and Fe(II) sulfate via co-precipitation method. Polyaniline was synthesized by chemical polymerization. Then, polyaniline was dissolved in formic acid and coated on the surface of magnetized cellulose via cast solution method. magnetized cellulose polyaniline nanocomposite was then applied for adsorptive removal of dye in a batch system. Congo Red was selected as a test probe for dye removal efficiency. FE-SEM, XRD, VSM and FT-IR techniques were employed for characterization of magnetized cellulose polyaniline nanocomposite. Different parameters such as pH, exposure time, adsorbent dosage, temperature, and initial dye concentration were investigated for obtaining the optimal dye removal conditions. The results showed that the removal percentage of Congo Red with 0.009 g of the adsorbent and the concentration of 150 mg/L at pH = 3 was more than 90%. Based on isothermal studies, it was found that the Congo Red adsorption follows the Langmuir model. Under optimal conditions, the maximum adsorption capacity of Cellulose/Fe_3O_4/Polyaniline nanocomposite was 1000 mg/g. Kinetic studies were not performed due to the high reaction rate (adsorption above 90% in the first minutes). Thermodynamic experiments showed that the adsorption of Congo Red on Cellulose/ Fe_3O_4 / Polyaniline was not temperature dependent and that the maximum amount of adsorption occurred at ambient temperature. Also, a negative ΔG value indicates that the process is spontaneous.

Keywords: Polyaniline, Adsorption, Dye, Magnetic cellulose, Nanocomposite

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Application of a developed approach of hydrogel-based spin column micro solid phase extraction for monitoring of trace concentration of antifungal drugs in blood samples

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In this study, a blended polyacrylamide-chitosan hydrogel was synthesized. The prepared sorbent was efficiently employed in a hydrogel-based spin column setup for the first time as a proper format. Due to the swelling property of hydrogels, when the hydrogels employed in spin column setup as the sorbent, it can swell easily, leading to imbibe large quantities of the desired sample and subsequently, more interaction between the sorbent and analytes. This fact can significantly improve the extraction efficiency [1, 2]. So, it suggests that spin column format is an efficient approach for hydrogels application in sample analysis, especially in case of biological matrices in which the common problems of clogging and back pressure are minimized [3, 4]. In this way, given the many remarkable features of hydrogels, a composite polyacrylamide-chitosan hydrogel was synthesized as a promising sorbent to take advantage of desired properties of these polymers [5]. Fourier transform infrared spectroscopy, field emission scanning electron microscopy, and X-ray diffraction were employed to characterize the synthesized hydrogel. The synthesized sorbent was efficiently implemented for spin column extraction of some antifungal drugs including ketoconazole (KZ), miconazole (MZ) and clotrimazole (CZ) in blood samples. To achieve the best analytical performance, effective adsorption and desorption parameters, including sorbent amount (20 mg), sample pH (5.0), number of adsorption cycles (4), eluent type (acetonitrile), eluent volume (150 µL), and the number of desorption cycles (4) were optimized with central composite design and one-variable-at-a-time approaches, respectively. Under the optimized conditions, limits of detection values were obtained between 0.2-5.0 ng mL^{-1}. Also, the calibration curves were found linear in the range of 15.0-1000.0, 1.0-1000.0, and 2.0-1000.0 ng mL^{-1} for KZ, CZ, and MZ, respectively, along with intra- and inter-day precision less than 8.4%. The preconcentration factors were obtained in the range of 6.0-8.0. The current method was successfully applied for micro solid-phase extraction of trace amounts of the studied antifungal drugs in human blood samples followed by liquid chromatography-tandem mass spectrometry. The satisfactory relative recoveries of 94.0-104.0 % were found, indicating method reliability. In overall, the developed method offers acceptable repeatability and accuracy, high reusability, and desirable applicability for determining antifungal drugs in complicated biological fluids.

Keywords: Hydrogel, Spin column, Micro solid-phase extraction, Antifungal drugs, Blood samples.

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Easy Applicable Approaches for Sensitive Analysis for Drug Molecules

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Sample preparation has been recognized as a major step in the chemical analysis workflow. As such, substantial efforts have been made in recent years to simplify the overall sample preparation process. Sensitive analysis of drug molecules in biological samples is a challenge due to low concentration of target molecules and comlexity of sample matrix [1]. Major focusses of these efforts have included miniaturization of the extraction device; minimizing/eliminating toxic and hazardous organic solvent consumption; eliminating sample pre-treatment and post-treatment steps; reducing the sample volume requirement; reducing extraction equilibrium time, maximizing extraction efficiency etc. All these improved attributes are congruent with the Green Analytical Chemistry (GAC) principles [2]. Classical sample preparation techniques such as solid phase extraction (SPE) and liquid-liquid extraction (LLE) are being rapidly replaced with emerging miniaturized and environmentally friendly techniques such as Solid Phase Micro Extraction (SPME), Stir bar Sorptive Extraction (SBSE), Micro Extraction by Packed Sorbent (MEPS), Fabric Phase Sorptive Extraction (FPSE), and Dispersive Liquid-Liquid Micro Extraction (DLLME). These techniques manifest a rapid development of sample preparation techniques in different fields, such as biological, environmental, food sciences, natural products, forensic medicine, and toxicology. In the biological and forensic fields, where a wide variety of drugs with different chemical properties are analyzed, the sample preparation is required to make the sample suitable for the instrumental analysis, which often includes gas chromatography (GC) and liquid chromatography (LC) coupled with mass detectors or tandem mass detectors (MS/MS)[3]. Application of magneic nanoparticles as high-performance extraction sorbents has undoubtedly elevated the extraction efficiency and method sensitivity of modern chromatographic analyses to a new level. Combining magnetic nanoparticles with many microextraction sorbents has opened up new possibilities to extract target analytes from sample matrices containing high volumes of matrix interferents. By developing this type materials, highly sensitive and selective analyzes can be performed easily and effectively even in laboratories with a conventional chromatographic system.

Keywords: Pharmaceutical analysis, Microextraction techniques, HPLC, GC, Biological samples

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The Label-free electrochemical-based oligonucleotide genosensor by hybridization process for highly sensitive determination of *Leishmania spp.* in biological samples

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Leishmania parasite identification is very important in clinical studies of leishmaniasis and its diagnosis. Though there are various clinical and epidemiological approaches to identifying *Leishmania spp*, due to some drawbacks of the clinical and conventional methods, sensitive techniques are needed and of great importance [1, 2]. In this study the label-free electrochemical-based oligonucleotide genosensing assay through hybridization process have been developed [3, 4]. For attaining an appropriate electrochemical signals, thermionic vacuum arc method has been applied. Various features of this new technique is being fast-fabricated, not being time-consuming, high vacuum regime, low surface roughness, high quality, and plasma-based technique for coating nano-dimension materials and providing an appropriate surface for electrochemical investigations. The roughness value was obtained 6 nm, and the FESEM image was shown a low amount compactness asymmetrical deposition of particles, flatness of the void- and the crack-free surface. The high transparency (76%) of and the refractive index of the electrode was enhanced that demonstrated higher impact, higher the electronic polarization of ions as well as localized zones due to successful graphene incorporation into Nb_2O_5 structure. Low detection (LOD) associated with the fabricated platform to detect *Leishmania spp* have been evaluated down to 1.12 fM. Moreover, the wide linear range of 100 nM to 10 fM demonstrates the capability of the designed platform. 1, 2, and 3-base mismatched sequences were investigated and also negative control samples clarified the high selectivity and better performance of the engineered assay. The values of recovery indexes and RSDs have been obtained in human serum samples. Furthermore, repeatability and reproducibility of the associated bio-assay have been studied. Consequently, the novel method is appropriate for rapidly and quantitatively detecting *Leishmania spp*, and is considered as a better candidate for advanced tests on biological samples.

Keywords**:** Genosensor, Leishmania spp, Physical properties, Optical properties

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Electrochemical Determination of 4-Nitrophenol Using a Cu/MOF Carbon Paste Electrode

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Recently, water contaminated by 4-nitrophenol (4-NP, a nitroaromatic compound) has become a severe problem due to its extensively used as a precursor and intermediate material in the manufacturing of dyes, pesticides, pigments, explosives, pharmaceuticals, engineering polymers, and anti-corrosion lubricants. 4-NP is the most toxic pervasive organic pollutant which is highly water-soluble and has strong chemical stability in nature that can quickly affect the human body through the respiratory system, mouth, skin, and digestive system. However, there is no facile and direct determination method for the sensitive determination of 4-NP in water samples. Until now, various analytical methods have been developed for the determination of 4-NP including the chromatographic method and spectrometric methods, and photo-electrochemical methods. The electrochemical methods have exhibited great potential for the analysis of 4-NP because of their simplicity, high sensitivity, inexpensive, short time, and quick response. Hence, the development of various modified electrodes with advantages including easy fabrication, inexpensive, sensitivity, and excellent reproducibility has grabbed much attention in electro-analytical chemistry research [1, 2]. Recently, metal-organic frameworks (MOFs), which are composed of metal ions with organic linkers, have become a hot research topic. These compounds provide tunable porosities, high thermal stabilities, large pore sizes, and extensive surface areas and can be easily synthesized by facile methods. The high porosity and large surface area of MOFs allow them to capture numerous analytes and seize the one with the desired size and configuration. The immobilization of metal nanoparticles into MOFs for application to catalytic reactions has been thoroughly explored because the MOF porous structure prevents the agglomeration of metal NPs, thereby increasing their catalytic activity. To the best of our knowledge, there are very few reports of the electrochemical detection of 4-NP by metal-based MOFs [3]. In this study, a novel modified carbon-paste electrode (CPE) with a new synthetic Cu/MOF was employed for 4-nitrophenol measurement by cyclic voltammetry, and differential pulse voltammetry (DPV), and chronoamperometric methods. Various parameters such as pH, modifier, and scan rate were optimized. The proposed electrode showed a good response towards 4- nitrophenol determination. Under the optimized conditions, the reduction peak current showed a good linear relationship with the nitrophenol concentration in the range comprised between 1×10−6 molL^{-1} and1×10−4 molL^{-1}. The developed electrode was successfully applied for the determination of 4-nitrophenol in water samples.

Keywords: Modified electrode, Mesoporous silicate, 4-Nitro phenol

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High throughput liquid phase thin film microextraction of estrogens by polyvinylidene fluoride membrane sheet

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In this study, n-octanol loaded polyvinylidene fluoride (PVDF) membrane sheet was introduced as extracting phase in high-throughput liquid phase thin film microextraction (TFME) for the rapid and simultaneous extraction of two steroid hormones, including estrone (E1) and 17β-estradiol (E2) in aqueous samples (water, waste water and urine samples) prior to liquid chromatographic determination. The proposed thin film membrane was characterized by FE-SEM, AFM, ATR and BET. Thin film membrane was prepared by non-solvent induced phase inversion method and pore generation using Polyvinylpyrrolidone (PVP). Optimum extraction/desorption conditions were found as: organic solvent: n-Octanol, Salt concentration: 16%w/v NaCl, stirring speed: 1600 rpm, pH 8, extraction temperature: 25 °C, extraction time: 35 min, desorption solvent: methanol and desorption time: 15 min. The figures of merit were obtained under the optimized conditions: the Linear Dynamic Ranges (LDRs): 6.70-100 µg L^{-1} and 4.18-100 µg L^{-1}, Limits of Detection (LODs): 2.21 µg L^{-1} and 1.38 µg L^{-1}, Limits of Quantification (LOQs): 6.70 µg L^{-1} and 4.18 µg L^{-1} for E1 and E2, respectively.

Keywords: Polyvinylidene fluoride (PVDF), High-throughput, Liquid phase thin film microextraction, Estrone (E$_1$), 17β-estradiol (E$_2$)

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Development of a hydrophobic deep eutectic solvent based on fatty acids for liquid-phase microextraction of a calcium channel blocker drug from plasma samples

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Liquid-phase microextraction (LPME) undoubtedly constitutes one of the most exploited strategies within modern analytical microextraction methods for sample preparations. Since the incorporation of the Green Analytical Chemistry guidelines in the sample preparation stage, the search for new solvents to improve the environmentally friendliness of LPME methods is one of the most important research lines in the field [1]. Deep eutectic solvents (DESs) have attracted attention in recent years as new green solvents. These solvents have properties like ionic liquids, with the advantage of presenting low-cost and straightforward synthesis. The production of DESs requires low-cost raw materials from renewable sources, which makes them alternative solvents of great interest for applications in extraction processes [2]. In this study, a new DES by combining various fatty acids which can concurrently act as both hydrogen bond acceptors (HBA) and hydrogen bond donors (HBD) was prepared. Adding a third component to classical two-component eutectic solvents allows to purposefully control the density, melting point, and viscosity of the synthesized solvents. The DES was used as an extraction solvent in the ultrasound-assisted emulsification-microextraction (USAEME) of amlodipine in plasma samples. Accurate and sensitive determination of amlodipine was accomplished with the combination use of USAEME-based DES and UV-Vis spectrophotometric detection. The central composite design combined with the desirability function was applied to find out the optimal experimental conditions providing the highest global extraction efficiency. The effect of important analytical variables such as pH of sample solution, the volume of the DES, amount of added salt, and sonication time was studied and optimized. According to the optimization criteria, the experimental conditions according to the maximum one in the desirability function were found to be: pH = 9.46; DES volume, 126 μL; NaCl, 16.69% (w/v); sonication time, 270 s. The established method was successfully applied to determine amlodipine in human plasma samples and saliva with satisfactory relative recoveries.

Keywords: Deep eutectic solvent, Microextraction, Amlodipine, Plasma

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Investigation of electrochemical behavior of pyrocatechol and utilizing a drug delivery system for loading and releasing of pyrocatechol in order to electrochemical signal amplification

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To date, signal amplified electrochemical biosensors have been widely used in the study of life science, biomedical research, food and environmental analysis, chemical analysis, etc [1]. Nowadays, hydrogels have been attracted a lot of interest due to their immense potential in different fields such as biomedicine and biotechnology [2]. Pyrocatechol can be electrochemically oxidized to o-quinone. Therefore, it can be used as an electroactive indicator for the detection of various biomarkers. In this research, the loading and releasing behaviour of pyrocatechol was investigated using the hydrogel and the optimized conditions were obtained. The surface of pencil lead electrode (PLE) was activated through different strategies (potentiodynamic and potentiostatic) to achieve the highest amplified signal. According to the results, the potentiostatic pretreatment exhibits better performance toward higher electrochemical responses. Compared to other electrode modification methods, electrochemical activation of PLE is a simple, more applicable and, less timeconsuming strategy that eliminates the employing of toxic substances for electrode surface modification [3].

Keywords: Hydrogel, Pyrocatechol, Loading and releasing, Pencil lead electrode, Signal amplification

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Use of room-temperature ionic liquid (1-ethyl-3-methylimidazolium tetrafluoroborate) as a non-aqueous, robust and conductive electrolyte to improvement of Li-O_2 battery performance

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Today, the main energy supplier comes from fossil fuels, such as coal, oil, and natural gas that their consumption causes a dramatic build-up of greenhouse gases in the atmosphere. In response, energy conversion from renewable sources has been considered as a promising solution to decrease CO_2 and other pollutant agent's emissions. However, rechargeable energy storage systems with high energy density and round-trip efficiency are urgently needed to capture and deliver renewable energy for applications such as electric transportation [1,2]. Lithium-oxygen batteries have received much attention in the past several years because of their large theoretical specific energy density, stable output voltage, cost-effective, energy-efficient, pollution free, and have broad application prospects [3]. The electrolyte is one of the crucial components of lithium-oxygen batteries and the electrochemical performance of the battery is determined by electrolyte to a great extent. Due to the react violently between lithium metal (as anode) and aqueous solutions as electrolyte solvent, it is not practical for Li-oxygen batteries to use directly an aqueous electrolyte. Here, capability of lithium-oxygen battery using hydrophobic ionic liquid consisting of 1-etyl-3-methylimidazolium as cation and tetrafluoroborate as anion was investigated. 1-ethyl-3-methylimidazolium tetrafluoroborate [Emim][BF_4], which has high conductivity and prevents hydrolysis of the lithium metal in anode, showed the satisfactory performance. The battery worked for 30 days in usual air condition, and the cathode carbon based showed high discharge capacity of 2340 mAh $\mathrm{g}^{-1,}$ which was about 540 mAhg^{-1} higher than battery with usual electrolyte. Furthermore, the usage of an ionic liquid as electrolyte leads to the increase of battery lifetime to more than 2 times. The over potential amount for this battery was 1.1 V and about 0.4 V was lower that battery with usual electrolyte. In summary, a durable, good discharge capacity, and low over potential were observed in electrochemical battery behaviour.

Keywords: Li-O_2 battery, Ionic liquid, Robust electrolyte, Improvement performance

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A green method for electrochemical synthesis of new benzofuran derivatives

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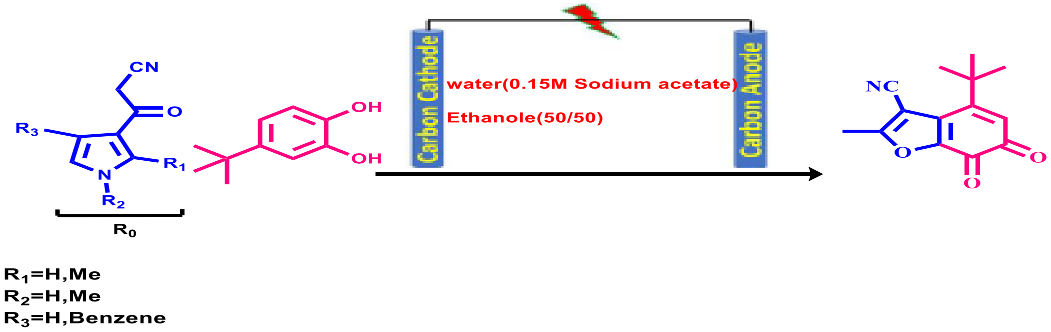
Today, electrochemical methods have found a special place in various fields of basic and applied research as well as in industry [1]. The efficiency of electrochemical methods in the synthesis of organic compounds has led to the replacement of many chemical methods with direct electrochemical methods. Other advantages of electrochemical methods in the synthesis of organic compounds include the following: 1) the reaction conditions can be improved by modifying the electrode surface, which improves the reaction progress. 2) Electrochemical syntheses usually have no contaminant effects. 3) Energy efficiency in these syntheses is high. 4) The reaction scale is easily controllable. 5) Electrodes as heterogeneous catalysts are easily separated from the reaction medium after the reaction. 6) Electrochemical reactions are performed under mild conditions such as room temperature and atmospheric pressure and using electric current [2]. Heterocyclic compounds have a wide range of application. They are predominantly used as pharmaceuticals, as agrochemicals and as veterinary products. They also find applications as sanitizers, developers, antioxidants, as corrosion inhibitors, as copolymers, dye stuff [3-4]. These derivatives were synthesized via constant current electrolysis in high yield, without need for metal catalyst and oxidant, using conventional equipment (simple cell and carbon electrode) under green conditions.



Scheme 1: Preparation of benzofurans.

Keywords: Electrochemical, Heterogeneous, Indolyl, Organic compounds.

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Application of magnetic MOF nanocomposite as SPME fibers coupled with HPLC for determination of NSAID drugs in biological fluids samples

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A novel solid-phase microextraction (SPME) fiber based on a capillary glass tube coated with magnetic Cobalt ferrite@Cu3(BTC)2 metal organic frameworks (MOF) nanocomposite was prepared by sol–gel technique. The magnetic Cobalt ferrite@Cu3(BTC)2 MOF nanocomposite were synthesized for first time by a simple coprecipation reaction and the resultant powder was mixed with sol–gel precursors to prepare sol–gel solution of the magnetic Cobalt ferrite@Cu3(BTC)2 coating material. In this study, glass tubes with a specific diameter were used as substrates. The magnetic Cobalt ferrite@Cu3(BTC)2 MOF nanocomposites coating was characterized using FT-IR, XRD, FE-SEM, EDX, TGA/DTA, BET and VSM. Then, the synthesized fiber as a novel SPME fiber combined with HPLC was applied for the determination and quantification of 9 non-steroidal anti-inflammatory drugs (NSAIDs) in real samples including human urine, serum and plasma. NSAIDs are the most commonly used analgesics worldwide today. They are used mainly to treat pain, inflammation, and fever in animal and human species and can decrease the risk of Alzheimer's disease, increase the human lifetime, and improve the quality characteristics of dairy products. However, they can lead to severe toxic side-effects in cases of overdose or chronic abuse [1]. To found optimum microextraction conditions, the influences of effective variables were investigated using one-factor-at-a-time experiments and the significant variables were optimized using a central composite design (CCD) combined with desirability function. Under optimized conditions, calibration graphs of analytes were linear in a concentration range of 0.1–700 μg L−1 with correlation coefficients>0.9975. Limits of detection (LOD) and quantification (LOQ) were in the ranges of 0.02–0.04 ng L−1 and 0.09–0.13 ng L−1, respectively. This procedure was successfully employed in determining target analytes in spiked human urine, serum and plasma samples with recoveries ranged from 95.2 to 101.7%.

Keywords: Solid-phase microextraction (SPME), Non-steroidal anti-inflammatory drugs (NSAIDs), HPLC, Biological fluids, Magnetic MOF Nanocomposites

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An Electrochemical Genosensor for gastric cancer cell detection

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A genosensor was fabricated for the early detection of miRNA-106a, the promising biomarker of gastric cancer. The sensor was made of a nanocomposite of reduced graphene oxide (rGO) and cerium oxide (CeO2) nanoparticles. For this purpose, surface of a glassy carbon electrode was first modified by polyaniline (PANI) and then rGO-CeO2 nanocomposite. It was next characterized through scanning electron microscopy, cyclic voltammetry and electrochemical impedance spectroscopy. A 22-base oligonucleotide sequences (miRNA-106a) previously reported as a biomarker of gastric cancer which is up-regulated in apatient plasma and also related with cancer stage, tumour size, and proliferation of tumour cells [1–3] was selected as a target molecule. Its ssDNA probe was immobilized on the modified surface via a strong interactions between CeO2 nanoparticles and the phosphate groups in the ssDNA. Detection of the biosensor signal was performed by square wave voltammetry (SWV) and $[Fe(CN)_6]^{3-/4-}$ as an electrochemical probe. In presence and absence of the target sequence, the electrochemical probe showed a different behaviour on the electrode surface. The developed genosensor could detect the of miRNA-106a sequence high selectively and sensitively, with in a good linear range of 10 fM to 10 nM.

Keywords: DNA biosensor, Genosensor, Gastric cancer, Cerium oxide nanoparticles, Reduced graphene oxide, Square wave voltammetry

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An alternative magnetic semi-solid sorbent composed of modified magnetic nanoparticles & supramolecular solvent in removal of Direct Black EX 122 from aqueous samples

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In this study, a new and interesting magnetic semi-solid sorbent has been introduced. In primary steps of this research, a compersion study on the extraction efficiency of three kinds of sorbents in dye remoal from aqueous solutions was performed.The three sorbents were: modified magnetic nanoparticle (modified-MNP), supramolecular solvent (SUPRA), and a sticky, viscose, and magnetic semi-solid phase composed of modified-MNP & SUPRA. Modified-MNP & SUPRA were prepared in our Lab, which have been reported before [1- 4]. The results of primary experiments showed that the magnetic semi-solid sorbent composed of modified-MNP & SUPRA, could act better than those of two other sorbents in dye removal. Since azo dyes are environmental pollutants and their removal also has been considered by all scientists [5], so the extraction conditions for the removal of Direct Black EX 122 from aqueous samples, were optimized. Direct Black EX 122 is an azo dye and used in textile industry. The effective variables such as: pH of dye solution, temperature, the amount and kind of the sorbent (both of modified-MNP & SUPRA), extraction time, the volume and concentration of dye solution were investigated. Under optimal condition, high extraction efficiency, facile removal, and low time-consuming separation of azo dye from water samples was observed.

Keywords: Magnetic, Nano particle, Supramolecular solvent, Semi-solid, Sorbent.

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Ultra-high conductive Inorganic quasi solid state electrolyte containing Li ion

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Considering the energy crisis, the Scientists' attention has been attracted to high-efficiency energy conversion, storage systems, and more especially electrolyte as an essential part of this field area [1]. However, some critical factors such as leakage and volatilization have limited the long-term performance and practical usage of liquid electrolytes [2]. Therefore, the quasi-solid-state electrolytes could be a suitable alternative for liquid electrolytes [3]. But, compared to liquid electrolytes, the quasi-solid-state electrolytes have less ionic conductivity [4]. Hear in, by addressing this issue, preparation of an ultra-high conductive quasi-solid-state electrolyte based on a bismuth-titanium gel composite containing lithium ions is reported. The prepared material is characterized by the use of EDX and TGA instruments to confirm the ratio of the materials. The ionic conductivity performance was measured by electrochemical impedance spectroscopy (EIS). The utilized electrochemical system was an asymmetrical cell consisting of two flat graphite electrodes and as-prepared electrolytes. After optimization of the ratio amount of electrolyte materials, conductivity was achieved at 555 mS cm-1 at room temperature which hasn't been already reported [5]. In addition, this electrolyte has some other advantages such as non-flammability, environment friendly, and flexibility.

Keywords: Quasi-solid-state electrolyte, Inorganic materials, Lithium ion, High conductivity

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Design an automated microextraction on a screw system coupled with high performance liquid chromatography.

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Opium alkaloids are a class of prescription drugs frequently used for chronic pain relief, especially of visceral origin. These drugs are well-known due to their addictive properties in that their prolonged usage can lead to mood-altering effects, sweating, nausea, vomiting, itching, and diarrhea. As a result of the immense illicit use of opioids, there are increasing demands to measure their trace levels in biological samples [1]. Up to now, chromatographic techniques coupled with a variety of solid phase microextraction methods (SPME) in order to extraction and preconcentration of opium alkaloids, have been widely applied. However, the published methods are operated off-line [1- 3]. Microextraction on a screw (MES) is a new important branch of SPME that is introduced by Yamini's group in 2019. It not only inherits the advantages of SPME including simplicity, and environment-friendliness, but also displays other attractive merits such as without back pressure, without clogging, easy automation, and online coupling with HPLC [4]. In the present work for the first time, on-line microextraction on a screw as a convenient, sensitive, and environmentally friendly sample pretreatment method, was introduced. The screw was coated with a polyaniline/carbon nanotube-COOH composite as an absorbent by the electrochemical method. The prepared screw was placed in a cartridge holder and located on loop position of a six-port two position injection valve of an HPLC instrument. The performance of the online MES–HPLC system was demonstrated by analyzing five alkaloids in biological samples. The extracted illicit drugs from biological samples were automatically transferred to HPLC-UV/Vis for separation and quantitative determination. The impact of experimental factors on the extraction performances of analytes was explored and optimized. Based on the obtained experimental results, the proposed MES–HPLC exhibits some advantages such as automation, cost-effectiveness, satisfactory sensitivity and precision, and good linear dynamic range. Therefore, the proposed method is a competitive alternative to the other microextraction methods in the analysis of trace levels of opium alkaloids in complex samples.

Keywords: Alkaloids of opium, Carbon nanotube, Microextraction on a screw, Poly aniline.

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Coacervation extraction of Co (II) from aqueous samples followed by smartphone based colorimetric determination

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Surfactants are composed of a polar head and a long non-polar tail, and may be classified to anionic, cationic, zwitterionic and non-ionic surfactants. With concentration increases, aggregates formed above the critical micelle concentration (CMC) are called micelles. Coacervates made up of vesicles and reversed micelles of alkyl carboxylic acids. Coacervates are also the extraction medium, called coacervative extraction (CAE). The coacervative phase formation is affected from various factors like temperature and pH [1]. In this study coacervative extraction of Co (II) as its complex with 1-(2-pyridylazo)-2-naphthol (PAN) using capric acid as surfactant and THF as solvent was optimized. After extraction of colored complexes in coacervate rich phase, colorimetric determination of the analyte was performed using digital RGB factors recorded by smartphone as analytical devise [2].

Under the optimum conditions, linear dynamic range of calibration curve was 25-250 μg L^{-1} and a regression coefficient (R^2) of 0.9923. The limit of detection (LOD) and quantitation (LOQ) were 7.18 and 25 μg L^{-1}, respectively. The proposed method was successfully applied for the determination of trace amounts of Co (II) in mineral water, well water and river water with recoveries of 105, 109 and 98%, respectively. The repeatability of the proposed method, expressed as the relative standard deviation (%RSD), was 4.45% for intra-day (n=5, 100 μg L^{-1}) and 5.34% for inter-day determinations (n=3).

Keywords: Smartphone , Colorimetry, Digital factors , Co (II), PAN

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SPE-trace Detection of Sulfasalazine Using a Cu(II) Modified Magnetic Chitosan Nanocomposite

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One of the environmental problems today is the leakage of high-consumption chemicals, especially pharmaceuticals, into the water and soil sources. Sulfasalazine (SSZ) is a sulfonamide, a gastrointestinal anti-inflammatory drug, that is used primarily for treating bowel inflammation, diarrhea, rectal bleeding, and abdominal pain in patients with ulcerative colitis [1, 2]. In this research a new method has been developed for efficient and sensitive analysis of SSZ in different samples by combination of a new magnetic solid phase extraction (MSPE) procedure and a simple colorimetric detection method. A cross-linked magnetic chitosan nanocomposite was prepared and its structure and morphology was characterised by different spectroscopic and microscopic techniques, respectively. The preliminary experiments showed that the adsorbent was efficient for the adsorption of SSZ when Cu(II) was present in the solutions. The optimization of the MSPE procedure was performed. Different parameters related to the adsorption and elution steps were considered during the optimization. The studies showed that a solution containing ammonia and sodium hydroxide was efficient on the both elution of SSZ (from the adsorbent) and colorimetric-detection of SSZ at 456 nm. The method introduced the linearity of absorbence against the SSZ concentration in the ranges of 2-50 ($R^2 = 0.9976$) and 50-2000 ($R^2 = 0.9956$) nmol L^{-1} for SSZ. Also, a limit of detection equal to 0.7 nmol L^{-1} was found. Further experiments showed that the accuracy, reproducibility, repeatability and selectivity of the method were excellent. Different soil and water samples were successfully analyzed according to the appropriate standard addition methods.

Keywords: Sulfasalazine, Glutaraldehyde cross-linked chitosan, Cu(II) modified magnetic solid phase extraction, Colorimetric detection.

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Microextraction on a screw for determination of trace amounts of alkaloids of opium by gas chromatography

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Abuse of psychotropic substances is a complicated worldwide issue, and the quantity and diversity of these drugs is growing on a daily basis. Hence, researchers have long been interested in the use of innovative techniques for the separation and measurement of these chemicals in complex tissues [1]. In last decades, new extraction and pre-concentration techniques have been established and suggested in order to generate more efficient and easy extractions. In 2019, the Yamini's Research Group introduced micro-extraction on a screw (MES) method to modify the defects of previous microextraction methods. The MES method is another kind of solid phase microextraction which provide impressive improvements including being without back pressure, fast and user-friendly, considerable extraction efficiency, and low cost [2, 3]. In the present work, the adsorbent of PAN/TMU31 nanocomposite was coated on the screw by the electrospinning method and used for the efficient extraction of three addictive drugs from urine samples. The extracted analytes were separated and determined by gas chromatography/mass spectrometry (GC/MS). The coating was characterized by powder x-ray diffraction (PXRD), Fourier transform infrared spectroscopy (FT-IR), and scanning electron microscopy (SEM) techniques. The parameters affecting the extraction efficiency of the analytes were examined and optimized. Under optimum conditions the obtained limits of detection (LODs) for codeine, papaverine, and thebaine were down to 2, 0.5, and 1 μg/L, respectively. The relative recoveries (RR%) of the proposed method were between 85.0 and 105.0% and the interday and intraday precision (n = 3), represented as relative standard deviation (RSD %), were between 5-7% and 7-10%, respectively. The extraction performances indicate that PAN/TMU31-MES has advantage like as repeatable, cost-effective, simple, and environmentally friendly that it can be efficiently used for the preconcentration of drugs in urine samples.

Keywords: Alkaloids of opium, Metal-organic framework, Microextraction on a screw

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Dispersive Micro Solid Phase Extraction of Bisphenol A, Using In Situ Nano Sorbent Formation

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Bisphenol A (BPA) is an important industrial chemical mainly used for the production of polycarbonate plastics, epoxy and polyester resins and also in various industrial products. It is one of the endocrine disruptors and has recently drawn a lot of scientific researches attention due to environmental issues [1-3]. This compound disrupts hormonal activities and adversely affects human health and aquatic organisms by disrupting growth, development, and reproduction. Due to the low concentration of the BPA in real samples, in this research, sample preparation using homogeneous solid-phase extraction (SPE) by the in-situ synthesis of zein biopolymer nano sorbent was developed to create a simple, green, sensitive and low-cost method before high-performance liquid chromatography (HPLC) analysis. The bio sorbent used in this method was prepared in situ during extraction from its alkaline solution and was also a zein bio polymer nano sorbent characterized by several instrumental techniques (XRD, FT-IR and SEM). The parameters affecting extraction efficiency including the dosage of sorbent, the volume of precipitation acid, the concentration of salt, type and volume of desorption solvent and desorption time were investigated and optimized. Under the optimal conditions, linearity was achieved in the linear range of 10-300 μg L^{-1} (R^2=0.9897), and the limit of detection (LOD) was calculated about 3.5 μg L^{-1}. The repeatability of the method was acceptable for five replications (RSD%= 2.7%, n=5) and satisfactory relative recoveries 86-102.9 %) were obtained in real samples which confirms the precision and accuracy of the method.

Keywords: High performance liquid chromatography, Bisphenol A, Zein, Homogeneous solid phase extraction, Biopolymeric sorbent

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Fabrication of high-performance symmetric supercapacitor based on polyaniline grafted multiwalled carbon nanotube onto anodized graphene oxide nanosheets/graphite electrode

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Nowadays, the utilization of supercapacitors has received much more attention in the field of materials and chemistry, which has had significant progress and success due to their high density and power [1, 2]. The load storage process in supercapacitors occur in two ways: 1) electrochemical double-layer capacitors(EDLCs) and 2) Faradaic or pseudocapacitors [3]. PANI-g-MWCNT/GO NSs/graphite electrode was prepared by electrodeposition aniline-functionalized multiwalled carbon nanotubes (An-fMWCNT) onto previously anodized graphene oxide nanosheets/graphite electrode, and subsequent grafting polyaniline chains onto An-fMWCNT through in situ chemical polymerization. SEM (Scanning electron microscopy) investigations proved that the PANI-g-MWCNT nanocomposite with a high surface area was uniformly polymerizated onto the anodized graphene oxide nanosheets/graphite electrode. The electrochemical measurements confirmed the MWCNT and polyaniline possess synergistic effect in capacitive behavior of the modified electrode and the other hand graphene oxide nanosheets with high surface area increase adhesion of PANI-g-MWCNT nanocomposite to the graphite electrode, leading to significant supercapacitive activity and long cyclic life. The PANI-g-MWCNT/GO NSs/Graphite electrode showed remarkable specific capacitance of about 880 F g^{-1}, a superb energy density of 68.4 mWh g^{-1} and an appropriate power density of 895.4 mW g^{-1} at a current density of 1.5 A g^{-1} in 1.0 M aqueous H_2SO_4 electrolyte. The observed superior capacity of the fabricated PANI-g-MWCNT/GO NSs/Graphite electrode can be attributed to the increased surface area by the graphene oxide nanosheets (GO NSs) and the synergistic effect of PANI-grafted-MWCNT. To show the fabricated supercapacitor device's practical application, we made a solid-state supercapacitor separated by PVA/H_2SO_4.

Keywords: Supercapacitor, Graphene nanosheet, Anodized Graphite, Multiwalled Carbon Nanotubes, Polyaniline

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Organic solventless liquid-liquid microextraction of Co(Ⅱ) and Ni(Ⅱ) from water using deep eutectic solvents

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Metal ions have long half-lives, and are non-biodegradable. Most of heavy metals are famous as toxic materials and can easily accumulate in living organisms [1]. Nickel above certain levels can cause serious health problems such as cardiovascular, pulmonary, fibrosis degeneration, dermatitis, skin disorder, and renal diseases [2, 3]. In this study an efficient, green and organic solventless liquid-liquid microextraction procedure was developed to determine of Co(II) and Ni(II) ions in water by flame atomic absorption spectrometry. Both of extraction and dispersive solvents of the method are deep eutectic solvents. Therefore, it was performed without using any organic solvent. Effect of various analytical parameters such volume of synthesized solvents, temperature, ionic strength, and pH of sample solution on extraction efficiency of the method were investigated and optimized. After optimization of the method, good linearity in the ranges of 0.29-40 μg L^{-1} (Co(II)) and 0.5-40 μg L^{-1} (for Ni(II) were obtained with a coefficient of determination ≥0.9919. Low limits of detection were obtained for Co(II) and Ni(II) (0.10 and 0.17 μg L^{-1}, respectively). Extraction recoveries of the method were 95.4 and 92.8% for Co(II) and Ni(II), respectively. To investigate validity of the method, SPS-WW2 as a certificate reference material was analyzed with the proposed method. Finally, the method was successfully applied to determine Co(II) and Ni(II) ions in different water and fruit juice samples.

Keywords: Liquid-liquid microextraction, Flame atomic absorption spectrometry, Deep eutectic solvent, Heavy metal ions

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Application of functionalized cobalt ferrite nano-particles in dispersive solid phase extraction of some heavy metals from aqueous samples prior to ICP-OES

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In recent years, environmental pollution by heavy metal ions has became a main concern in the world-wide, because of their persistence, carcinogenic effects, high toxicity, and global distribution in soil, water, and air. Also, the ions tend to accumulate in food chains with a low decomposition rate [1–3]. In this study a simple dispersive solid phase extraction method based on $CoFe_2O_4$ nano-particles modified by deep eutectic solvents was used to extract some heavy metals ions from aqueous samples. For this purpose, deionized water spiked with the studied analytes or sample solution was taken and transferred into a glass test tube. After adjusting its pH, NaCl was dissolved in the solution. Then the prepared sorbent was added into the solution and it was vortexed. Then the mixture was placed on top of an external magnet and the sorbent was collected on the bottom of test tube. The supernatant phase was discarded and the adsorbed metalic ions onto the sorbent surface were desorbed by acetic acid solution. The eluent was taken and injected into ICP–OES system for determination of the studied cations. After optimization of the method, good linearity in the range of 1.80-200 ng mL^{-1} was obtained with coefficient of determinations ≥0.994. Low limits of detection were obtained for analytes in the range of 0.54-1.30 ng mL^{-1}. The extraction recoveries of the method were between 72 and 90%. Finally, the method was successfully applied to determine the concentration of the selected analytes in different fruit juices.

Keywords: Dispersive solid phase extaction, Deep eutectic solvent, Heavy metal, Cobalt ferrite

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Determination of Antiepileptic Drugs at Trace Levels via HPLC-PDA System after Solid Phase Extraction

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Epilepsy is one of the most common chronic neurological diseases affecting 50 million people worldwide. It can be defined by recurrent spontaneous seizures, the main goal of epilepsy treatment is to provide complete seizure-free treatment without side effects [1]. A sustained antiepileptic activity is required for this, but will only be achieved if plasma and brain drug concentrations remain at sustained therapeutic levels [2]. Analysis of drugs in biological samples and pharmaceutical products is gaining importance due to the need to understand the therapeutic and toxic effects of drugs and efforts to develop more selective and effective drugs. Knowledge of drug levels in body fluids such as serum and urine can optimize pharmacotherapy and provide a basis for studies on patient compliance, bioavailability, pharmacokinetics, and co-drug effects [3]. In addition, therapeutic drug monitoring based on measurements of drug concentration in the blood can be used to improve patient care. The developed method is based on magnetic solid phase extraction (MSPE), which has been widely used in the literature in recent years and offers application practicality. A new magnetic material was synthetized by means of a well-known procedure including a chemical reaction between Fe(II) and Fe(III) ions in basic medium. The developed extraction method provides a very efficient and green sample preparation technique by successfully integrating the advantages of easy phase separation and reusability. Analysis of drug molecules were successfully carried out with a conventional C18 column under gradient elution mode by means of acetonitrile, methanol, and 0.1 % TFA as the mobile phase. The calibration graphs for target molecules were obtained as linear in the range of with 50-800 ng mL^{-1} with correlation coefficient of 0.9966. Finally, the developed method was applied to simulated urine samples with satisfactory reproducibility with relative standard deviations less than 6.5 %.

Keywords: Antieplectic Drugs, Solid phase extraction, HPLC, Simulated urine samples

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Application of different mathematical models for further investigation of in vitro drug release mechanisms based on magnetic nano-composite

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The purpose of this study is to investigate drug release mechanisms on the novel pre-synthesized magnetic nano-composite based polyurethane and develop a kind of appropriate model to forecast quantitatively targeted drug delivery for in vitro breast cancer therapy. A newly presented analytical instrument, Ion Mobility Spectrometry, was used to investigate loading and release procedures for two pharmaceutical cancer agents (Doxorubicine and Methotrexate) for breast cancer treatment. Loading percentages on the nano-composite 0 were obtained 94% and 98% for Doxorubicine and Methotrexate, respectively. In vitro drug release data were obtained in two different pHs (4.7 and 7.4) in various continuously time intervals to follow release procedure [1,2]. Cumulative release profile was drawn and consequently quantitatively correlated and interpreted with varied mathematical models, viz. zero-order model, first-order model, Higuchi model, Hixson–Crowell model and Korsmeyer–Peppas model. The calculated parameters of mentioned models including r^2, slope and intercept were used for evaluation and describing the kinetics of drug release. The criterion for the most suitable model was based on the high degree of correlation coefficient of nano-composite drug release profile [3]. Hence, finally it is concluded that the best fitted drug release pattern between all proposed methods is Higuchi kinetic model which explains the drug-diffusion-diffuse controlled manner.

Keywords: Kinetic models, Ion mobility spectrometry, Nano-composites, Higuchi, Korsmeyer–Peppas.

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Sensitive Analysis Duloxetine Molecules as an Antidepressant Drug by Using HPLC-DAD System

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Antidepressant drugs are widely and effectively used in the treatment of many mood disorders, especially depression, psychotic disorders and substance-dependent mood disorders. It is also used in the treatment of sleep, anxiety and eating disorders, pain syndromes, arrhythmias and some immune dysfunctions[1]. Currently, most of the monitoring of low concentrations of antidepressant drugs, especially in biological samples, with high sensitivity, good selectivity and high efficiency is performed by liquid chromatography-mass spectrometry (LC-MS) based analysis methods. Sample preparation methods provide both an enrichment with their ability to increase the concentration of target molecules to a certain level, and a kind of separation because they remove many species that have the potential to disrupt the analysis in the environment[2,3]. A new separation and preconcentration method for the trace determination of Duloxetine (DUL) in urine samples was developed based on HPLC-DAD analysis after magnetic solid phase extraction (MSPE). In the proposed method, target drug molecules were retained on the newly synthetized magnetic sorbent in the presence of buffer (pH 10.0) and then were desorbed into a lower volume of acetonitrile prior to the chromatographic determinations. Before HPLC analysis, all samples were filtered through a 0.45 µm PTFE filter. Experimental parameters such as interaction time, desorption solvent and volume, and pH were studied and optimized in order to establish the detection limit, linearity, enrichment factor and other analytical figures of merit under optimum operation conditions. By using the optimum conditions, limit of detections for DUL molecules was 3.35 while the limit of quantifications was 9.46 ng mL^{-1}, respectively. Relative standard deviations (RSD%) for triplicate analyses of model solutions containing 100 ng mL^{-1} target molecules were found to be less than 4.6 %. Finally, the method was successfully applied to urine (both simulated and real healthy human) samples, and quantitative results were obtained in recovery experiments.

Keywords: Duloextine, Magnetic solid phase extraction, HPLC, Urine samples

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Novel and Efficient Method for Lead Ions Biosorption from Aqua Solution by Artemia Cysts

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The eco-friendliness and affordability of biosorption as a water treatment method to eliminate hazardous heavy metal ions, has stimulatedthe interest of many scholars that explore this arena [1,2]. The study proposes Artemia cysts (A.C.) as a new and efficient biosorbent for the elimination of lead ion contaminants which can continuously produce new and multifold cysts as a sorbent in every cycle. Cyst of Artemia is composed of multiple layers covered with a porous surface and numerous functional groups that are capable of vigorous encapsulation of lead ions[3,4]. Actually, this research suggest a novel, continuous system to use cysts for cleaning the contaminated waters that is able to uptake contaminated lead ions without extra cost. Also, cyst shells are waste with no economic value. Fourier transform infrared spectroscopy (FT-IR) and scanning electron microscopy (SEM) used to assert surface properties of the cyst. The most vital parameters in evaluating adsorption rate such as pH, contact time and initial concentration of lead ions proved that rapid and robust biosorption occurred during these experiments.The most astounding result to appear from the data was that batch experiment showed the maximum uptake of 94.40% at pH 5.8 in less than 1 min with 50mg.L^{-1} of initial concentration of lead ions. Kinetics models well fitted by Langmuir isotherm. The results confirmed the efficient and straightforward performance of Artemia cysts in purifying contaminated water with lead ions. this novel method integrates merits of simplicity, time-optimization and affordability in addition to the reusability, good biodegradability, low cost, high efficiency and the possibility of metal recovery.

Keywords: Artemia cyst, Biosorption, Lead ions

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Fabrication of Fe_3O_4@ZnO-MWCNTs-TiO_2 for efficient photocatalytic removal of Ibuprofen and caffeine under visible light

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A novel core–shell covalently functionalized Fe_3O_4 coated ZnO decorated multi-walled carbon nanotubes (Fe_3O_4@ZnO-MWCNTs) adsorbent was synthesized and then coated TiO_2. The prepared photocatalyst characterized by SEM, FT-IR, XRD, and VSM measurements. Results show that the prepared photocatalyst exhibits excellent photocatalytic degradation efficiency for the removal of Ibuprofen and caffeine from water, for which nearly 98% and 92 % of Ibuprofen and caffeine is degraded within 60 min under visible light, respectively. Higher adsorption of Fe_3O_4@ZnO-MWCNTs-TiO_2 observed for Ibuprofen and caffeine than the other synthesized photocatalyst may be attributed to the synergistic effect of the ZnO and TiO_2 [1, 2]. This shows that the Fe_3O_4@ZnO-MWCNTs-TiO_2 is effective for the degradation of Ibuprofen and caffeine. The pseudo-second-order kinetic and Langmuir isotherm models adjusted better to the experimental data. Meanwhile, the Fe_3O_4@ZnO-MWCNTs-TiO_2 photocatalyst displayed beneficial reusability and stability to Ibuprofen and caffeine degradation. The easy separation from the treated solution and its recyclability make it a promising photocatalyst.

Keywords: Photocatalyst, Ibuprofen, Caffeine, Isotherm, Multi-walled carbon nanotubes.

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Synthesis of magnetic Cu MOFs modified hydroxyapatite as new adsorbent for magnetic solid-phase extraction of brucine from human urine

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A magnetic Cu metal–organic framework (Fe_3O_4@CuMOF) was modified with hydroxyapatite (Fe_3O_4@CuMOF@HAp) and then successfully employed as adsorbent of magnetic solid-phase extraction (MSPE) for the determination of brucine in human urine sample coupled with high performance liquid chromatography. The as-prepared Fe_3O_4@-CuMOF@HAp was characterized by SEM, F-IR, XRD, VSM, and zeta potential analysis. Important operation parameters for MSPE that could affect the extraction efficiencies of brucine were investigated in detail. Under the optimal experimental conditions, the proposed method provided low limits of detection (0.08 ng mL^{-1}) and quantification (0.2 ng mL^{-1}), good linearity (R^2= 0.995) in the range of 0.50-1000.0 ng mL^{-1}, and excellent reproducibility (4.7-6.2%).The promising results demonstrated that Fe_3O_4@CuMOF@HAp composite could be employed as magnetic adsorbent for efficiently extract of brucine from human urine sample [1, 2].

Keywords: Magnetic Cu metal–organic framework, Hydroxyapatite, Brucine, Magnetic solid phase extraction

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Novel deep eutectic solvent-assisted electrochemical synthesis of TGA capped CdSe@Cu_2Se core-shell cauliflower quantum dots on the graphene-modified electrode as a catalytic platform for the determination of pyrazinamide

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A novel electrochemical synthesis of CdSe@Cu_2Se core-shell cauliflower quantum dots is applied in deep eutectic solvent to modify surface of graphene film-coated glassy carbon electrode. This synthesis method of CdSe@Cu_2Se quantum dots in deep eutectic solvent creates a green and environment-friendly processes. Tuberculosis (TB) is a major infectious diseases has led to the death of many people in the world. There are many drugs to control and treat of TB such as isoniazid, rifampicin and etc [1]. Pyrazinamide (PZA) is one of the important drugs used for short period treatment of TB. The PZA elimination from human body is very low, which causes to some side effects like liver and kidney problems, fever, sideroblastic anemia and etc [2]. Therefore, This selective electrochemical sensor was used to determination of PZA by differential pulse voltammetry method under optimized conditions with the detection limit of 0.37 µM (0.4 -10 µM). The proposed quantum dots-based sensor has good advantages in comparison with spectrophotometric and different chromatographic [3–5] like simplicity, accurate, low cost, fast and short time analysis as well as indicates high reproducibility and recoveries (95.17-103.27%) in the pharmaceutical tablets and biological samples.

Keywords: Pyrazinamide, CdSe@Cu_2Se/graphene/GCE, Deep eutectic solvent, Green electrochemical synthesis

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Magnetic in-tube solid phase microextraction of some herbicides

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Triazines herbicide can be used to control of grasses and broadleaf weeds in agricultural land containing plants as corn, soybean, barley and sorghum. These herbicides can pollute soil and specially ground waters [1]. Because of toxicity of triazine and wide spread usage of them, they are dangerous for human health and even for environment [2]. Therefore, determination of trace amounts of triazine is crucial. In-tube solid phase microextraction coupled to HPLC (IT-SPME-HPLC) is the efficient technique for extraction trace amounts of the analytes and increases precision, accuracy and reduce the analysis time. Magnetic nanoparticles can be used in IT-SPME technique as a sorbent [3]. In this study, magnetic nanocomposite of cross-linked poly(styrene/divinylbenzene) was synthesised. The characterization of the prepared material was fully investigated using various techniques including SEM, VSM, TGA, and FT-IR. They were used as an absorbent for the magnetic IT-SPME. The absorbent was kept in a tube by applying a magnetic field. Separation and determination of the analytes were performed by HPLC-UV. The effects of sample pH (6), extraction time (20 minute), type and volume of elution solvent (500 µL methanol) and extraction flow rate (2 mL min^{-1}), desorption flow rate (50 µL min^{-1}) and salt addition (15%) and applying magnetic field on the extraction efficiency of triazine were examined and optimized. Under optimal conditions, calibration curves were found to be linear in the range of 0.3-500 µg L^{-1} for cyanazine, simazine and propazine. The LODs were 0.1 µg L^{-1} for cyanazine, simazine and propazine. Finally, the developed method was successfully applied for extraction and determination of triazines herbicides in fruit and vegetable juice sample and recoveries in the range of 52.1 to77.4 were obtained. Magnetic IT-SPME-HPLC-UV was developed for preconcentration and quantification of trace amount of triazines.The advantages of this method is the usage of small amount of sorbent and high extraction efficiency and the good reusability of the sorbent.

Keywords: Magnetic in-tube solid phase microextraction, Triazine, Magnetic nanoparticles

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Extraction and determination of parabens from fruit juice with µ-solid phase extraction using yolk−shell ZIF-8-based material ($ZnO@SiO_2@C/Ni$)

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Parabens are lipophilic, inert, odourless, tasteless, colourless and stable compounds in a wide range of pH [1]. The antimicrobial and intracellular properties of these compounds make them suitable to be used in different products like cosmetics, bath gels and tooth-pastes, food and drugs as preservatives [2]. The use of parabens in costumer products has recently given rise to concern about their long-term issues and side-effects on human health and even on aquatic organisms [3]. Developing of simple, fast and precise analytical methods for determination of parabens is essential [4]. Hollow or yolk−shell nanostructures with a low density, high surface area, good chemical and mechanical stability have attracted special attention. So $ZnO@SiO_2@C/Ni$ can be used as an efficient sorbent [5]. In this study, a rapid and highly efficient sample preparation, dispersive micro solid phase extraction (D-µ-SPE) method, followed by HPLC-UV was developed for the extraction, preconcentration and determination of parabens from aqueous solutions. Compositional modulation of ZIF-8 derived hybrids comprised of metallic Ni nanoparticles and silica as interlayer, was used as adsorbent in D-µ-SPE method. The effects of sample pH (6), extraction time (20 min), type and volume of elution solvent (600 µL methanol), break through volume (20 mL), absorbent weight (10 mg), desorption time (4 min) and salt addition (0%) on the extraction efficiency of parabens were examined and optimized. Under optimal conditions, calibration curves were found to be linear in the range of 0.1-800 µg L^{-1} for methylparaben, ethylparaben and propylparaben. The LODs were 0.05 µg L^{-1} for all of the studied parabens. Finally, the developed method was successfully applied for extraction and determination of parabens in fruit juice sample and recoveries in the range of 46.8 to 82.6 were obtained. The combination of $ZnO@SiO_2@C/Ni$ sorbent and D-µ-SPE with HPLC-UV, because of high surface area and good structure for π-π interaction, is a useful method for determination trace amounts of parabens in juice sample.

Keywords: D-µ-SPE, Parabens, ZIF-8 based material

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Application of newly synthesized layered double hydroxides in pre-concentration of heavy metals from aqueous samples using ICP-OES

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Toxic heavy metals have been introduced into the environment from both human activity and natural origin. Water and soil pollution with toxic heavy metals is of phenomenal concern nowadays, due to the fact that they are not eco-friendly and can be accumulated in living tissues causing serious diseases and disorders [1]. Direct determination of heavy metals, due to low concentration in aqueous samples, is a challenging task. Therefore, the need for a sample preparation step is an integral part of most analytical methods to solve this problem. Sample preparation procedures such as liquid-liquid extraction (LLE) and solid phase extraction (SPE) are usually used for the preconcentration of the analytes. But these techniques, due to requiring large amounts of poisonous organic solvents and a large volume of samples are not suitable. In recent years, much attention has been paid to the use of the dispersive micro-solid phase extraction (D-µ-SPE) method due to reduction the consum in ption of adsorbent amounts, short extraction time, being eco-friendly and simplicity [2]. Among the various adsorbents used in the D-µ-SPE method, layered double hydroxides (LDHs) have become very important due to their properties such as ease to synthesize, low cost, high specific surface area, environmental compatibility, structural variability, chemical stability, and large interlayer space (high porosity) [3]. The newly synthesized GO@Co-Al/LDH@Fe_3O_4 adsorbent was used for preconcentration of heavy metals Cu(II) and Cd(II) in aqueous samples, by the D-µ-SPE method, and detection was accomplished with ICP-OES. In order to investigate the effective parameters for the extraction recovery of the mentioned metals, the central composite design (CCD) method was used. Under optimized conditions, the method provided considerable repeatability (RSD% 3.9), with a preconcentration factor (121 and 114 for Cu(II) and Cd(II), respectively) and it exhibited a wide linear range (0.9-250 ng mL^{-1}). The results obtained show that the GO@Co-Al/LDH@Fe_3O_4 adsorbent has a high ability to measure ultra-trace amounts of metals mentioned in various aqueous samples.

Keywords: Layered double hydroxides, Dispersive micro-solid phase extraction, Heavy metals, ICP-OES.

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Design and Custom-Build of Portable Fluorimeter

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Fluorimeter is an important instrument to qualitatively and quantitatively analyze substance in modern analytical chemistry [1]. A Portable fluorometer coupled with a smartphone as a simple and compact device has been developed and analytical figures of merit such as sensitivity, linear dynamic range, detection limit, and selectivity were determined. This device has a light emitting diode with a wavelength of 495 nm as an excitation source. A lens is used to focus the source light on the sample. The sample container is made of plastic with four transparent sides. In this system, two detectors are used for detection and measurement. The first detector is a photodiode which uses a fluorescent light receiver, an Arduino board and a display to display the voltage. The second detector is a smartphone which takes a photo using its camera and then the image is analyzed by RGB software.Both photodiode and smartphone detectors are located at 90-degree angles to the light source and minimize the effect of the source light. After the sample container, lenses have been used to focus emission light on the detectors. All components of this system were made of poly methyl methacrylate (Plexiglas) .The height and distance between the holder components can be adjusted to optimize the intensity of the signal. Finally, the system was compacted in a box made of polyvinyl chloride (PVC) .The walls inside the box have been blackened to reduce the noise. This system has dimensions with a length of 27, width of 24 and height of 25.3 cm. The weight of the device is approximately 4 kg, which makes it portable(figure below).

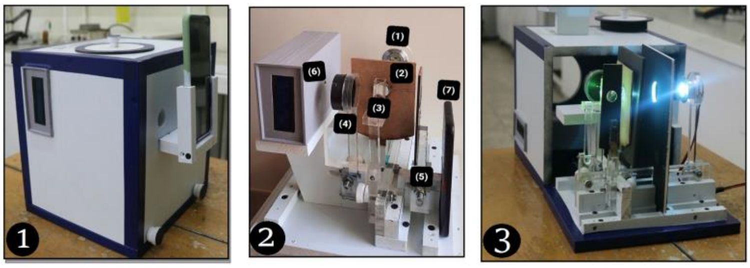

Fig: The external (1) and internal (2)(3) configurations of the custom-built fluorimeter. Experimental setup in fig (2): (1) cyan LED with a wavelength of 495 nm (2) plano convex lens (3) sample container (4) and (5) Bi-convex lenses (6) photodiode detector (7) smartphone detector.

Keywords: Smart phone,L-cost fluorimeter, Fluorescence, Analytical chemistry

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Preconcentration of naproxen in biological samples by three-phase hollow fiber liquid-phase microextraction coupled to HPLC-UV

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Naproxen is a non-steroidal anti-inflammatory drug that for the treatment of many diseases, like degenerative joint disease, rheumatoid arthritis, ankylosing spondylitis, acute gout, and primary dysmenorrhea. Chemiluminescence, spectrofluorimetry, high-performance liquid chromatography (HPLC), voltammetry, etc. are the ordinary methods of naproxen determination [1]. However, determination of analytes in complex matrices is a challenging task. The challenges are mainly due to the low concentration of analytes in biological samples as well as the existence of a wide variety of interferences, which can mask the analytical signals of analytes and pose several problems on analytical instruments. To solve these problems, one needs a sample preparation step which is an integral part of most analytical methods. Among the various sample preparation methods, three-phase hollow fiber liquid-phase microextraction (HF-LPME) has always been considered due to its inexpensive procedure, insignificant consumption of organic solvents, good clean-up, and high preconcentration factor. In three-phase HF-LPME, the organic solvent is immobilized in the pores of a porous hydrophobic hollow fiber and the aqueous acceptor phase is introduced into the lumen of the hollow fiber by a microsyringe. Then, the system is located in the aqueous sample solution and mass transfer is also accomplished by a stirring magnet in the sample container [2]. In this work, 12-cm long pieces of the HFs were washed by sonication in an acetone bath for 5 min and left to dry in the air. To impregnate the pores of the HF, it was dipped into 1-octanol as organic solvent (a time interval of 10 s was found to be optimal), and the residual organic solvent expelled from the fiber lumen by the air exhaled from a syringe. Thereafter, the prepared HF was filled with the acceptor phase in optimized pH (approximately 60 μL). Both ends of the fiber were inserted into the syringe needle and, then, the U-shaped fiber was introduced into a 10-mL glass vial with 8 mL of sample solution (sample phase) adjusted at the optimized pH. The extraction was carried out in direct immersion mode for 45 min at 700 rpm. After that, the extract was collected from the lumen HF by syringe, and a 25-μL portion was injected into HPLC-UV. This study demonstrates the applicability of three-phase HF-LPME for the determination of naproxen in complicated biological matrices such as urine. The method provided considerable repeatability (RSD% 2.9), and it exhibited a wide linear range (2.0–1000 ng mL^{-1}). The results obtained show that the three-phase HF-LPME method provides a high pre-concentration and noticeable extraction clean-up.

Keywords: Hollow fiber liquid-phase microextraction, Naproxen, Complex matrices, HPLC-UV.

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Effect of thin film in acceptor phase on electromembrane extraction of some cationic dyes from aqueous solutions

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The use of synthetic dyes in aquaculture and various industries has raised serious concerns due to the complex structure and low biodegradability of them [1]. Therefore, in recent decades, designing and developing methods for identifying and measuring trace amounts of artificial colors in blue environments have been a challenging problem [2]. In the present study, a thin film coated with polyaniline/graphene oxide composite was located in acceptor phase of electromembrane extraction (EME) on a chip. The device contained two single channels on two separate polymethylmethacrylate (PMMA) plates. The upper channel was dedicated to sample solution flow pass and the underneath channel was provided as a compartment for stagnant acceptor solution. A slide of fluorine doped tin oxide (FTO) was placed in the bottom of the acceptor phase channel. A thin layer of polyaniline/graphene oxide composites was electrochemically deposited on the FTO surface to create the required thin film for thin film solid phase microextraction (TF-SPME). Also a slide of FTO was embedded in the donor phase channel and stainless-steel wires were attached on the surface of the two FTO. The channels were separated by a piece of polypropylene sheet as membrane. The membrane was impregnated with 1-octanol containing 10% (v/v) DEHP. By applying 30 V voltage across the supported liquid membrane (SLM), analytes migrated from sample solution towards the acceptor phase and then adsorbed on the thin film. Finally, the analytes were desorbed by successive movement of a desorption solvent in the acceptor phase and the desorption solution was injected into HPLC-UV for further analysis. The applicability of the proposed method was represented by extraction of the cationic dyes: methylene blue, rhodamine B and malachite green from various samples. All of the effective parameters on the efficiency of the EME and TF-SPME including Composition of the SLM, pH of acceptor and donor phase, the quantity of the applied voltage, sample solution flow rate, type and volume of desorption eluent and eluent flow rate were investigated and optimized. And Under optimized conditions the figures of merits of the method was reported. The method was applied for extraction and determination of the analytes in real samples and satisfactory results were obtained.

Keywords: Electromembrane extraction, Thin-film solid phase microextraction, cationic dyes

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Fabrication of Impedimetric Sensor Based on Metal Nanoparticle for Determination of Mesna Anticancer Drug

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Monitoring the levels of anticancer drugs in real samples would allow dose optimization. Mesna is the sodium salt of 2-mercaptoethane sulfonate, a thiol-containing drug. MESNA was proved to be effective in preventing hemorrhagic cystitis induced by high doses of several chemotherapeutic regimens such as cyclophosphamide and ifosfamide. Because of the increased level of interest in using Mesna for treating various disorders, a new and sensitive method was needed to understand the pharmacokinetics of this drug. Therefore, the determination of Mesna in real samples is very important and essential [1]. Electrochemical impedance spectroscopy (EIS) is a powerful method to investigate the surface of electrodes in detail. many EIS-based electrochemical sensors are based on measuring the charge transfer resistance (R_{ct}) of redox probes at the surface of electrodes to monitor the binding of target molecules have been reported [2]. Mesna determination by conventional electrochemical methods was not reported. In this research, we developed a novel impedimetric sensor based on glassy carbon electrode (GCE) modified with oxidized multiwalled carbon nanotubes (MWCNTs)/gold nanoparticle(AuNPs) (denoted as Au NPs/MWCNTs/GCE) for impedimetric determination of Mesna anticancer drug. The modified electrode was characterized by field emission scanning electron microscopy (FESEM), energy dispersive X-ray (EDX), and EIS. The EDX spectrum confirmed that the presence of carbon, gold and oxygen elements in the prepared composites.The detection mechanism of the proposed impedimetric sensor was based on the increase in the $[Fe(CN)_6]^{3-/4-}$ charge transfer resistance (R_{CT}) as an electrochemical probe in the presence of the target analyte. Under the optimum condition, the calibration curve at the Au NPs/MWCNTs/GCE covered two linear dynamic ranges, 0.06−1.0 and 1.0−130000.0 nM, with a detection limit of 0.02 nM. Eventually, in order to test the analytical investigation, the practical application of the as-prepared Au NPs/MWCNTs/GCE was used for the determination of Mesna anticancer drug in real urine and serum samples. The results indicated that satisfactory recoveries in the range 90% and 113%, were achieved. Therefore, the modified electrode can be employed for Mesna determination in biological real samples.

Keywords: Impedimetric sensor, Multiwalled carbon nanotubes, Au nanoparticles, Mesna, Anticancer drug.

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Combination of dispersive solid phase extraction using MIL–88A as sorbent and deep eutectic solvent–based dispersive liquid–liquid microextraction for the extraction of some pesticides from fruit juices

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Nowadays, consistent consumption of fruit juices that are the main sources of essential vitamins, antioxidants, minerals, and polyphenols is recommended by nutritionists. The use of fruit juices can minimize the menace of various types of cancer and cardiovascular diseases [1]. But the fruit juices need to be free of any chemical component like pesticides and heavy metals that can threat the consumers health [2]. Unfortunately, pesticides can remain on the surface of products or even penetrate into their tissues and pollute them [3]. Referring to these points, there is an increasing demand for the continuous monitoring of pesticides in agricultural products and their by–products like fruit juices. In the present work, a metal organic framework–based dispersive solid phase extraction combined with dispersive liquid–liquid microextraction has been developed for the extraction of some pesticides (diazinon, haloxyfop–R–methyl, hexaconazole, diniconazole, and tebuconazole) from fruit juices before their determination with gas chromatography–flame ionization detection. In the extraction process, first, synthesized MIL–88A as sorbent (at mg–level) was added to the aqueous solution and the mixture was vortexed to adsorb the analytes. In the following, the sorbent was eluted with a water–miscible deep eutectic solvent. This phase was taken and used in a dispersive liquid–liquid microextraction step to further preconcentrate the analytes. Under the best extraction conditions, satisfactory analytical results such as wide linear ranges ($235–1 \times 10^6$ ng L^{-1}), high enrichment factors (255–315) and extraction recoveries (51–63%), and low limits of detection (70–89 ng L^{-1}) and quantification (235–290 ng L^{-1}) were acquired. Lastly, the offered procedure was utilized for the quantification of the opted pesticides in fruit juices. Based on the results, the investigated samples were free of studied pesticides.

Keywords: Dispersive solid phase extraction, Deep eutectic solvent, Metal organic framework, Pesticide, Gas chromatography–mass spectrometry

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On chip electromembrane surrounded solid phase microextraction of antidepressants using PEDOT-GO nanocomposite coating

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Tricyclic antidepressants (TCAs) are commonly used for clinical treatment of major depressive disorder, anxiety and certain personality disorders as well as chronic pain. Amitriptyline, nortriptyline, imipramine, desipramine, maprotiline and sertraline are known as the most conventional class of antidepressants. However, some adverse health effects have frequently occurred such as mind confusion, dry mouth, and constipation. In addition, due to the relatively narrow therapeutic/toxic index and low therapeutic window of TCAs, monitoring the concentration of these compounds in biological fluids is imperative [1]. Sample preparation has always been one of the most challenging steps for the analysis of different analytes from various complex matrices. In the recent few decades the perspective of these methods has been focused on miniaturization and minimization of the organic solvent usage and lowering the limits of detection. In order to achieve these goals, electromembrane surrounded solid phase microextraction (EM-SPME) has been introduced as proper and effective extraction method. It is stated that this method overcame the drawbacks of direct immersion SPME and the limitations of EME. High cleanup ability, appropriate extraction efficiency, high preconcentration and coupling with gas chromatography are some advantages of EM-SPME for extraction of compounds from complicated matrices in low concentrations [2]. In the present work, EM-SPME on chip was developed to extract antidepressant drugs from various complex matrices. Therefore, poly(3,4-ethylenedioxythiophene)-graphene oxide (PEDOT-GO) nanocomposite was electrochemically synthesized on SPME fiber as a conductive polymer. Consequently, the SPME holder has been injected in acceptor phase and the fiber has played the negative electrode role during the extraction. Likewise, after electromembrane extraction, thermal desorption was applied to transfer the drugs in to the column in gas chromatography-mass spectrometry. Effective parameters on extraction efficiency were investigated and optimized. Under optimum conditions, the limits of detection of the analytes were in the range of 0.005-0.025 µg L^{-1}. Linearity of the method was obtained within the range of 0.010-500 µg L^{-1} for imipramine and sertraline, 0.025-500 µg L^{-1} for amitriptyline, nortriptyline and desipramine, and 1.000-250 µg L^{-1} for maprotiline with coefficients of determination better than 0.9984. Moreover, the precision of the method is suitable with relative standard deviations lower than 6.2%. The method was applied for extraction of the mentioned drugs from biological fluids such as bone marrow aspirate, urine and plasma samples; and satisfactory relative recoveries between 96 and 105% were obtained.

Keywords: Electromembrane extaction, Solid phase microextraction, On chip, Antidepressants.

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Efficient Extraction of Pb (II) by Microextraction by packed sorbent Method based on Modified Composite Adsorbents of MOFs

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Lead is one of the most important heavy and toxic element that even in small amounts has a serious threat on human health and the environment [1]. It can accumulate in the brain, kidneys and nervous system, which may cause organic damage and dysfunction on central nervous systems [2]. Various methods have been reported for the determination of lead such as chemical precipitation, membrane filtration, ion-exchange, biological, electrochemical and adsorption methods [3]. Among them, adsorption is the most modern method, that has a wide application. In this work, we propose novel Thiourea-functionalized copper-based metal organic frameworks (MOFs) as a sorbent for Microextraction by packed sorbent (MEPS) of trace amounts of Pb(II) in water samples. Successful composite grafting was confirmed by Fourier transform infrared spectroscopy (FTIR), isoelectric point (IEP), field emission scanning electronic microscopy(FESEM) and energy dispersive X-ray spectrometer (EDS). Various experimental factors were investigated on the percentage of lead ion recovery (II) including pH, adsorbent amount, number of sample loading cycles, number of solvent loading cycles, sample volume, solvent volume. The Thiourea-MOFs showed higher adsorption capacity than that of the pristine MOFs in pH=6. The adsorption mechanisms is proposed to be the coordination interaction between the amino groups (–NH_2) and Pb (II). Therefore, the Thiourea-MOFs has demonstrated a great potential in the treatment of heavy metal wastewater.

Keywords: MOFs, Thiourea, Microextraction by packed sorbent

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A survey on antioxidant activity of Iranian shrimp waste [Penaeus Semisulcatus]

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Shrimp waste, as an important source of natural carotenoids, is produced in large quantities in seafood processing industry. The robust association between seafood consumption and beneficial health effects has been well documented [1]. Shrimp is the main resource in crustacean fisheries [2], in terms of nutritional value and great economic importance [3]. One of the important characteristics of carotenoids is their ability to act as antioxidants, thus protecting cells and tissues from damaging effects of free radicals and singlet oxygen. The aim of this study was to find effective method for carotenoid extraction [Enzymatic and alkaline treatment] from shrimp waste in sunflower oil. The sunflower oil was exposed to three concentration of extracted carotenoid [470, 235 and 118 mg/kg] and synthetic antioxidants. The inhibition of lipid peroxidation was evaluated for Malondialdehyde and peroxide value. The mean values of carotenoid extract were 243 and 170 mg/kg for enzymatic and alkaline treatment, respectively. So the highest efficacy of carotenoid extraction was obtained from enzymatic extraction. The oil samples containing 470 ppm carotenoid, which extracted by alcalase as the default treatment, exhibited the less peroxide value and higher antioxidant potential than the oil samples containing synthetic antioxidants.

Keywords: Shrimp waste, Carotenoids, Edible oil, Oxidation

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Selective and green separation of RDX and HMX explosives using ammonium acetate/diethylene glycol deep eutectic solvent

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Deep eutectic solvents (DESs), owing to their ease and low cost of synthesis, environmental friendliness, limited volatility, high solubility, and adaptable structural design, have been developed as green new solvents in adsorption and separation procedures. DESs are typically prepared by combining a hydrogen bond donor (HBD), including alcohols, amides, and carboxylic acids, with a hydrogen bond acceptor (HBA), like quaternary ammonium salts (QASs), quaternary phosphonium salts, and imidazolium-based salts [1,2]. In this research, a DES composed of ammonium acetate (AS) and diethylene glycol (DEG) was chosen for selectively separating and purifying cyclotetramethylene tetranitramine (HMX) explosives from cyclotrimethylene trinitramine (RDX). The influence of DES on the solubility of two explosives was investigated, as well as the interaction of DES components was evaluated using Fourier transform infrared spectroscopy (FT-IR). The inductance-capacitance-resistance (LCR) meter was used to measure the electrical conductivity and dielectric constant of various DES solutions over 100.0 Hz – 1.0 MHz. Additionally, solubility characteristics for RDX and HMX in the suggested solvent were determined, including solubility coefficient, dissolution enthalpy, and mixture enthalpy. The solubility of two compounds in DES was modelled employing central composite design (CCD) of experiment in mini-tab software in relation to two factors of temperature and ammonium acetate concentration. Analysis of variance (ANOVA) and statistical assessments revealed a suitable correlation between the empirical and projected solubility findings. Additionally, empirical findings indicated that the dissolution ratio of RDX to HMX varied between 10.0 and 30.0 times. This enables the development of a specific and successive approach with temperature control for the separation of two chemically identical compounds with separation efficiency of > 98.0 % and a purity of HMX >99.5%. High-performance liquid chromatography (HPLC), laser-induced breakdown spectroscopy (LIBS), and FT-IR analysis of the final product revealed the elimination of impurities of ammonium acetate and ethylene glycol. The suggested approach allows the separation of high-energy RDX and HMX compounds in an effective, safe, and environmentally friendly manner.

Keywords: Deep eutectic solvent, HMX, RDX, Explosive, Separation.

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Phytoremediation of PAHs from indoor air by pelargonium domesticum plant

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Poly aromatic hydrocarbons (PAHs) are carcinogenic contaminant. It is therefore important to remove them from the environment. In this study, phytoremediation of PAHs from polluted air by pelargonium domesticum was investigated under controlled environment using a Plexiglas chamber. According to the physiological and morphological tests, no toxicity effects on the plants were found at these concentrations. Entire plant, growing media in PAHs were evaluated by continuously introduction of different concentrations of PAHs into the chamber (0.25–14.56 mg m-3) each over a 72 -h period. Findings showed that the plant efficiently removed PAHs from polluted air by 70-99%, depending on the inlet concentrations, for a long time exposure. A maximum elimination capacity of 1.52 mg/m2.h was achieved with an inlet PAHs concentration of 12.42 mg m-3. The plants could remove more PAHs in light rather than dark environment. Concentrations up to 14.56 mg m-3 were not high enough to affect the plants growth. It can be concluded that the plant's application is a green and environment-friendly technology to remove PAHs from the polluted indoor air.

Keywords: pelargonium domesticum plant, Phytoremediation, PAHs, Indoor air

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Determination of acrylamide in tahdig prepared with the most common edible liquid and solid oils

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Acrylamide (2-propenamide) is a known neurotoxic compound found in the year 2002 by research groups from the Swedish National Food Administration (SNFA) and the University of Stockholm that was detected in carbohydraterich fried or baked food samples. Acrylamide has been classified into Group A2, possibly carcinogenic to humans, by the International Agency for Research on Cancer [1]. The main reaction in acrylamide formation in heated foods is the Maillard reaction. Maillard reaction is a chemical reaction between free amine groups of protein and the glucoside hydroxyl group of reducing sugars or carbonyl compounds, such as aldehydes and ketones that are produced by the oxidation of lipids [2]. Due to the heating of amino acids with edible oils to high temperatures, different amounts of acrylamide are produced. The purpose of this study was comparative investigation of acrylamide amount formation in tahdig prepared with the most common liquid and solid eatable oils, including sunflower oil, corn oil, canola oil, frying oil without palm and household solid oil. The tahdig was prepared in the traditional baking of rice under the same conditions of temperature and time and different oils. Acrylamide isolation was performed on a solid phase extraction (SPE) method by cartridge and determination of acrylamide was performed using HPLC-UV system. The highest amount of acrylamide was observed by sunflower oil (194.091 mg /Kg) and the lowest amount of acrylamide was obtained by solid household oil (48.54 mg /Kg).

Keywords: Acrylamide, Tahdig, Liquid and solid edible oils

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Determination of Polycyclic aromatic hydrocarbons (PAHs) in indoor air by monolith adsorbent micro extraction copled to GC-FID method

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People spend most of their lives in indoor spaces; in this regard, knowledge of indoor air quality will help us improve the quality of the air we breathe. Polycyclic aromatic hydrocarbons (PAHs) or poly-nuclear aromatic hydrocarbons (PNHs) refer to a large group of resistant aromatic compounds (including more than 100 compounds) with two or more benzene aromatic rings that are dispersed in air, water, and soil. These compounds have been classified in the list of hazardous compounds according to the US environmental protection agency (USEPA) and the world health organization (WHO) [1-3]. In this study, a solid-phase microextraction (SPME) method was utilized by an integrated carbon nanofiber to measure polycyclic aromatic compounds in indoor air. The microextraction conditions were optimized. The correlation coefficient of the compounds ranged between 0.9991-0.9996 with the detection limit range of 0.014-0.032 mg/m^3 and a standard deviation of 6.38-8.95%. This method was finally applied to measure analytes in indoor spaces using gas chromatography with a flame ionization detector (GC-FID)

***Keywords**:* Multiwalled carbon nanotube, Headspace solid-phase microextraction, Polycyclic aromatic hydrocarbon, Capillary gas chromatography, Indoor air.

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Combination of mixed mode dispersive solid phase extraction with magnetic ionic liquids based dispersive liquid–liquid microextraction for the extraction of anticoagulant drugs from urine samples

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Blood clotting is a widespread phenomenon observed in many patients who suffered from atrial fibrillation and venous thromboembolism [1]. In recent years, direct oral anticoagulants (DOACs) are considered as the substitute drugs to warfarin and prescribed to prevent from venous thromboembolism or stroke [2]. DOACs are known as the powerful inhibitors of the activated coagulation factor. Apixaben, anagrilde, rivaroxaban, dabigatran, and edoxaban are the most famous DOACs agreed by the European Medicines Agency or United States Food and Drug Administration [3]. According to these benefits, the use of DOACs is increasing and their accurate therapeutic monitoring in biological fluids is significant for clinical trials. In this report, combination of a mixed mode dispersive solid phase extraction with dispersive liquid–liquid microextraction has been performed in order to the effective isolation of three anticoagulant drugs (anagrelide, betrixaban, and apixaban) from urine sample. The extracted drugs were quantified by high performance liquid chromatography–diode array detector. Firstly, analytes were adsorbed onto a mixture of octadecylsilane, graphitized carbon black, and primary secondary amine sorbents which their composition was obtained by a simplex centroid design. To increase the adsorption efficiency of sonication of the solution and sorbents mixture was performed. The loaded analytes onto the sorbent surface were washed employing a water–miscible organic solvent which was utilized as a disperser in microextraction process. The microextraction step was done using a magnetic ionic liquid (as an extractant) and the droplets were sedimented at the bottom of tube with the aid of magnetic field. Satisfactory analytical results such as wide linear ranges (0.21–250 ng mL^{-1}), high enrichment factors (223–247) and extraction recoveries (76–84%), and low limits of detection (0.04–0.06 ng mL^{-1}) and quantification (0.16–0.21 ng mL^{-1}) were obtained using the optimum experimental situations. Lastly, the offered procedure was utilized for the quantification of the opted analytes in urine sample.

Keywords: Dispersive solid phase extraction, Dispersive liquid–liquid microextraction, Urine, Anticoagulant drugs, High performance liquid chromatography

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Potential use of Dunaliella Salina as biosorbent for bioremediation of saline water ions

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The aim of the present research was to culture Dunaliella salina in the saline groundwater located in the county of Taqiabad near Mashhad. The growth curve was compared with the growth curve in Artificial Seawater. The results showed that Dunaliella salina cells is able to grow gradually without adding main nutrients to the culture medium. The biomass produced in 22 days was 1.3 g/l. During the Dunaliella salina cultivation, electrical conductivity and total hardness were monitored. Each graph of the electrical conductivity and changes in total hardness indicated a maximum and a minimum respectively on the eighth day. In this study, the amount of total hardness changed from 812 to 521 ppm of CaCO3. Therefore, the total hardness reduction by Dunaliella salina was 35.83 percent. Biosorption of chloride and sulfate ions from sampled saline groundwater was also calculated after cultivation and was 12 and 48 percent respectively. On the other hand, biosorption isotherm of calcium ion using live Dunaliella salina cells was mainly investigated. Biosorption isotherm was normalized and fitted with Langmuir, Freundlich, and D-R models. According to the results, the biosorption of calcium ion follows Langmuir model better than Freundlich and D-R models. Fourier transform infrared analysis revealed the presence of several functional groups on the biomass surface, including carboxyle, aromatic, and hydroxyl groups bound to calcium and magnesium ions whereas ether functional group has not been involved in the biosorption process. The characterisrics obtained from Scanning Electron Microscope combined with Energy-dispersive X-ray spectroscopy clearly indicated that calcium and magnesium ions have been biosorbed by live cells of Dunaliella salina. Finally, the images recorded by Optical microscope proved that there had not been any microorganism contamination.

Keywords: Adsorption isotherm, Biosorption, Dunaliella salina, Biomass, Growth curve

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Determination of hypochlorite in milk using a portable photometer

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The short shelf life of Milk has always been a problem. Some small business milk producers utilize various adulterations to increase the shelf life, potentially risking the health of end-users [1]. These adulterations may include the addition of hypochlorite [2]. As a result of the bleach solution's contact with the milk components, chemical reactions occur [3]. The determination of bleach solution adulteration in milk by the present methods in Iran were not applicable for this aim due to the fast reaction of ClO^- anions with milk compounds and the low residual concentration of it in the milk received by the end-users. Then, the determination of bleach adulteration in milk is by a developed method critically important. Paired emitter-detector diodes (PEDD) based on photometers provide low fabrication cost, low power consumption, ease of miniaturization and a high signal-noise ratio response in a large wavelength range [4]. This paper reports on developing a cheap but efficient paired emitter-detector diode (PEDD)-based photometer. The photometer consists of a white light-emitting diode (LED) as the emitter diode, an RGB LED as the detector diode and a multimeter for recoding the signal. The developed PEDD-based photometer was used for the determination of liquid bleach adulteration in cow milk samples. N, N-Diethyl-p-phenylenediamine sulfate aqueous solution (pH=6.0) was used as a probe to monitor the presence of residual active chlorine in milk. Finally, the calibration curve for determining sodium hypochlorite by using the developed method covered a linear dynamic range, 0.5 to 20.0 ppm, with a detection limit of 0.14 ppm and quantification limit of 0.46 ppm. Real sample analysis results showed that “maybe” liquid bleach adulteration in milk is the case for local distributors of raw milk and some pasteurized milk products.

Keywords: Paired emitter-detector diode-based photometer, Miniaturization, Milk adulteration, Liquid bleach adulteration, Point-of-use testing.

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Green Synthesis and characterization of gold nanoparticles using aqueous extract of Mentha pulegium

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In this research work, the results of two existing methods for synthesizing gold nanoparticles, The green method and The chemical method called Turkovich, were compared and studied. In the green method, the extract of aboveground organs of the medicinal plant Mentha pulegium was used as a reducing agent. The properties of gold nanoparticles synthesized by both method were investigated by SEM, TEM, UV-VIS, EDX, and DLS. The results showed that the size of the green synthesis of gold nanoparticles was smaller and more stable than the Turkovich method. The SEM and TEM results show the morphology of all nanoparticles spherical and the size of nanoparticles synthesized by sodium citrate to be 10.3 nm. The size of nanoparticles synthesized by Mentha pulegium extract is 9.6 nm. The UV-VIS results showed approximately absorption at 526 nm for gold nanoparticles synthesized by sodium citrate and at 421 nm for gold nanoparticles synthesized by Mentha pulegium extract.

Keywords: Green chemistry, Medicinal plants, Mentha pulegium, Gold nanoparticles

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Preparation of a Novel Thin Film Based on Graphene Oxide-Chitosan Nano-biocomposite for Thin Film Microextraction of Fluoxetine from Biological and Environmental Samples

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In this research, for the first time, graphene oxide-chitosan (GO-CS) nano-biocomposite (NBC) [1] is designed and prepared as a novel adsorbent for thin film microextraction (TFME) [2] and was employed for extraction of fluoxetine followed by determination applying high performance liquid chromatography (HPLC) [3]. The properties of the prepared nano-biocomposite were characterized using ATR-FTIR, XRD, TGA and FESEM techniques. The extraction capability of GO-CS NBC toward fluoxetine has been evaluated and the obtained results revealed that incorporation of GO into CS has led to higher extraction efficiency in comparison to CS thin film, and the highest efficiency has been achieved at GO doping level of 5%. The important parameters influencing the extraction efficiency have been investigated via one at a time approach. These parameters have included GO doping level, desorption solvent, extraction time, desorption time, pH and salt content. After optimizing the effective factors in extraction efficiency, the figures for the developed method have been evaluated in which the method's linearity is in the range of 0.4-800 ng ml^{-1} (R^2= 0.996) and the limit of detection (LOD) was 0.1 ng mL^{-1}. The repeatability of the developed method has been investigated in the term of intra-day, inter-day and inter-thin film precision and RSD% values for six replicate experiments were obtained 8.6%, 8.4% and 5.7%, respectively. The applicability of the developed method has been investigated by applying it for extraction and determination of fluoxetine in wastewater, plasma and urine samples and the relative recoveries (RR%) of 91.1%, 82.9% and 72.65% have been resulted, respectively.

Keywords: Thin film microextraction, Graphene oxide-chitosan nano-biocomposite, Fluoxetine, High performance liquid chromatography

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A Paired Emitter-Detector Diode-Based Photometer for the Determination of 2,4,6-Trinitrotoluene (TNT) in Soil Samples

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Visible light-emitting diodes (LEDs) were developed in 1962, containing p-n junctions emitting a narrow band of light wavelengths. LEDs have found a wide application for the miniaturization of optical sensors due to their low cost, small size, robustness, and high efficiencies. They are also used as light detectors since, upon light incident, a potential difference is generated across the p-n junction [1]. Therefore, LEDs can be used as both the light source and the detector in paired emitter-detector diodes (PEDD) optical sensors [2]. PEDD-based photometers provide low fabrication cost, low power consumption, ease of miniaturization, and a high signal-noise ratio response in a large wavelength range [3]. Furthermore, their output is a direct pulse-duration-modulated signal, eliminating the need for a costly analog-to-digital converter. These advantages have led to the utilization of PEDD-based optical sensors in various miniaturized photometers as well as a flow-through optical sensor for chromatography and flow analysis. This paper reports on developing a cheap but efficient PEDD-based photometer. The photometer consists of a white light-emitting diode (LED) as the emitter diode, an RGB LED as the detector diode and a multimeter for recoding the signal. The developed PEDD-based photometer was used for the determination of 2,4,6-trinitrotoluene (TNT) in soil samples. A Meisenheimer complex in acetonitrile was used as a probe to monitor the presence of residual TNT in soil samples. The calibration curve was linear in the concentration range of 1.5 to 97.0 μM, with a detection limit of 0.32 μM and quantification limit of 1.05 μM. Analysis of the soil samples collected from an Iranian cinema town using the developed method showed considerable residual of TNT.

Keywords: Paired emitter-detector diode-based photometer, Determination, Soil analysis, TNT, Point-of-use testing.

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Synthesis and comparison of the electrocatalytic performance of NiCo-X nanodiscs (X = OH, S, Se, P) as an electrochemical platform

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Nanostructures including two various metal elements have reportedly performed better than their single metal counterparts. For example, the electrocatalytic behavior of bimetallic nanostructures containing nickel and cobalt is improved compared to their single metal nanostructures. Several factors such as the combination of electron states, more redox reactions, and the synergistic effect of cobalt and nickel ions are effective in improving electrocatalytic behavior. Therefore, the introduction of novel and efficient bimetallic catalysts has received much attention [1]. So far, different nanomaterials of first-row transition metals such as hydroxides [2], phosphides [3], sulfides [4], and selenides [5] have been reported. However, the electrochemical application of these nanomaterials with disc-like morphology and comparison of their nanodiscs has not been reported so far. The existence of comparative reports can provide useful information to researchers in this field.

In this paper, the NiCo-X (X= OH, S, P, Se) nanodiscs (NDs) were synthesized and characterized. The electrocatalytic performance of the mentioned nanodiscs is compared in the electrochemical determination of isoprenaline (IP) as a templet. The results showed that NiCo-Se NDs show better electrocatalytic activity compared to other nanodiscs studied. The NiCo-Se NDs modified glassy carbon electrode (NiCo-Se NDs/GCE) showed a low detection limit (0.16 µM) and wide linear range (0.5-750 µM) of IP. The proposed substrate for measuring IP in human blood serum samples was successfully used. This study provides insights into the development of polymetallic nanodiscs in the field of electrochemical applications. In addition, our results are promising for usage in other electrochemical applications.

Keywords: Nickel-cobalt selenide, Nanodiscs, Phosphidation, Electrochemical sensor

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Synthesis of new Metal-Organice Framework (MOF) and its applications for detection of antibiotics by fluorescence method

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Antibiotics are a large group of drugs that have been widely used in the treatment of bacterial infections in humans and animals [1]. Excessive use of antibiotics has caused numerous environmental problems; Which can cause some diseases and their complications [2]. Many of the antibiotic compounds used in humans, livestock, and aquatic animals have high percentages of unchanged excretion or drug metabolites. The important point is that only less than 10% of drugs in the body are deformed and the rest are excreted from the body without any changes, and therefore cause pollution and various environmental problems; That's why identifying them is so important[3]. we present an analytical method for detection of metronidazole, an overused antibiotic that has a significant and challenging impact on the environment and health. Solvothermal method was used for synthesis of Zn-2ATA (MOF) as flurophore using zinc nanoparticles and 2-methyl imidazole and 2-amino terephthalic acid as organic ligands. The chemical and physical properties of the synthesized compound have been studied by different spectroscopy methods and microscopic imaging techniques. Then, the fluorescence properties of the prepared compound as fluorophore for analysis of the metronidazole were investigated. Fluorescence data show that the metronidazole drastically reduces the PL emission of the Zn-2ATA metal-organic framework and the fluorescence intensity decreasing with increasing antibiotic concentration. The proposed fluorescence assay was used for detection of metronidazole at concentration range of (5µM-1035µM) with detection limit of 0.5 µM. Fast response, high stability and selectivity along with cheapness and availability are the advantages of the presented fluorescence assay.

Keywords: Metal-Organic Framework, PL photoluminescence, Solothermal synthesis, Antibiotic detection, Metronidazole.

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Simultaneous preconcentration and determination of multiclass pesticides residues in mango and cantaloupe by an in situ electropolymerized solid phase microextraction fiber coating

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Herein, a pencil lead graphite fiber coated with nanostructured polythiophene by a fast, facile and in situ electrochemical method have been developed for solid–phase microextraction and determination of multiclass pesticide residues in summer fruits [1]. The effective parameters in electrochemically synthesis were investigated and optimized [2]. The effective parameters on extraction process including the type of extraction solvent, adsorption time, desorption time, pH, ionic strength, and stirring speed were studied and optimized. Under the optimized conditions, the proposed SPME fiber provided wide linear range (0.1–600 µg L^{-1}) with good correlation coefficients ($R^2 \geq 0.997$) and low limits of detection (0.03–0.15 µg L^{-1}). Relative standard Deviations at concentration of 200 µg L^{-1} of each analyte (n= 5) were estimated ≤7.9 and ≤8.4% for inter– and intra–day precisions, respectively. The proposed method was successfully applied for trace analysis of studied pesticides in fruits matrices and satisfactory relative recoveries were obtained (87.5–117.3 %). The repeatable electrochemically fabrication of proposed fiber, provide a homogeneous coating with high stability and long life time. The cost effective proposed method was demonstrated good extraction efficiency in complex food matrices.

Keywords: Multiclass pesticides, Solid–phase microextraction, Electropolymerization, Nanostructured polythiophene, Fruits

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Trace analysis of some polycyclic aromatic hydrocarbons in food and vegtables using electrochemically fabricated graphene oxide/ polythiophene nanocomposite coating on pencil lead graphite SPME fiber

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Herein, a graphene oxide/ polythiophene nanocomposite coating were successfully synthesized on pencil lead graphite by an in-situ electrochemically method [1], moreover; it was applied for solid phase microextraction and determination of some polycyclic aromatic hydrocarbon (PAHs) resides in honey and celery real samples. The effective parameters on coating electropolymerization and extraction conditions (type of extraction solvent, adsorption time, desorption time, pH, ionic strength, and stirring speed) were studied and optimized. Under the optimized conditions, the proposed SPME fiber provided wide linear range (0.05–99µg L^{-1}) with good correlation coefficients ($R^2 \geq 0.998$) and low limits of detection (0.015–0.10 µg L^{-1}). Relative standard Deviations at 25ml of a mixed standard PAHs solution (phenanthrene: 5, anthracene: 2.5, fluoranthene: 16.5 and pyrene: 12.5 µg L^{-1} and n= 5) were estimated ≤4.7 and ≤6.4% for inter– and intra–day precisions, respectively. The proposed SPME fiber was successfully applied for trace analysis of PAHs in the honey and celery samples which was obtained satisfactory relative recoveries (70.15–110.4 %). The proposed cost effective SPME fiber provided a homogeneous coating with high stability and long life time which can be used for preconcentration of the PAHs in various complex matrices [2].

Keywords: Polycyclic aromatic hydrocarbon, Solid–phase microextraction, Electropolymerization, Graphene oxide, Polythiophene

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Preparation of superhydrophobic rock wool for oil-spill clean-up

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Oil-spill accidents and organic wastewater discharge have caused serious environmental issues. In this regard, the cleanup strategies of oil spill should be implemented to significantly reduce the environmental damages. Conventional strategies including skimming, bioremediation, *in situ* burning, and adsorption have been widely employed for oil-water separation [1]. Among these approaches, adsorption is considered the most effective method for oil pollutions removal [1]. Several adsorbent materials such as carbon aerogels and graphene sponges have been used for this purpose [2, 3]. However, complicated preparation processes, high costs, and scalability challenges restrict the practical applications of these adsorbent materials. In this regard, the use of 3D porous materials such as wools and sponges are more effective. The present work reports the preparation of a superhydrophobic rock wool (RW) for efficient clean-up of oil and organic solvents. The modified RW was prepared by coating a commercial RW with reduced graphene oxide (RGO) nanosheets under hydrothermal treatment. However, modified RW with RGO can be degraded in high-viscosity oils because of weak adhesion between RGO and RW surface and the poor mechanical stability of the rough surface structure. To further enhance hydrophobicity and recyclability, chloroprene rubber (CR) was deposited on the RW surface followed by the second modification with RGO. The elasticity of CR is crucial for preparation of recyclable modified RW. The modified RW possessed superhydrophobicity and superoleophilicity with a water contact angle of 152.4° and it was used for separation of oil-water mixture. The modified RW exhibited the adsorption capacity from 520 to 1030 wt%, depending on the density and viscosity of the oils and organic solvents. The modified RW exhibited excellent mechanical elasticity and durability when compared with commercial one, and the adsorbed oils was recycled by a simple squeezing technique. Its oil adsorption capacities were maintained above 95%, after several compression cycles. After five cycles of recycling, the adsorption capacity decreased. This may be attributed to slight damage of the surface structure in the repeated squeezing and drying process. Importantly, the modified RW exhibited excellent photothermal properties which is beneficial for the separation of high-viscosity oils. Owning to low costs, versatility and scalability in production, the modified RW can be regarded as a suitable choice for large scale oil/water separation.

Keywords: Superhydrophobic rock wool, Reduced graphene oxide, Chloroperene rubber, Oil/water separation

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Assessment of organophosphorus pesticides residues in honey samples using a new mode of dispersive liquid–liquid microextraction method combined with HPLC–UV

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Pesticides are an important part of the modern industry including agricultural food sector. Organophosphorus pesticides (OPPs) are widely used in agricultural areas to prevent crop losses from any pests and improve the product quality, yield, and appearance [1]. However, extremely use of these harmful substances can cause insecticides to accumulate in environment, water and food samples and then they can negative effects on human and animal health even at low levels [2]. OPPs may cause different health problems in humans such ascoma, headache, dizziness, muscle cramps, nausea, and even death in higher concentrations [3]. Therefore, development of an easy, safe, selective, sensitive, fast and green analytical method for the simultaneous extraction, and determination of OPPs residue levels in various food samples is critical. In this work, gas–controlled evaporation–assisted solidification of floating organic droplet–based dispersive liquid–liquid microextraction method has been employed for the extraction of some OPPs (parathion–methyl, triazophos, parathion, diazinon, and phoxim) from honey samples. In this method, briefly, a mixture of chloroform (as a volatile solvent) and menthol: phenylacetic acid DES (as an extraction solvent) was added to honey solution placed into a narrow–bore tube (55 cm × 6 mm i.d.) through the septum using a microsyringe. In the following, nitrogen gas was bubbled into the tube through a glass syringe barrel connected to a needle. During this stage, chloroform was evaporated and a cloudy state was obtained because of releasing and dispersing the droplets of DES. Consequently, the droplets of DES (extraction solvent) containing the extracted analytes were collected and solidified as a single drop on the top of the solution. The drop was transferred into a vial with a spatula and dissolved in ACN. Finally, the resulted solution was taken and injected into HPLC–UV for quantitative analysis. Under the best experimental situations, satisfactory results such as low limits of detection (0.17–0.37 ng g^{-1}), high extraction recoveries (69–87%), and good repeatability (relative standard deviations equal or less than 5.9%) were acquired. At the end, the suggested approach was applied for the quantification of the selected OPPs in ten various honey samples sold in Tabriz, Iran. Considering the outcomes, parathion was detected in three honey samples.

Keywords: Dispersive liquid–liquid microextraction; Organophosphorus pesticides, Honey, High performance liquid chromatography

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Assessment of heavy metal ions in agricultural soil, water, and vegetables in the Kashaf Rud riverside, Razavi Khorasan Province, Iran.

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Nowadays, because of the danger associated with eating vegetables contaminated with heavy metal ions, the safety of vegetables for consumption is becoming an increasing concern to consumers. Industrialization, unrestrained human population, urbanization, and over-usage of pesticides are often the key reasons for heavy metals (HMs) contamination in the food chain. The current study was conducted to quantify some heavy metal ions and to assess their sources and health risks in various samples. Samples used in this study were alfalfa, barley leaves, beet, and beet leaves. Additionally, these samples' agricultural soil, irrigation water, and treated and untreated wastewater of Charmshahr Industrial Town of Mashhad were analyzed for heavy metal ions including Fe, Co, Cd, Zn, Cu, Cr, Pb, and Ni by inductively coupled plasma – optical emission spectrometry (ICP-OES) and were compared with the permissible amounts given by the food and agriculture organization (FAO) and also the world health organization (WHO) for human consumption. Results showed that while samples of beet leaves indicated the highest number of HMs including 1839.69 ppm Fe, 1.43 ppm Co, 48.77 ppm Zn, 18.78 ppm Cu, and 9.33 ppm Cr, the beetroot had concentrations of 22.65 ppm Co, 56.08 ppm Zn, and 20.53 ppm Cu that were exceeding the permissible amounts. Therefore, the leaf of vegetables contained more HMs as compared with the vegetable itself. Moreover, 664.71 ppm Fe, 30.50 ppm Zn, 18.46 ppm Cu, and 3.09 ppm Cr were the concentrations that exceeded the acceptable levels for alfalfa, whilst for barley these HMs were Zn, Cu, and Cr with the concentration of 63.32 ppm, 24.64 ppm, and 1.33 ppm, respectively. In addition, the only HM greater than the permissible level for all water samples was Cr with concentrations of 1.39 ppm for alfalfa and barley irrigation water, 1.36 ppm for the water before purification, and 0.47 ppm for the water after treatment. It is clear that the concentrations of chromium in most samples were beyond the allowable level, which indicates the existence of several tanneries around the river.

Keywords: Industrial effluents, Agricultural samples analysis, Heavy metal ions, Inductively coupled plasma – optical emission spectrometry spectrometry (ICP-OES)

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Solid-phase extraction based on sodium dodecyl sulfate-coated nanomagnets with HPLC determination of sunitinib malate in biological samples

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Sunitinib is a novel oral multitargeted tyrosine kinase inhibitor with antitumor and antiangiogenic activities. Sunitinib was recently approved for the treatment of advanced renal cell carcinoma and for the treatment of gastrointestinal stromal tumors after disease progression or intolerance to imatinib mesylate therapy [1, 2]. Therefore, in this work, for the first time, we used the magnetic solid-phase extraction (MSPE) method based on magnetic extraction as a simple and sensitive method for monitoring sunitinib malate in biological samples. In this work, magnetic solid-phase extraction (MSPE) based on sodium dodecyl sulfate (SDS)-coated Fe_3O_4 nanoparticles was investigated as a novel method for the extraction and determination of sunitinib malate in biological samples prior to HPLC-spectrophotometry determination. The main factors affecting the extraction of analysts, such as pH, surfactant and adsorbent amounts, ionic strength, extraction time, and desorption conditions were studied and optimized. Under the selected conditions, the sunitinib malate was quantitatively extracted. The accuracy of the method was evaluated by recovery measurements on spiked samples, and good recoveries of 95% and 89% were observed for urine and plasma respectively. Proper linear behaviors over the investigated concentration ranges of 2–16 and 2–14 mg/L with good coefficients of determination, 0.997 and 0.995 were achieved for urine and plasma samples, respectively. LODs were 1.13 and 0.97 mg/L and LOQs were 3.52 and 2.94 mg/L for urine and plasma samples, respectively. Also RSD % was 10.21 and 9.02 for urine and plasma samples, respectively. The obtained results demonstrated that the prepared sorbent due to the high surface area has an excellent adsorption capacity and satisfactory extraction recoveries.

Keywords: Sunitinib, Magnetic solid-phase extraction, Magnetic nanoparticles, Sodium dodecyl sulfate.

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Magnetic dispersive solid phase extraction of some tetracycline and fluoroquinolone antibiotics from milk samples prior to their determination by HPLC-DAD

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Today, different kinda of veterinary drugs (e.g. tetracyclines, quinolones, macrolides, sulphonamides, and etc.) are used in animal husbandry to promote a rapid growth of livestock and treatment or prevention the different diseases [1]. These drugs are administered orally as feed additives or administered directly by injection [2]. However, widespread use of antibiotics can cause their residues in dairy and animal-derived foodstuffs that is one of the main concerns of food safety and can threat consumer's health and cause problems such as allergic reactions, liver damage, and carcinogenic or teratogenic effects [3]. Thus, the development of green, simple, reliable and highly sensitive analytical methods is highly recommended. In this work, folic acid magnetic nanoparticles were synthesized and used as sorbent in magnetic dispersive solid phase extraction of some tetracycline and fluoroquinolone antibiotics (doxycycline, tetracycline, oxytetracycline, ciprofloxacin, and enrofloxacin) from milk samples. For this purpose, after precipitating the proteins of milk by using zinc sulfate solution, the supernatant phase was taken and mixed with an appropriate amount of magnetic sorbent. Afterward, the resulted mixture was vortexed to disperse the sorbent in the whole of solution. Then, the sorbent particles containing the adsorbed analytes were separated in the presence of magnet and eluted with the mobile phase under sonication. Finally, in the presence of magnet, the supernatant phase was taken and injected into HPLC–DAD. Satisfactory analytical results such as wide linear ranges (2.13–2000 ng mL^{-1}), high extraction recoveries (69–87%), and low limits of detection (0.63–0.96 ng mL^{-1}) and quantification (2.13–3.21 ng mL^{-1}) were obtained using the optimum experimental situations. Lastly, the offered procedure was utilized for the quantification of the opted analytes in twenty–one milk samples marketed in Tabriz, Iran. Considering the outcomes, oxytetracycline was found in five of the investigated milk samples in the range of 11-52 ng mL^{-1}.

Keywords: Magnetic dispersive solid phase extraction, Milk, Antibiotic, High performance liquid chromatography

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Microextraction in packed syringe using ion monitoring graphene oxide-mesoporous silica nanosheets as sorbent for extraction and determination of Cr (VI) from real samples.

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Cr (VI) considered as one of the toxic heavy metals, which can cause damage to the human health, like lung cancer, liver, kidney and gastric damage [1]. For this reason varios treatments have been studied. Adsorption is a common treatment applied to remove Cr (VI) [2]. A large number of adsorbents have been utilized in Cr (VI) removal, including activated carbon, chitosan, nanoscale zero-valent iron, magnetic nanocomposite, ion-imprinting technique and other substances [3-5]. In this study, chromium (VI) ion-imprinted polymer (Cr(VI)-IIP) was prepared using surface ion imprinting technique on graphene oxide-mesoporous silica (GO-MS) nano sheets with 3-(2-amino ethyl amino) propyl trimethoxysilane. Absorbent nanosheets produced were characterized by Fourier transform infrared spectroscopy (FT_IR), scanning electron microscopy (SEM), X-ray diffraction (EDAX), and thermal balance analysis (TGA) techniques. The influences of pH of aqueous sample, adsorbent amount, number of sample loading cycles, number of solvent loading cycles, sample volume, solvent volume on the adsorption performance of Cr(VI)-IIP were investigated. The method has a linear range of 100-1400 ppb and detection limit (LOD) of 4.88 ppb. In the selectivity study, it was found that the synthesized adsorbent shows high efficiency in adsorption of chromium (VI) ions in competition with other metal anions and cations.

Keywords: Ion-imprinted polymer, Cr(VI), Graphene oxide, Mesoporous silica

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Adsorbtion Study of Alizarin Yellow GG on a Cu(II) Modified Magnetic Nanoadsorbent

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Dyes are risky hazardous materials and are one of the most important pollutants of soil and water resources. They cause serious problems to aquatic creatures. In addition, dyes are widly produced in chemical plants and are employed increasingly in various industries related to textile, cosmetics, paper, food, paint, printing and pharmaceuticals. The scientific resources have mentioned a total of more than 50000 ton of dyes are discharged annually into the environment [1]. Magnetic nanoparticles (MNPs) have been extensively studied as an efficient adsorbent with large surface area causing small diffusion resistance for the separation of pollutant chemicals such as dyes, metals and pharmaceuticals [2]. Moreover, MNPs cause advantages on ease of separation and fast recovery by employing an external magnet due to prevention of the additional centrifugation or filtration processes [3]. Alizarin yellow GG (AY) is an anionic dye having carcinogenic effects that are used in large quantities in dyeing of woven fabrics, wool and cotton textiles. AY causes many environmental problems. In this work a cross-linked chitosan@Fe_3O_4 nanomaterial was prepared and its charactersitics were studied by appropriate spectroscopic and microscopic techniques. Then, the magnetic nanoadsorbent was used to study the adsorption and extraction of AY from the effluents in the presence of Cu(II). The results of the experiments revealed that a 95% removal of AY was achieved at the optimal adsorbent dosage of 0.4 mg mL^{-1} and Cu(II) concentration of 0.25 mmol L^{-1} for 6 min. The experimental results were fitted with various adsorption isotherms. As a result, the equilibrium data were well fitted to the Langmuir isotherm model (a monolayer adsorption pattern with homogeneously distributed adsorption sites). Moreover, it was observed that a solution containing ammonia was efficient on the relatively complete recovery of AY (from the adsorbent). The applicability of the nanoadsorbent on the AY separation from lake, well and river water samples was evaluated. The separation yield was in the range of 94-97%. A certain amount of the magnetic nanoadsorbent (20 mg) was employed for 6 consecutive adsorption and elution (with ammonia) steps. The results showed that the adsorption and elution yields of AY were about 98% and 95-97%, respectively.

Keywords: Alizarin yellow GG, Adsorbtion study, Cu(II) modified magnetic nanoadsorbent.

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Electrosynthesis of layererd double hydroxides on the surface of graphene electrodes

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Layered double hydroxides due to their high structural flexibility, high anion exchange capacity, large surface area has found various applications in catalysts, photochemistry, pharmacy, removing of pollutants from the environment and drug delivery. Due to some problems with older synthesis methods, many scientists are interested in synthesizing LDHs with electrochemically controlled reactions. Therefore, in this work, different LDHs were precipitated on different graphene-based substrates and their electrocatalytic behavior were investigate in details [1]. Cyclic voltammetry or constant potential techniques can be used to prepare LDHs electrochemically. Here, we have used a constant potential for the LDHs synthesis. For this purpose, LDH-related precursors are placed in the electrochemical cells with certain concentrations and by applying a constant potential for a certain period of time, we perform the electrodeposition process. The prepared LDHs were characterized with XRD, SEM and cyclic voltammetry in details [2]. For example, to prepare Fe / Ni LDH, 0.09 M $Fe(NO_3)_3.9H_2O$, 0.12 M $Ni(NO_3)_2.6H_2O$ and 0.15 M KNO_3 were placed in an electrochemical cell and a constant potential of -0.8 V for 100 s were applied to the surface of electrode. The results showed that the electrodeposition of LDHs have the advantage of fastness, low cost, ability to control the synthesis and also high electrocatalytic properties for measuring some species.

Keywords: Electrosynthesis, Layered double hydroxides, Graphene

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Classification of CC Chemokine Receptor Inhibitors: A Computational Journey Leading to Drug Discovery

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CC chemokine receptors are introduced as integral membrane proteins that particularly attach and respond to cytokines of the CC chemokine family representing one subfamily of chemokine receptors, a large family of G protein-linked receptors. Four member of CCR family, CCR1, CCR2, CCR4 and CCR5 have been distinguished on the surface area of monocytes, activated memory T cells, B cells, and basophils in humans [1] binding several inflammatory/inducible CC chemokines [2], whereas undoubtedly the most important CC chemokine receptor called CCR5 is expressed on multiple cell types and it is defined as an essential coreceptor implicated in susceptibility to HIV-1 infection [3]. The given article illustrates the characterization of molecular features that induce selectivity for inhibition of CCR1, CCR2, CCR4 and CCR5, in which the number of 7294 molecules were collected from Binding Database and 3224 molecular descriptors for each molecule were calculated via Dragon Talete 5.5. Moreover, the best feasible subset of molecular descriptors were selected utilizing Variable Importance in Projection (VIP), providing the opportunity to classify the mentioned targets based on their therapeutic features and activities. Two various classification methods namely SKN and CPANN were used so as to find the relationship amongst molecular structures of chemicals, their activities and selectivities. Generally, the performances of classified models were evaluated according to the statistical parameters derived from the given confusion matrices. Additionally, both dependability and predictability of the conducted models were estimated by the tenfold cross-validation techniques and test sets. Sensitivity, specificity, precision, accuracy and non-error rate are mostly equal in CPANN and SKN classification results and in both are mostly over 80% which can either be meticulously found handful in order to design brand new drugs with selective inhibitory activities toward mentioned CCRs or much more efficacious in pharmaceutical aspects of miscellaneous medical treatments for self-immune diseases.

Key words: Chemokine receptors, Self-immune disease, Ligand-based classification models, Variable importance in projection, Discriminative models

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Magnetice nanoparticles coated with tannin as a new sorbent in dispersive solid phase extraction using deep eutectic solvent for extraction of phenolic compounds from industrial wastewater samples prior to GC-MS/MS determination

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Industrial procedures and human activities cause numerous types of pollutant in the environment that can lead to serious problems to human health and environment. Phenolic compounds released to environment is as a result of their broad use in petrochemicals, paper, dyes, pesticides, resin and plastic production within a various concentration range [1–3]. Here, a D-µSPE coupled with AALLME approach was established for extraction and preconcentration of some PCs from industrial wastewater samples perior to GC-MS/MS. For this purpose, a sorbent, was prepared as a magnetic sorbent in D-µSPE step for the first time. In addition, the AALLME step was performed using an DES as an extraction and elution solvent. The effective parameters on extraction effeciency such as amount of sorbent, agitation mode, and volume of extraction solvent were studied by "one-parameter-at-one-time" in details and the validated method was established for determination of the PCs from industrial wastewater samples before gas chromatography-tandem mass spectrometry (GC-MS/MS) analysis. A high enrichment factor and extraction recovery (79-86%), low limits of detection (0.002-0.009) and quantification (0.007-0.027 ng/mL) of results demonstrated a satisfactory performance of the present approach. Finally, the proposed method was successfully implemented to detect the studied phenolic compounds in water samples from different areas.

Keywords: Magnetice nanoparticles, Dispersive magnetic solid phase extraction, Phenols, Gas chromatography-tandem mass spectrometry, Water samples

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Quantification of individual and total major sterols contents of butter by gas chromatography

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Sterols are organic compounds, which are subgroup of steroids. Sterols and related compounds play essential roles in the physiology of eukaryotic organisms [1]. This investigation describes the preparation and extraction of the unsaponifiable matter from butter oils. The extracted oil of butters, with added an internal standards (I.S.), are saponified with potassium hydroxide in ethanolic solution and the unsaponifiable matter is then extracted with diethyl ether. The different alcoholic compounds fractions are separated from the unsaponifiable matter either by thin-layer chromatography (TLC) on a basic silica gel plate. The fraction recovered from the silica gel separation is transformed into trimethylsilyl ethers and then analysed by capillary column gas chromatography [2]. The developed method was validated according to international guidelines.

Keywords: Sterol, GC, TLC.

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Carbon selenide nanofilms supported on a wearable conductive textile as a freestanding sensing interface for pethidine detection

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Pethidine (PTD), known as meperidine (ethyl, 1-methyl-4-phenylpiperidine-4-carboxylate hydrochloride), is a synthetic opiate in the category of phenylpiperidine with many side effects. PTD use has been banned by many organizations like the International Olympic Committee (IOC) because of the disorder of vital biological activity of the body and, even worse, death by the drug interactions of PTD or its overdose [1-3]. Due to the importance of PTD tracking in biofluids, the clinical and judicial organizations have recently boosted many demands for a selective and real-time sensor, especially through a noninvasive method. Herein, the impregnation of carbon cloth with carbon selenide nanofilms (CSe_2NF/CC) has been proposed for the electrochemical sensor fabrication for PTD monitoring in the human blood, urine and saliva samples. Accordingly, Se was doped in the carbon skeleton to provide the CSe_2NF/CC as the sensing interface and embed a sizeable electroactive surface area of 4.61 cm^2 compared to the unmodified CC (0.094 cm2). By optimizing some important parameters, including the effect of accumulation time, the amount of Se powder, scan rate, pH and the supporting electrolyte type, the CSe2NF/CC catalyzed PTD with an oxidation current of 18-times higher than unmodified CC at 0.97 V. This electrochemical behavior revealed that CSe2NF onto CC surface as a sensing interface has an acceptable catalytic effect for PTD oxidation. The developed flexible sensor exhibited a detection limit (LOD) of 19.3 nM and two linear PTD concentration ranges (29 nM to 1.9 µM and 1.9 µM to 181.8 µM) by the excellent stability of 93.2% after 30 days. PTD analysis in the non-spiked and spiked real samples by the developed sensor was validated by HPLC analysis as the reference method using a t-test statistical method at the confidence level of 5%. The results ascertain the applied strategy in the flexible sensor design as a model may be a convenient method for the fast, non-invasive addict diagnosis in the biofluids of suspicious people.

***Keywords**:* Carbon selenide nanofilms, Carbon cloth electrode, Flexible sensor, Pethidine, Opiate

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Dispersive micro solid phase extraction of several ultraviolet filters from hygiene samples using deep eutectic solvent-modified graphene oxide nanoparticles prior to their determination by HPLC-MS/MS

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Overexposure to ultraviolet (UV) radiation can induce serious skin disease such as skin inflammation or skin burns, immunosuppression, or even skin cancer [1, 2]. As a result, nowadays there are many cosmetic products (sun screen, lotions, lipsticks, hair dyes, shampoos, etc.) produced in order to protect the skin from UV rays, which included in UV filters in their formulation. Octocrylene, 4-methylbenzylidene camphor and Avobenzone are one among them, have the ability to absorb or reflect in both UV ranges [3]. In this work, a simple, sensitive and efficient preparation method based on dispersive micro solid-phase extraction (D-µSPE) is developed to extraction and preconcentration of UV filters (avobenzone, octocrylene, 3-(4-methylbenzylidene) camphor) before their quantification by high performance liquid chromatography- tandem mass spectrometry (HPLC-MS/MS) in hygiene samples. Therefore, deep eutectic solvent-modified graphene oxide nanoparticles was applied as a simple and green sorbent to extract the selected UV filters Effects of different parameters on extraction efficiency were studied and optimized. The proposed D-µSPE method provided the precise detection of the UV-filters in hygiene samples, with high enrichment factors between 69-82, low limits of detection 0.12-0.39 ng g^{-1} and proper repeatability (RSD≤ 5.3%). Finally, the proposed method was successfully employed to determination trace amount of UV filters in three hygiene samples with complicated matrix.

Keywords: Dispersive micro solid phase extraction, Ultraviolet filters, Deep eutectic solvent, Hygiene samples, High performance liquid chromatography-tandem mass spectrometry

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Determination of nitrite in water samples based on a starch adhesive-iodide system using a simple spectrophotometric method

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In recent years, environmental pollution by nitrogen compounds, such as nitrite, nitrate, ammonia, and organic compounds [1], has attracted considerable attention. Among the above-mentioned compounds, nitrite (NO_2^-) is known as the most hazardous and important anionic analyte. Nitrites are largely used in food preservatives, fertilizers, detergents, wood pulping and dyes and thus can be released into the environment, leading to the contamination of soils, groundwater, rivers, and lakes. According to the World Health Organization (WHO), the maximum permissible amount of nitrite ions in drinking water is 3 mg L^{-1} [2] . Thus, sensitive, selective, and precise methods are required for the determination of nitrite ions in water samples. In this work, a simple method has been developed for determination of nitrite in different aqueous samples based on spectrophotometry and colorimetric methods. The method is based on the reaction of nitrite with potassium iodide in acid medium to liberate iodine. This liberated iodine reacts with starch adhesive to form a dark blue complex with a maximum absorption of 570 nm. The effect of different parameters on the proposed method was investigated and optimized. Under the optimal conditions, the calibration graph was linear in the range of 0.05-1 mg L^{-1} with the limit of detection (LOD) of 0.02 mg L^{-1}. Relative standard deviation for determination of 0.3 and 0.5 mg L^{-1} of nitrite was obtained 7.5% and 5.5, respectively, for six replicates. After investigating of interference of common cations and anions, the proposed method was successfully utilized for the determination of nitrite ions in different water samples (rain water and tap water) with satisfactory recovery ranged from 93% to 95%.

Keywords: Nitrite, Spectrophotometry, Starch adhesive, Water samples

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Estimated intake of sweeteners, Aspartame and Acesulfame-k in Soft Drinks by HPLC-DAD

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The most popular non-nutritive sweeteners are acesulfame potassium, aspartame. Acesulfame potassium is the potassium salt of acesulfame (6-methyl-1, 2, 3-oxathiazine-4(3H)-one 2,2-dioxide), an acidic cyclic sulfonamide groups in sucrose which is 600 times sweeter than sucrose [1]. In this study, acesulfame potassium and aspartame quantified in some soft drinks with optimized procedure. A simple and rapid sample pretreatment method was used to remove fat and protein from the test solution with Carrez clearing regent precipitant knows to be effective for protein and fat removal [2]. The pretreated samples were simulative detected by high performance liquid chromatograph using a Reverse phase C18 column (5 ㎛, 4.6 × 250 mm). The validated results showed good correlation with FDA community.

Keywords: Sweeteners, Acesulfame potassium, Aspartame, HPLC.

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Development of dispersive solid phase extraction based on a super hydrophobic metal organic framework for the extraction and preconcentration of several pesticides from fruit juices prior to HPLC-MS/MS determination

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Pesticides are generally used in agriculture to increase crops yield and reduce the damage of weeds, insects, and diseases on the agricultural products [1]. Pesticide residues, left to variable amounts in the food materials after harvesting, are beyond the control of customer and have long-term toxic effects on human health (e.g., lacrimation, seizures, headaches, and abdominal pain) [2, 3]. Considering this, determination of pesticide residues in fruit juices is important. Because of the complicated matrix and low concentration of pesticide residues in food samples, development of an efficient and sensitive preparation method for their determination is required. In the present study, a superhydrophobic MOF was synthesised and used as a sorbent in DSPE of selected pesticides from fruit juice samples prior to their determination by high performance liquid chromatography-tandem mass spectrometry (HPLC-MS/MS). For this purpose, NH_2-UiO-66(Zr) MOF was functionalized by trimethylchlorosilane to increase its hydrophobicity and it was used in DSPE approach. Effective parameters were investegated by “one-parameter-at-one-time” and the validated method was used for determination of the analytes in fruit juice samples. The method was linear within the range of 0.29-500 ng mL^{-1}. The limits of detection, intra- and inter-day relative standard deviations, and extraction recoveries were in the ranges of 0.02-0.1 μg L^{-1}, 2.9-8.8%, 6.8-14.4%, and 74-89%, respectively. Appling the method on the selected samples showed that they were free of the analytes. This method could help to monitor the studied pesticides in juice samples as well as improve our understanding of the safety of foods.

.***Keywords:*** Metal-organic framework, Dispersive solid phase extraction, Pesticides, High performance liquid chromatography-tandem mass spectrometry, Fruit juice

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MXene/NiONPs nanolayer as an efficient supporting substrate in the electrochemical aptasensor fabrication for methamphetamine detection

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Methamphetamine (MAMP), one of the recreational industrial opiates with sever damage, is commonly abused to create a feeling of extreme pleasure in youth and teenagers. Taking high doses of this famous street opiate leads to the increased heart rate and blood pressure, respiratory problems, stroke and death [1, 2]. To control the epidemic problems of MAMP abuse, the developing a reliable method for the selective and on-site screening of biofluids and seized ecstasy drugs is essential for the legal and medical authorities. Herein, a glassy carbon electrode (GCE) modified with nickel oxide nanoparticles (NiONPs) anchored on MXene has been applied as a supporting substrate to load more aptamer sequences as the MAMP receptors. The GCE modified with NiONPs/MXene nanocomposite as the aptasensor exhibited more surface area and higher current than the bare GCE. The fabricated aptasensor detected MAMP electrochemically for 40 min with a linear concentration range of 1 pM to 50 mM and a limit of detection (LOD) of 0.02 pM. The proposed system indicated a desirable selectivity in the presence of other possible interferences such as cocaine (COC), methadone (MET), tramadol (TRM), pethidine (PTD) and codeine (COD). The aptasensor detected MAMP in some human serum, urine and saliva samples, with the acceptable recoveries ranging from 98.51%-105.94%, 96.80%-100.75% and 97.07%-103.68%, respectively. According to the results the proposed strategy is promising for the fabrication of other electrochemical aptasensors to monitor other opiates to open a new way of dealing with the global problem of addiction.

Keywords: Methamphetamine, MXene, Nickel oxide nanoparticles, Aptamer, Aptasensor

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Application of riboflavin as a green sorbent in dispersive µ-solid phase extraction combined with deep eutectic solvent based dispersive liquid-liquid microextraction for sample preparation of some pesticides from vegetable samples prior to GC-FID and GC-MS

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Vegetables are a good source of dietary fiber, minerals, antioxidants, vitamins, and etc. A diet rich in vegetables and fruits can lower blood pressure, reduce the risk of heart disease and stroke, prevent some types of cancer, obesity, diabetes, and cardiovascular diseases [1]. Increasing population growth, followed by increased demand for agricultural products, different groups of pesticides have been widely used to repel, prevent, or control pests [2]. However, excessive use of pesticides is a serious threat to the environment and human health [3]. Therefore, to remove health concerns, determination of pesticides at low concentrations in vegetables is essential. The main goal of this study is develop a preparation method based on coupling D-µ-SPE with DLLME for the extraction and preconcentration of pesticides at trace amounts. In the peresent work, riboflavin was used as a green sorbent for the first time in D-µ-SPE step. In following, the DLLME step was performed using an DES as an extraction solvent. The effects of different parameters on extraction efficiency in both steps were investigated and optimized. In following, the proposed method was applied in the extraction and preconcentration of the selected pesticides from vegetable samples. Under optimized conditions, wide linear range were achieved.The limits of detection obtained by gas chromatography-flame ionization and gas chromatography-mass spectrometry were in the ranges of 0.35-0.78 and 0.01-0.09 ng mL^{-1}, respectively. Finally, the developed methods were applied successfully for analysis of the selected pesticides in vegetable samples.

Keywords: Dispersive µ-solid phase extraction, Dispersive liquid-liquid microextraction, Deep eutectic solvent, Pesticide, Gas chromatography

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Preparation of Monolithic Membrane Sorbent based on Polyethersulfone-Natural Polymers Composite and its Application in the Extraction of Bisphenol A

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Bisphenol A (BPA) is an industrial chemical used in synthesis of poly esters, poly sulfones and poly ether ketones and is a key monomer in production of poly carbonate plastics and epoxy resins. Poly carbonate plastics are used in production of water and milk bottles, sports equipment, medical and dental equipment, dental composites, contact lens and electric home appliances. According to the epidemiological studies, bisphenol A is found in urine samples of 90% of world population. Bisphenol A is an environmental pollutant and disturbs nitrogen fixation process in plant roots. In this study a novel analytical method based on solid phase microextraction using monolithic membrane fiber for extraction of bisphenol A from bottled mineral water was developed. Factors affecting extraction efficiency like physical and chemical nature of the fiber, extraction time and temperature, solution pH, salt effect were optimized by surface response methodology based on central composite design (CCD). Proposed method has linear dynamic range between 1-150 μgL^{-1} with regression coefficient of 0.9993. Limit of detection (LOD) and limit of quantification (LOQ) were 0.33 and 1 μgL^{-1}, respectively. Repeatability of fiber preparation (n=2) and repeatability of extraction (n=3) were 5.77 and 3.87%, respectively. Proposed method was applied for determination of bisphenol A in bottled mineral water and 95.62±8.05 % recovery value of the method made it a suitable method for extraction and determination of bisphenol A.

Keywords: Monolithic sorbent, Liquid chromatography, Bisphenol A, Membrane, Polyether sulfone

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Ferrofluid-based liquid-liquid microextraction method for separation and determination of uric acid in biological samples

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Uric acid is the most important nitrogenous compound in urine. At a certain pH, uric acid ionizes and mostly forms urate ions. When the concentration of urate in the body exceeds the solubility level, sodium urate crystallizes in soft tissues and joints, leading to serious diseases such as hyperuricemia, hypertension, gout, kidney disorder and arthritis [1]. As a result, the determination and quantification of uric acid in biological samples in order to control and prevent side effects of this compound is extremely neededIn this study, $CoFe_2O_4$ magnetic nanoparticles were synthesized by hydrothermal method [2] and characterized by Fourier transform infrared (FT-IR) spectroscopy, vibrating sample magnetometer (VSM), field emission scanning electron microscopy (FE-SEM) and energy dispersive X-ray (EDX). Ferrofluid-based liquid-liquid microextraction consisting of cobalt ferrite nanoparticles coupled with UV-Vis spectrophotometry (LLME-FF-UV-Vis) as a green and efficient approach was used for extraction and determination of uric acid. Four parameters of pH, ferrofluid volume, temperature and ultrasonic time were selected as effective factors on the process and optimized by central composite design (CCD) [3]. Under optimized conditions, the linear range 0.07–40 mg L^{-1}, limit of detection 0.02 mg L^{-1} and the relative standard deviation (R.S.D) %2.1 were obtained for target analyte. Finally, the proposed method was successfully applied for preconcentration and determination of uric acid in human urine sample.

Keywords: $CoFe_2O_4$ magnetic nanoparticles, Ferrofluid, Uric acid, Central composite design, Biological samples.

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Trace quantification of dimethyl phthalate in fruit juice and water samples based on STA-12(Fe) as an efficient sorbent

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Dimethyl phthalate (DMP) belongs to the family of phthalates or phthalic acid esters (PAEs). These compounds are widely used as plastic additives, especially in poly (vinyl) chloride (PVC) and polyethylene terephthalate (PET) to improve properties such as flexibility, transparency and durability of products produced with these polymer matrices [1]. Human exposure to phthalates can occur as a result of direct contact with and use of them, or indirectly through the washing of other products or general environmental pollution[2]. PAEs are known to be potential endocrine disruptors, accumulate in tissues, and are not well degradable. Therefore, determination of DMP is an important analytical task. In this study, STA-12 (Fe) was synthesized and characterized by Fourier transform infrared spectroscopy (FT-IR), x-ray diffraction spectroscopy (XRD)[3]. STA-12 (Fe) as adsorbent, in dispersive micro-solid phase extraction (Dμ-SPE) as green, simple and efficient method was used for trace quantification of dimethyl phthalate. Four independed parameters of pH, adsorbent amount, temperature and ultrasonic time were selected as factors influencing the process and optimized by central composite (CCD) design[4]. Under optimal conditions, linear range of 600-30 ng mL^{-1}, detection limit of 8.68 ng mL^{-1} and relative standard deviation (R.S.D) of 0.81% were obtained for the target analyte. Finally, the proposed method was successfully used for preconcentration and determination of dimethyl phthalate in fruit juice and water samples.

Keywords: Dimethyl phthalate, Preconcentration, STA-12 (Fe), Fruit juice samples, Experimental design

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Deep eutectic solvent-based emulsification liquid-liquid microextraction method for separation and determination of allura red in food samples

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Synthetic dyes contain azo functional groups and aromatic ring structures that are harmful to human health. Some studies show that the use of these pigments causes health problems such as recurrent headaches in adults, neurotoxicity, genetic toxicity and carcinogenesis. Allura red is one of the artificial colors that is found in beverages, juices, gelatin, puddings, condiments, confectionery products and so on [1]. Therefore, the determination of allura red in food samples in order to control and prevent the mentioned complications is very important. This study reports the application of deep eutectic solvents (DES), as a new generation of environmentally friendly solvents for the emulsification liquid-liquid microextraction of allura red in food samples. The DES used in this work was synthesized with choline chloride and phenol (molar ratio 1:4). Affecting parameters such as volume of DES, volume of tetrahydrofuran (THF), pH and ultrasonic-extraction time were optimized by central composite design (CCD) [2]. Under optimized conditions, the calibration curve was linear in the concentration range from 15-1200 μg/L, relative standard deviation (RSD) and limit of detection were obtained 3.59% and 4.31 μg/L, respectively. The proposed method was successfully applied for preconcentration and determination of allura red in food samples.

Keywords: Deep eutectic solvents, Allura red, Emulsification liquid-liquid microextraction, Food sampels, Central composite design

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Evaluation of activated charcoal infused dental floss as a viable sorbent for preconcentration and extraction of pesticide residues from fruit juices

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Pesticides are extensively used in agriculture to increase crop production and control pests [1]. Unfortunately, pesticide residues in fruit juice can introduce during planting and preservation process and pose many adverse effects on human health including cancer and detrimental effects on reproductive and nervous systems [2]. Gas chromatography [3] and Liquid chromatography [4] are the conventional instrumental techniques for pesticide detection and determination. This study describes the development of a solid phase extraction approach based on the use of activated charcoal infused dental floss as an efficient, economic, and easy–accessible carbon fiber sorbent. The fiber is used to extract residue of some pesticides including chlorpyrifos, haloxyfop-R-methyl, clodinafop-propargyl, fenpropathrin, diniconazole, oxadiazon, and fenoxaprop–P–ethyl from various fruit juices. In this method, activated charcoal infused dental floss is cut into 50-cm pieces and washed with acetonitrile for conditioning and dried at room temperature. Then it is immersed into the sample solution and vortexed. By this action, the analytes are adsorbed on the sorbent. The sorbent is removed by a pence. Then the analytes are desorbed using an appropriate solvent. After that, the eluate is enriched with a dispersive liquid–liquid extraction procedure. The enriched analytes are quantified with gas chromatography–mass spectrometry. Under the best extraction conditions, limits of detection and quantification were found in the ranges of 0.02–0.06 and 0.09–0.22 μg L^{-1}, respectively. Enrichment factors and extraction recoveries of the analytes ranged from 245–394 and 49–79%, respectively.

Keywords: Carbon fiber sorbent, Dispersive solid phase extraction, Pesticides, Fruit juice

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Sono Fenton degradation of phenazopyridine by $FeMnO_3$ magnetic nanocomposite

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Pharmaceuticals, pesticide and cosmetic products are usually find in wastewater and since these compounds destroyed hardly, they never remove completely. Among these polluters, pharmaceuticals residue in wastewaters, were known as emerging contaminants [1-2]. Thus removal of these materials from waste water is more important. Fenton process is an advanced oxidation process that is used for degradation of organic pollutants. Both of Fenton process and Ultrasonic waves are used as separate method for degradation of the pollutants.

This study is an experimental research in a laboratory scale with the aim of evaluating the efficiency of the new $FeMnO_3$ magnetic nanocomposite for the degradation of phenazopyridine in the presence of H_2O_2 as a heterogeneous Fenton- like catalytic degradation in aqueous solution. So $FeMnO_3$ magnetic nanocomposite was synthesized by hydrothermal method. The synthesized catalyst was identified using methods such as Fourier transform infrared spectroscopy(FTIR), X-ray diffraction(XRD), energy dispersive X-ray spectroscopy (EDS), Field emission scanning electron microscopy (FESEM), Transmission Electron Microscopy (TEM), and visible-ultraviolet spectroscopy, and the results confirmed the catalyst structure. The parameters such as pH, nanocomposite dose, hydrogen peroxide concentration and contact time were investigated in the degradation of phenazopyridine. Based on the results after optimizing the parameters, the maximum degradation efficiency of phenazopyridine by the synthetic catalyst was 96%. The results indicated that the Fenton process has a good performance in degradation of phenazopyridine [3-4].

Keywords**:** Magnetic nanocomposite, Phenazopyridine, Heterogeneous fenton- like

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Detection of HER2 breast cancer biomarker using an antibody-based label-free electrochemical immunosensor

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The most prevalent and diverse women's cancer is breast cancer, which annually affects 2.06 million women leading to the highest number of deaths. Human Epidermal growth factor Receptor 2 (HER2) is a specific cancer related biomarker used in clinical settings. Abnormal HER2 levels are particularly significant since its overexpression is related to invasive and aggressive breast cancer-types [1]. The traditional analytical techniques, currently available for the control of HER2, provide complete information, but they have significant constraints in terms of low selectivity and sensitivity, complexity, cost and duration of time [2]. However, we need fast-response systems to control in situ HER2 level. To obtain direct, rapid, and amplification-free detection of HER2 with satisfactory specificity an ultrasensitive and label-free electrochemical immunosensor for early breast cancer diagnosis was designed. In this study, a biosensor based on a specific antibody (Ab) against the coat protein of the HER2 on the protein G (PG) immobilized on Cysteine (CYS) functionalized high surface area gold electrode (Au/CYS) using covalent conjugation (Au/CYS/PG/Ab) was developed for the detection of HER2. It is based on label free techniques (Low-wave platform and electrochemical admittance), which allow an in situ monitoring of HER2 in the range of 10 pM to 1 nM with the limit of detection of 0.008 nM. This biosensor has desirable performance with HER2 in human serum samples which confirms its highly promising potential for early clinical breast cancer diagnosis.

Keywords: Breast cancer, Cysteine adaptable linkage, Electrochemical detection, HER2 biomarker, Label-free immunosensor

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Monitoring of pyrethroid pesticides in commercial fruit juices using a magnetic dispersive solid phase extraction combined with dispersive liquid–liquid microextraction and gas chromatography–mass spectrometry

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Nowadays, food safety that can affect the quality of human life is the main priority of human societies [1]. Pesticides are widely utilized in order to increase the crop's yield and quality and reduce the damages caused by insects, weeds, and diseases [2]. Regardless of the several merits of pesticides using, most of them are highly stable in the environment and can remain in soils, plant tissues, fruits, and vegetables [3]. Considering this point, controlling the pesticide content of fruits and their by–products like fruit juices that are extensively used is crucial. In the current work, a magnetic dispersive solid phase extraction in combination with ferrofluid–based dispersive liquid–liquid microextraction was used for the extraction of some pyrethroid pesticides (bifenthrin, phenothrin, tetramethrin, cyhalothrin, permethrin, and cypermethrin) from fruit juices. In the extraction process, first a few milligrams of a synthesized magnetic sorbent (Fe_3O_4@polythiophene) was added into a sample solution and the resulted mixture was stirred at high rate to disperse it throughout the sample solution. After stopping the stirring process, the particles containing the adsorbed analytes were rapidly returned onto the stir bar and eluted with acetonitrile to desorb the analytes. In the following, this phase was taken and mixed with a few microliters of a synthesized ferrofluid and the mixture was quickly injected into deionized water placed in a conical glass test tube for more enrichment. The ferrofluid droplets were settled down in the presence of magnet and the analytes were back-extracted into *n*–hexane. This phase was injected into gas chromatography–mass spectrometry for quantitative analysis. Under the optimum situations, low limits of detection (4–12 ng L^{-1}) and quantification (14–40 ng L^{-1}), high extraction recoveries (69–83%) and enrichment factors (1380–1660), and good repeatability (relative standard deviations equal or less than 7.1% for intra– and inter day precisions) were acquired. Finally, the offered method was employed for the determination of the studied pesticides in various fruit juices and cypermethrin was detected in one apple juice sample.

Keywords: Magnetic dispersive solid phase extraction, Dispersive liquid–liquid microextraction, Fruit juice, Gas chromatography–mass spectrometry

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Functionalized silica particles by MPTS as a novel sorbent for microextraction in packed syringe of Pb(II) ions prior to determination by graphite furnace atomic absorption spectroscopy

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Lead ion is considered one of the toxic heavy metals and is concentrated in aquatic ecosystems and poses a serious hazard to human health, even at trace levels [1]. Numerous diseases are related to Pb(II), such as respiratory, anemia, cardiovascular and endocrine systems[2]. The maximum allowable level of lead in drinking waters by the US Environmental Protection Agency (EPA) and the European Union (EU) are respectively 15 ppb and 10 ppb. So, the determination of Pb(II) in water sources is necessary. Owing to the low concentration of Pb(II) in real samples and complex matrices, a preconcentration and purification step is necessary before instrumental detection. Various methods have been used for the extraction and preconcentration of Pb(II). Microextraction in a packed syringe (MEPS) is a new technique for miniaturized SPE that was introduced by Abdel-Rehim in 2004 [3]. This method's advantages include high extraction efficiency, low consumption of organic solvents, and convenience of operation. Generally, sorbent plays an important role in selectivity and sensitivity. In this study, the silica particles were modified with 3-Mercaptopropyltrimethoxysilan (MPTS) as a sorbent for microextraction in a packed syringe (MEPS) of Pb(II) from aqueous solutions. The lead ions were eluted using 500 µL HCl 0.5 M and analyzed via graphite furnace atomic absorption spectroscopy. Scanning electron microscopy (SEM), Fourier transform infrared spectroscopy (FT-IR) and X-ray energy diffraction (EDX) spectroscopy methods were used to characterize the obtained sorbent. Under optimal experimental conditions, the method had a linear range of 0.1–50 µg/L.

Keywords: Pb(II), Microextraction in packed syringe, Graphite furnace atomic absorption spectroscopy

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Fe (III) doped TiO_2 nanoparticles prepared by high energy ball milling as sensitive electrochemical sensor

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Paracetamol (PC) is a secure and effective analgesic drug that is applied to lessen pain, including muscular aches, headaches, post-surgical, arthritis, and joint pains. The recommended dosage of paracetamol exhibits no serious side effects, but overdose consumption of PC causes fatal liver harm via accumulation of toxic metabolites. Thus, an accurate and rapid analytical method is required for the determination of PC concentration in pharmaceutical and biological samples. Several different semiconductors like ZnO, Fe_2O_3, WO_3, SnO_2, CdS, CdSe, and SnO_2, but TiO_2 has shown remarkable performance compared with the other materials until now. TiO_2 is trusted as one of the most promising chemicals due to its non-toxicity, high oxidation efficiency, chemical inertness, and high photostability [1-4]. In this research work, pure and Fe (III) doped TiO_2 nanoparticles were prepared in order to fabricate a nano sensor for electrochemical sensing of paracetamol. TiO_2 nanoparticles were synthesized using a solvothermal method and doped with Fe (III) by mechanochemical planetary ball mill method. For structural and chemical characterization of the as-synthesized nanoparticles, techniques such as X-ray diffraction (XRD), energy dispersive X-ray (EDX), and transmission electron microscopy (TEM) were employed. The performance of the modified electrode was characterized with cyclic voltammetry, differential pulse-voltammetry techniques. The Fe (III)TiO_2/GCE modified electrode represents excellent electrocatalytic activity for paracetamol detection in phosphate buffer (pH=7) solution, with a considerable enhancing of the peak current and decrease of overvoltage in comparison with the bare GCE. The response of the nano sensor was linear over the paracetamol concentration range of 1.50–10.2 μM and 10.2–62 μM. The limit of detection (LOD) was calculated to be 0.52 μM. The advantages of this method include good sensitivity, selectivity, stability, reproducibility, fast response, wide linear range, low detection limit. This nano sensor was successfully used to determine paracetamol in pharmaceutical and biological samples.

Keywords: Titanium dioxide, Paracetamol, Doping, Cycle voltammetry, Differential pulse voltammetry

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Development of a magnetic dispersive solid phase extraction method combined with DES based AALLME for the extraction and preconcentration of phthalate esters from milk samples

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Today, food safety that can affect the quality of human life is the main priority of human societies [1]. Phthalate esters are extensively employed in food packaging and drink bottles to enhance flexibility and persistence of the polymeric materials [2]. Nevertheless, these chemicals can migrate into foods and drinks. The residue of these compounds can disrupt hormones and have negative effects on reproductive system [3]. Therefore, development of an easy, safe, selective, sensitive, fast, and green analytical method for the simultaneous extraction and determination of them in various foods and beverages is critical. In the present work, first, the proteins of milk samples were precipitated using zinc sulfate solution. After centrifugation, the supernatant phase was taken and mixed with urea–formaldehyde @ Fe composite (as sorbent). After sonication the mixture, the magnetic particles were separated in the presence of magnet and eluted using tetrabutylammonium bromide: menthol deep eutectic solvent (DES). Then, whole of the DES was taken and injected into 5 mL of deionized water. The mixture was aspirated into a glass syringe and dispersed to the tube for three times. During this step, the DES was decomposed and menthol was released as tiny droplets in whole of the sample solution. After centrifugation, 1 µL of the collected phase was taken and injected into gas chromatography–mass spectrometry. Under optimal conditions, the method was linear within the range of 0.16–1000 ng mL^{-1}. The limits of detection, intra– and inter–day relative standard deviations, and extraction recoveries were in the ranges of 0.05–0.19 ng mL^{-1}, 3.1–6.0%, 4.4–7.5%, and 80–91%, respectively. Lastly, the suggested procedure was used for the quantification of the opted analytes in twenty–one milk samples marketed in Tabriz, Iran.

Keywords: Magnetic dispersive solid phase extraction, Air assisted liquid–liquid microextraction, Milk, Gas chromatography–mass spectrometry

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Experimental and density functional theoretical modeling of pesticides extraction by Mxene as a DSPE sorbent before HPLC-MS/MS analysis

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In this research, a convenient, fast, and green dispersive solid phase extraction procedure based on Mxene nanosheets was developed for effective enrichment of some triazole pesticides prior to high performance liquid chromatography-tandem mass spectrometry. The pesticide residues in food products are becoming an increasingly hot topic with new information that pesticides can disturb the immune system and endocrine at lower-than-expected concentrations [1, 2]. Characterization of the etching sorbent was carried out in detail. Adsorption and desorption steps have been optimized in detail to obtain efficient phase separation and reliable analytical results. Under optimized conditions, the presented method exhibited a wide working range (0.52-1000 ng mL^{-1}), low detection limits (0.03-0.3 ng mL^{-1}) and acceptable extraction recoveries (70-75%). The precision of the method was evaluated by intraday and interday studies for three different concentrations of triazole pesticides. The matrix effect was investigated by the recovery study. Following validation studies, the presented method was successfully applied to the extraction and determination of the studied triazole pesticides from fruit juice samples. The adsorption mechanism was supported by theoretical studies. The interactions between the studied pesticides and Ti2C nanosheets were investigated with the help of density functional theoretical calculations. The calculations supported the obtained experimental results.

Keywords: MXene, Dispersive solid phase extraction, Liquid chromatography-tandem mass spectrometry, Pesticides; Theoretical studies

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Development of a pH-induced dispersive solid phase extraction method with dispersive liquid-liquid microextraction; Application in the extraction of Cu(II) and Pb(II) ions from water and fruit juice samples

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Heavy metals are introduced in environment and organisms via natural origin and human activity [1]. Heavy metals are not eco-friendly and because of their accumulation in living tissues, they can cause serious disorders and diseases [2,3]. Therefore water and food pollution with heavy metals is of extraordinary concern nowadays. In this study, a new pH-induced dispersive solid phase extraction method has been proposed for the extraction of Cu(II) and Pb(II) ions from water and fruit juice samples. The effect of important parameters on the extraction efficiency of the method such as pH, folic acid amount, the amount of complexing agent, dimethylformamide volume, ionic strength, and centrifugation conditions were studied.Under optimized conditions, the developed method showed linear ranges of 0.20-40 and 0.25-40 µg L-1 for Pb(II) and Cu(II) ions, respectively. Limits of detection of Pb(II) and Cu(II) were 0.07 and 0.08 µg L-1, respectively. The relative standard deviations (intra- and inter-day precisions)were between 3.8 and 5.4%. Efficiency of the proposed procedure was evaluated by analyzing Pb(II) and Cu(II) ions in various water and fruit juice samples. The proposed procedure was sensitive, efficient, easy to use, reliable, and rapid for the extraction of the selected metallic ions from aqueous samples. Besides the analysis of one certified reference material and several water and fruit juice samples indicated that the suggested procedure provided precise and accurate results.

Keywords: Dispersive liquid-liquid microextraction, Heavy metal ions, Flame atomic absorption spectrometry

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Improving the antimicrobial activity of Apigenin loaded into shellac nanoparticles

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In this study, we constructed a natural nanocarrier consists of shellac as drug delivery system for improving the therapeutic index of antimicrobial drugs loaded on it. The purpose of this research is to enhance the antimicrobial activity of apigenin by loading on shellac nanocarrier. The nano-shellac particles were prepared by steric repulsion effect using poloxamer188 surfactant accomplished with reducing the pH to 5. To improve their adherence to the surface of microorganisms. The DLS results showed that the size of nano-shellac was (50.82) nm, with zeta potential of (-6.28) mV at 0.2 wt% shellac with 0.15wt% polymerase 188 at pH5. The nano-shellac loaded apigenin had average sizes of (77.23) nm with zeta potential of (-10.7) mV. The encapsulation efficiency of 0.03 wt.% of apigenin was (98.33%) with drug loading (9.33%). FESEM test showed that shellac nanocarrier has spherical shape. Fourier FTIR and UV-Vis spectroscopy techniques were used to prove the apigenin loading on the shellac nanoparticles. the nanocarriers were coated with CTAB to convert the charge. The biological activity of apigenin loaded shellac nanoparticles was detected against E. coli, and Staphylococcus aureus, as well as the anticancer activity was studied on A375 melanoma cells [1,2].

Keywords: Shellac, Poloxamer 188, Apigenin, DDS, Nanoparticles

Microgram use of MOF-70 in a developed adsorbent-based analytical method for the preconcentration and extraction of pesticides from fruit juices

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Detection and quantitative determination of pesticides in beverages are of great importance [1]. Conducting this deed requires sample preparation methods inevitably [2]. The application of metal organic frameworks in this field can be so promising due to their inherently beneficial properties [3]. In the present research, a sample preparation method called dispersive micro solid phase extraction followed by dispersive liquid-liquid microextraction was developed based on MOF-70 as a highly efficient adsorbent for the extraction of seven pesticides including chlorpyrifos, haloxyfop-R-methyl, oxadiazon, diniconazole, clodinafop-propargyl, fenpropathrin, and fenoxaprop-P-ethyl from various fruit beverages (orange, pineapple, pomegranate, grape, and cherry beverages). In the first step, the pesticides are loaded on the MOF particles from the sample solution by vortexing and then settled down by centrifugation. Then, they are desorbed by acetonitrile from the MOF surface. In the next step, the obtained acetonitrile phase is mixed with µL-level of 1,1,1-trichloroethane and injected into deionized water. After the final centrifugation, the sedimented phase is collected and an aliquot of the obtained phase is injected into a gas chromatograph equipped with a flame ionization detector. MOF-70 is carefully synthesized and characterized using X-ray diffraction, Fourier transform infrared spectrophotometry, scanning electron microscopy, energy dispersive X-ray, and nitrogen adsorption/desorption analysis. After optimization of the process, satisfactory figures of merit were obtained such as high extraction recoveries (35-96%) and enrichment factors (175-480), low relative standard deviations (4.5-8.5%), wide linear ranges, and low limits of detection (0.20-0.76 µg L^{-1}) and quantification (0.65-2.47 µg L^{-1}). The developed approach can be introduced as a highly efficient analytical method based on MOF-70 for the analysis of various pesticides in juice samples.

Keywords: Metal organic framework, Gas chromatography, Fruit beverage, Diffusion-based synthesis, Pesticide analysis

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Application of MIL-68 (Al)-based dispersive micro solid phase extraction method followed by dispersive liquid-liquid microextraction for the detection and determination of plasticizers

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Quantitative determination of plasticizers in beverages stored in plastic-packed containers is of great importance due to the various illnesses they result in [1]. The accomplishment of this action needs sample preparation due to the matrix complexity of real samples [2]. The application of metal organic frameworks in this field can be so promising due to their inherently beneficial properties [3]. The current study aims at extraction and preconcentration of some plasticizers including dimethyl phthalate, diethyl phthalate, di-*iso*-butyl phthalate, di-*n*-butyl phthalate, di (2-ethylhexyl) adipate, and di-*iso*-octyl phthalate migrated into different samples (mineral water, injection serum, orange juice, and carbonated soft drink) using MIL-68 (Al) in a dispersive micro solid phase extraction method prior to dispersive liquid-liquid microextraction. The sorbent was characterized using X-ray diffraction, Fourier transform infrared spectrophotometry, nitrogen adsorption/desorption, scanning electron microscopy, and energy dispersive X-ray analyses. At first, the analytes are adsorbed on MIL-68 (Al) from a solution having dissolved Na_2SO_4. Then, the sorbent particles are separated from the aqueous medium by centrifugation. Methanol is utilized as an elution solvent to desorb the plasticizers from the sorbent. Then, the eluent is mixed with carbon tetrachloride at µL-level and injected into an aqueous solution containing dissolved Na_2SO_4. The obtained cloudy solution is centrifuged and an adequate of the sedimented extractant is injected into the gas chromatograph equipped with a flame ionization detector. Satisfying figures of merit including high extraction recoveries (50-93%) and enrichment factors (251-466), wide linear ranges of the calibration curves, and low limits of detection (0.63-1.86 µg L^{-1}) and quantification (2.08-6.14 µg L^{-1}) were achieved in the present approach. Also, a little amount consumption of the sorbent and organic solvents were the highlights of the developed method.

Keywords: MIL-68 (Al), Dispersive liquid-liquid microextraction, Dispersive micro solid phase extraction, Plasticizers

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Introduction of a sample preparation procedure using MIL–53 (Fe) for the extraction of pesticides from different fruit juices

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Detection and quantitative determination of pesticides in beverages are of great importance [1]. Conducting this deed requires sample preparation methods inevitably [2]. The application of metal organic frameworks in this field can be so promising due to their inherently beneficial properties [3]. For the first time, this research aims to develop a MIL–53 (Fe)–based dispersive micro solid phase extraction method prior to dispersive liquid–liquid microextraction for the extraction and preconcentration of some pesticides and their analysis using a gas chromatography–flame ionization detector. For performing the extraction procedure, MIL–53 (Fe) was added to an aqueous solution containing the analytes and vortexed to be dispersed in the solution and adsorb the analytes. After centrifugation, the analytes loaded on the adsorbent were eluted using acetonitrile. Then, µL–level of carbon tetrachloride, as an extractant, was mixed with the obtained acetonitrile phase and injected into deionized water. One microliter of the sedimented phase after centrifugation was injected into the separation system. Satisfactory analytical results such as wide linear ranges, high enrichment factors (250–380), reasonable extraction recoveries (50–76%), and low limits of detection (0.63–2.05 µg L^{-1}) and quantification (2.11–6.83 µg L^{-1}) were obtained. Using only 5.0 mg MIL–53 (Fe) as the sorbent, 0.5 mL acetonitrile as the elution/disperser solvent, and 40 µL carbon tetrachloride as the extractant makes the analytical approach so precious. Also, using a green metal, iron, as the central ion of the metal organic framework is another beneficial aspect of the research.

Keywords: Metal organic framework, Gas chromatography, Fruit beverage, MIL-53 (Fe), Pesticide analysis

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Development of an extraction method based on UiO-66 for the detection and determination of some pesticides in juice samples using GC-FID

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The presence of pesticides in juice samples is dangerous. On average, about 14000 tons of agricultural pesticides are annually used in Iran. Herbicides constituted the largest volume (43%), followed by insecticides and acaricides (37%) and fungicides (19%) [1]. Thus, controlling the pesticide content of fruit-based beverages seems to be of great importance [2]. Performing this requires sample preparation methods [3]. The application of metal organic frameworks in this field has been seen to be influential [4]. The proposed analytical method tries to illustrate a new approach for the extraction of some pesticides from different fruit beverages (orange, pineapple, cherry, and mango) using UiO-66 as a capable adsorbent. Further preconcentration for heightening enrichment factors of the analytes was accomplished using a dispersive liquid-liquid microextraction. The synthesized adsorbent was carefully characterized using nitrogen adsorption/desorption, X-ray diffraction, MAP, Fourier transform infrared spectrophotometry, energy dispersive X-ray, and scanning electron microscopy analyses. The performed analyses proved the successful formation of the desired compound. After the sorption of the target compounds onto UiO-66 particles by vortexing, the adsorbent was separated by centrifugation. The analyte-loaded adsorbent was treated with 1.0 mL of acetonitrile for the aim of desorption. The obtained eluate containing the desorbed pesticides was mixed with 38 µL of 1,1,1-trichloroethane and hastily injected into sodium chloride solution. After the centrifugation, an aliquot of the sedimented phase was injected into a gas chromatograph equipped with a flame ionization detector. Satisfactory figures of merit obtained in this survey consisted of high enrichment factors (215-275), acceptable extraction recoveries (43-55%), low limits of detection (1.10-2.35 µg L^{-1}) and quantification (3.66-7.82 µg L^{-1}), low relative standard deviations (≤ 7.8%), and wide linear ranges. Also, the proposed method benefits from the high surface area of the adsorbent and low matrix effect.

Keywords: UiO-66, Gas chromatography, Fruit beverage, Adsorbent, Pesticide analysis

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Synthesis of a magnetic sorbent; application in the extraction of Cu (II) and Pb (II) ions from milk performed in a narrow-bore tube

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According to the Environmental Protection Agency (EPA) guidlines, lead and copper are among the most common heavy metals pollutants [1] and can have detrimental effects on human health even at trace levels [2]. In the present work, an efficient magnetic sorbent has been prepared and used in dispersive solid phase extraction of Cu(II) and Pb(II) from high volume of milk samples performed in a narrow-bore tube.The purpos of this study was to develop an environmentally friendly extraction method based on magnetic solid phase extraction performed in a narrow-bore tube coupled with FAAS for the extraction, preconcentration, and determination of Pb(II) and Cu(II) in milk samples. The important parameters such as the sorbent amount, type and volume of elution and extraction solvents, vortex time, pH, and ionic strength were studied. Under optimized conditions, the proposed method showed linear ranges of 0.50-40 and 0.75-40 μg L^{-1} for Cu(II) and Pb(II) ions, respectively. Limits of detection were obtained 0.16 and 0.22 μg L^{-1} for Cu(II) and Pb(II), respectively. Enrichment factors of 182.5 and 173.7 and extraction recoveries of 95.8 and 91.2% were obtained for Cu(II) and Pb(II), respectively. The relative standard deviations (intra- and inter-day precisions) for 5 and 25 μg L^{-1} of each cation were between 2.4 and 4.3%.

Keywords: Magnetic solid phase extraction; Dispersive liquid-liquid microextraction; Milk; Flame atomic absorption spectrometry

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Magnetic solid phase extraction of Ni(II) with Fe_3O_4@ Diaion HP-2MG particles as the adsorbents prior to flame atomic absorption spectrometry

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Heavy metal pollution increasing due to human activities and especially the problems experienced in trace level detection are increasing gradually. While heavy metals negatively affect the soil, food and water ecosystem, they also accumulate in the body through the air, skin or digestive system [1]. Nickel is an essential element for human metabolism, but high nickel intake is toxic. Therefore, the analysis of Ni(II) especially in complex matrices is important. Accelerating technological developments, even if analytical devices that can perform heavy metal analysis such as FAAS, ICP-MS and X-Ray fluorescence spectroscopy have been developed, they often do not allow analysis later because they are less sensitive than the detector can detect in the analysis of trace species. For this purpose, separation-enrichment methods are needed. Magnetic solid phase extraction method has been developed due to its high enrichment factor, low cost, low reagent consumption, ease of automation and environmental friendly features [2]. In this study, magnetic Diaion HP-2MG resin was synthesized for rapid extraction, enrichment and determination of trace amounts of Ni(II) ions. Diaion HP-2MG polymer with polymethacrylate matrix is relatively hydrophilic. Among the parameters affecting the Ni(II) extraction efficiency, pH, resin amount, matrix effect, sample volume, eluent type and volume were optimized and analyzes were performed in the FAAS device after pre-concentration [3]. After optimizing the analytical parameters such as LOD, LOQ, PF and reusability, the accuracy of the developed method was applied to natural water and food samples by adding-recovering increasing Ni(II) and validation was carried out with water and food certified reference material analyzes with known Ni(II) content.

Keywords: Nickel, Diaion HP-2MG, Magnetic solid phase microextraction, Separation-preconcentration, FAAS

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Determination of trace amount of As(V) in water samples based on a new Liquid phase microextraction and molybdenum blue method

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The importance of measuring As species has been appreciated for a long time because the toxicity of As varies depending on its redox state and its chemical form [1,2]. In this work, a green extraction method was developed for determination of trace amount of As(V) in various water samples. This method is based on the formation of β-molybdoarsenate blue complex followed by cetyltrimethylammonium bromide (CTAB) based microextraction. The analysis of final extraction phase was done using spectrophotometric measurement at $\lambda_{max} = 810$ nm. The effects of different parameters on the micrextraction and the complex formation were investigated and optimized. Under optimized conditions, the linear range was obtained 10-90 μg L^{-1} with a correlation coefficient of 0.997 and limit of detection (LOD) was 0.17 μg L^{-1}. Relative standard deviations for determination of 10 and 50 μg L^{-1} As(V) were obtained 2.1 and 3.9% for six replicates, respectively. The proposed method was successfully applied for determination of As(V) in various water samples with satisfactory recovery ranged from 89 to 95% .

Keywords: As(V), Cetyltrimethylammonium bromide, Molybdenum blue method, Aqueous samples

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Preconcentration of As(III) by chitosan graphene quantum dots via microextraction in packed syringe followed by quantitation through graphite furnace atomic absorption spectrometry

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Arsenic contamination is a leading environmental problem. thus, levels of this toxic metalloid must be constantly monitored by reliable and low-cost methodologies[1]. Arsenic contamination can cause serious health problems; including cardiovascular disease, type II diabetes, canser of skin, lung and kidney. Arsenic affects human health through drinking water or eating foodstuffs, so the link between arsenic and our health is not only limited to scientific research but also have been turned into a worldwide critical public concern [2]. Existing methods for analysis of As (III) including various spectroscopic, ICP and electrochemical teqniques [3]. Such as electrothermal atomic absorption spectrometry (ETAAS) [4] chromatographic separation coupled with ICP-MS [5]. Because the currently accepted upper limit for arsenic in water is 10 ppb, very sensitive and selective detection strategies must be developed[1]. In this study, chitosan graphene quantum dots is synthesized as packed sorbent in syringe for microextraction of As(III) in water and real samples. As(III) ions are adsorbed on chitosan graphene quantum dots because of the functional groups on chitosan and very small absorbent particles. The analyte ions were eluted using acid and analyzed via graphite furnace atomic absorption spectroscopy. The prepared sorbent was characterized using X-ray diffraction (XRD), scanning electron microscopy (SEM) and Fourier transform infrared (FT-IR) techniques. Several factors that may affect the preconcentration and extraction process, including sample pH, sorbent amount, number of sample loading times and number of desorption times were optimized.

Keywords: Chitosan graphene quantum dots, As(III), Preconcentration , Graphite furnace atomic absorption spectrometry

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Electrochemical study of orthotolidine and its use in electrosynthesis of new derivatives

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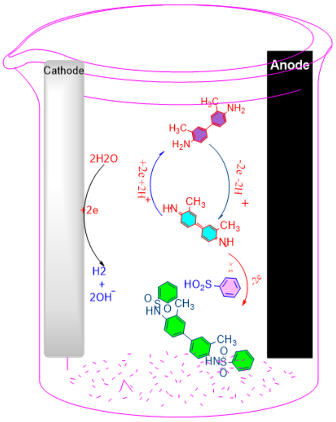
Electrochemical redox reactions produce high reactive intermediates, such as: anions, cations, radical ions, radicals and nucleophilic as well as electrophilic groups. In this work, the pH dependent anodic behavior of 3,3'-Dimethylbenzidine (OTD) was investigated. Our data shows that the E_{pA}–pH diagram indicates the presence of three predominant regions. The predominant species across all regions were identified. Furthermore, the electrochemical oxidation of orthotolidine in the presence of 4-methylbenzenesulfinate as a nucleophile has been investigated. The controllable electron transfer process causes to change the electron-poor and electrophilic character of a functional group to be nucleophilic or vice versa. The synthesis of this compound was performed by anodic oxidation of 3,3'-Dimethylbenzidine (OTD) in the presence of benzenesulfinic acid (BSA) in aqueous acetate buffer solution, using a carbon electrode. The cyclic voltammogram of OTD shows an reversible anodic peak corresponding to two-electron oxidation of OTD, while, the CV of the mixture of OTD and BSA two anodic irreversible peak which is a confirmation of the reaction between electrogenerated OTD_{ox} and BSA. Based on the electrochemical evidence, The synthesis of the desired derivative was conducted in aqueous buffer (pH =1.0, $HClO_4$ c = 0.1 M), by controlled potential method (at 0.57 V vs. Ag/AgCl electrode), under green conditions. Product formation was confirmed by using IR, MS and NMR spectra.

Keywords: Electrochemical oxidation, Orthotolidine, Electrosynthesis, Benzenesulfinic



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Characterizing rGO@ZIF-67 Nano-MOF as an Enhanced Visible Light-Harvesting and Fast Charge Carrier Separation for Effective Surface Photoreaction on Photodegradation of Methylene Blue

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Engineering of advanced highly efficient and stable photocatalysts for solving environmental pollution is desired. In fact, the driving force that directly enlarges the light-absorption and harvesting area, facilitates the adsorption of pollutant molecules on the photocatalyst surface, and transfers and separates electron-hole pairs are the most significant factors in the synthesis heterostructure of the photocatalysts [1-3]. In this regard, first, the rGO@ZIF-67 was synthesized and characterized by different characterization methods, including SEM, BET, TEM, XPS, and DRS analyses. Afterward, the photocatalytic activity of the as-prepared rGO@ZIF-67 was evaluated for methylene blue photodegradation. The factors affecting the degradation yield, for instance, pH, ionic strength, type of buffer, irradiation time, and amount of photocatalyst were optimized. After optimized experimental conditions, the results showed a high degradation yield of 99.5%. The cycling stability of the as-prepared rGO@ZIF-67 was also evaluated as one of the most important features of a catalyst, revealing that the photodegradation yield was slightly reduced after 4 cycles and reached 85%, showing high stability of the as-prepared photocatalyst. Also, the photocatalytic degradation of methylene blue was tested in real samples such as drinking and river waters.

Keywords: Photocatalyst, rGO@ZIF-67, Light-absorption, Electron-hole pairs, Methylene blue.

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Column solid phase extraction and determination of trace amounts of chromium by modified zeolite

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With the development of the chemical industry, various toxic pollutants are released into the environment that endanger the health of humans and other organisms. Chromium is one of the most widely used heavy metal which is created from industries such as metal working and tanning leather, etc [1-3]. In this research, a column solid-phase extraction using SDS modified zeolite was used for the preconcentration and separation of trace amount of chromium before determination with flame atomic absorption spectrophotometry. For this purpose, several parameters such as modifier dose, adsorbent amount, preconcentration time, sample flow as well as the nature and amount of releasing agent were optimized. Moreover, the effect of other cations and anions was studied on the recovery and selectivity of purposed method. The obtained results showed that SDS-modified zeolite as a very cheap adsorbent can be used for selective separation of chromium with high pre-concentration coefficient in very short time. The proposed method was successfully used for the determination of chromium in different water samples.

Keywords: Determination, Chromium, Solid-phase extraction, Zeolite, Flame atomic absorption

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Hydrophobic thymol-based natural deep eutectic solvents as a green extraction media for air-assisted homogeneous liquid-liquid micro-extraction of phenol and di hydroxyl benzens

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Phenolic compounds are pollutants present in wastewater from different kinds of industries, including oil refineries, coke plants, plastics, leather, chemical, paint and pharmaceutical industries [1,2]. In this study, a green sample preparation method using a Natural deep eutectic solvent-based Air assissted homogeneous liquid-liquid microextraction (NADES-AA-HLLME) followed by HPLC-UV was developed for preconcentration and determination of phenol and di hydroxyl benzens in aqueous environmental samples. This new method is performed by using THY as a hydrogen bond acceptor with six medium-chain fatty acids (C6, C7, C8, C9, C10, and C12) as the hydrogen bond donors and optimized by experimental design applying response surface methodology (RSM) to check the optimal conditions of both HPLC separation and extraction. The method was successfully applied to three different types of real surface water samples. Without toxic volatile organic solvents, the developed method allows for safe and rapid and reliable analysis of phenolic compounds. Under optimum conditions, calibration graphs of target analytes were found to be linear in the concentration of range of 1-300 µg. L^{-1} with correlation coefficients (r^2) of more than 0.9990.

Keywords: Deep eutectic solvent, Homogeneous liquid-liquid microextraction, Air assissted, Response surface methodology (RSM)

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In-syringe dispersive micro-solid phase extraction method for the HPLC-UV determination of dopamine, epinephrine and norepinephrine

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Catecholamines dopamine, norepinephrine and epinephrine serve as the most important neurotransmitters in the central and peripheral nervous systems [1]. Several psychiatric, neurological and cardiovascular diseases are associated with dopamine, epinephrine and serotonin levels and their concentrations in plasma are often useful for diagnosis and monitoring of therapeutic and pharmacodynamics effects. [2,3]. In presented work, dispersive micro solid phase extraction (DMSPE) was applied. In DMSPE in order to extract target analytes, the defined amount of solid sorbent is dispersed in the aqueous sample solution by ultrasound energy, a magnetic stirrer or a vortex device. In the following, for detection analytes high performance liquid chromatography (HPLC-UV) was used. For the sensitive and selective extraction and determination of target analytes, MNPs have been combined with the syringe–to–syringe magnetic solid–phase microextraction (SS–MSPME) method. The sorbent was characterized using fourier transform-infrared (FT-IR) spectroscopy, scanning electron microscopy (SEM) and energy dispersive X-ray (EDX). Various parameters affecting the extraction efficiency such as pH, ionic strength of sample solution, amount of sorbent (mg), volume of eluent solvent (µl), adsorption and desorption time (min) were optimized. Under optimum conditions, calibration graphs of target analytes were found to be linear in the concentration of range of 0.5-300 µg. L^{-1} with correlation coefficients (r^2) of more than 0.9990.

Keywords: Dispersive micro solid phase extraction, Syringe–to–syringe, HPLC-UV

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Fabrication of a magnetic dual-template molecularly imprinted polymer based on modified magnetic graphene oxide

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In this article, a new dual template molecularly imprinted polymer(DT-MIP) based on modified magnetic graphene oxide was synthesized and employed for the determination of organic compounds by a dispersive micro-solid phase extraction (DMSPE) method. The imprinted layer was introduced on the surface of a core–shell magnetic modified graphene oxide as a substrate. Molecularly imprinted polymers (MIPs) with predictable structures, specific recognition abilities and universal applications have become attractive adsorbents and have been widely applied in sample pretreatment and chromatographic separation to specifically extract the template molecules from complex matrices [1-4]. The sorbent was characterized by Fourier transform infrared (FTIR) spectroscopy, scanning electron microscopy (SEM), vibrating sample magnetometry (VSM), X-ray powder diffraction (XRD), energy dispersive X-ray (EDX) and methods. The effects of various parameters such as the pH, ionic strength of the sample solution, amount of sorbent (mg), volume of eluent solvent (mL), vortex time, and ultrasound time (min) were optimized by a Box–Behnken design. Under optimum conditions, the calibration graph of the analyte was linear in the concentration range of 1–300 µg L^{-1}, with a correlation of determination (r^2) of 0.9927. The limit of detection and quantification were 0.2 and 0.66 µg L^{-1}, respectively. This procedure was successfully applied to the determination of the analyte in a real sample and spiked real sample followed by high performance liquid chromatography (HPLC) analysis. The relative mean recoveries ranged from 95 to 104%.

Keywords: Extraction, HPLC-UV, DT-MIP, Box–Behnken design

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Electrochemical Study of Azoxybenzene and its Application in the Electrosynthesis of New Azoxybenzene Derivatives

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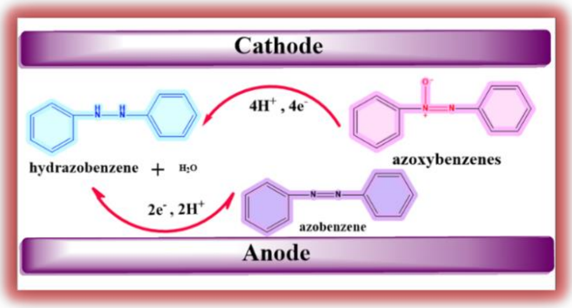
Organic compounds with a nitrogen-containing functional group play an exceptional role in natural and technological processes. In particular, such compounds are highly useful for medicinal purposes, dyes, pesticides, explosives, etc. The great theoretical and practical importance of these compounds has stimulated the study of the chemical properties of nitrogen-containing functional groups. Among organic nitrogen compounds, Azoxybenzenes (AZB) occupy a special place. As a result of their high thermal and chemical stabilities, all the compounds containing a nitrogen atom attached to the benzene ring can be ultimately converted into AZBs via oxidation or reduction reactions [1]. AZBs are widely applied in pharmaceuticals, oxidants, polymer inhibitors, and stabilizers. In light of their importance, the development of AZB derivatives has become a hot topic for a long time. Therefore according to the mentioned features, the electrochemical behavior of AZB at a glassy carbon electrode in the different aqueous buffered solutions was studied via cyclic voltammetry (CV), chronoamperometry, and chronopotentiometry techniques. The CV of AZB showed that azoxybenzene undergoes an irreversible 4e/4H+ reduction reaction and converts to Hydrazobenzene (HYB), which then undergoes a reversible $2e/2H^+$ oxidation reaction to generate azobenzene [2]. In this regard, Differential pulse voltammetry (DPV) was used to determine the number of transferred electrons. For more data, the diffusion coefficient of AZB was obtained using the chronoamperometry method. In the last decades, electrosynthesis has been known as a green and powerful tool for developing environmentally friendly synthetic processes [3]. In this work, we have also synthesized the new AZB derivative by reduction of AZB in the presence of Benzenesulfinic acid (BSA) in an aqueous buffered solution (pH = 2.0, C = 0.2 M H3PO4) via the controlled potential electrolysis (-0.78 V vs. Ag/AgCl electrode) under green conditions and with three plate graphite electrodes. The isolated products were identified and characterized via ^{1}HNMR, ^{13}CNMR, and FTIR spectra.



Keywords: Azoxybenzene, Azobenzene, Electrochemical reduction

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Removal of Crystal violet from wastewater by magnetic HKUST-1 metal-organic framework

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Dye in industrial wastewater is one of the most serious environmental concerns due to its potentially harmful effects on human health [1]. Many industrial dyes are carcinogenic, toxic, and teratogenic. Removal and recovery of hazardous dye from the effluent requires an efficient adsorbent [2]. This study surveys the removal of Crystal violet dye using magnetic metal-organic framework adsorbent, $MgFe_2O_4$-HKUST-1. This magnetic adsorbent was synthesized at room temperature. The Fourier transform infrared spectroscopy (FTIR) and X-ray powder diffraction (XRD) were used to characterize the prepared adsorbent. The effect of different parameters such as pH (3-10), contact time (0-25 min), and adsorbent dosage (0.001-0.0055 g/l) on the removal of dye was investigated. The optimized values were found to be: pH=5, contact time 5 min and adsorbent dosage 0.0055 g at room temperature. The removal efficiency of the adsorbent was studied by determining of dye concentration at a wavelength of 590 nm. The results showed maximum removal of dye (76.58%) in dye concentration of 5.30 mg/l at 5 min. The adsorption equilibrium isotherm and kinetic model were plotted and results showed that the adsorption process is consistent with the Langmuir model and follows the pseudo-second-order adsorption kinetics. This study shows that magnetic composite $MgFe_2O_4$-HKUST-1 has good potential for removal of Crystal violet dye from water in a short time and it is easily separated from the solution by a magnetic field due to its magnetic property.

Keywords: Crystal violet, HKUST-1, Magnetic metal-organic framework, Removal

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Determination of Vancomycin in Plasma Samples Using Magnetic Solid-Phase Extraction Coupled to Liquid Chromatography-Tandem Mass Spectrometry

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Vancomycin is an antibiotic of the glycopeptide class. This antibiotic has a broad spectrum of action against gram-positive and anaerobic bacteria. Adequate serum vancomycin concentration is between 5 and 10 mg/L. Higher levels are toxic, which mainly cause kidney toxicity and threaten the health of the body [1]. Concerns about health and the rational and controlled use of antibiotics are essential to minimizing antibiotic resistance. As a result, it is important to set up a sensitive analytical method for measuring antibiotics to monitor the patient's required dose [2]. Hence, in the present work, the magnetic solid phase extraction-liquied chromatography-tandem mass method is developed to determine vancomycin in human plasma as a quick and easy-to-use method to achieve the plasma concentrations of vancomycin. The present study was devoted to synthesizing Fe_3O_4/SiO_2 nanocomposites via silica nanoparticles obtained from rice husk waste and then its functionalization using amines to obtain Fe_3O_4/ SiO_2-NH_2 as a new sorbent by improving selectivity in vancomycin sorption. The structure and morphology of the synthesized sorbent were characterized by X-ray diffraction, scanning electron microscopy, and Fourier transform infrared spectroscopy. Some important parameters affecting the extraction of the vancomycin were optimized. Under the optimized experimental conditions, the method provided a linear range of 5 to 250 ng/mL with the correlation coefficients (R^2) of 0.995. The intra-day (n = 3) and inter-day precisions (n = 3 working days) calculated in the form of percent relative standard deviations (%RSDs) were below 5%. The proposed method was successfully practiced for the analysis of vancomycin in several human plasma samples, with recoveries in the range of 97.0–102.5% for the spiked samples.

Keywords: Magnetic solid phase microextraction, Liquid Chromatography, Mass spectrometry, Vancomycin

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Determination of vitamins B1 and B6 in infant formula and food supplement samples using magnetic Mg/Fe layered double hydroxide nanoadsorbent before liquid chromatography-tandem mass spectrometry

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Water-soluble vitamins primarily belong to the vitamin B complex group, essential nutrients in foods, especially infant formulas. These vitamins have been engaged in metabolic pathways and show significant health benefits when added to our daily diet [1]. According to the Food and Drug Administration (FDA) and food and supplement manufacturers, there are daily nutritional requirements for these vitamins, so quantitatively assaying the vitamin amount in such products is necessary. However, simultaneous measurement of these two vitamins in food is complicated due to the complexity of the sample environment and the small concentration of vitamins [2]. A magnetic Mg/Fe layered double hydroxide (magnetic LDH) nanocomposite was successfully prepared and used as a suitable adsorbent to simultaneously extract vitamins B1 and B6 from complex infant formula and food supplements. As-prepared nanoadsorbent was successfully in magnetic solid phase extraction setup with no hazardous solvents and extraction performed in 6 min. The structure of nanoadsorbnet is lamellar, providing a wide surface to extract the analytes. The quantification of the analytes was accomplished using the liquid chromatography-tandem mass (LC/MS-MS) technique. Under optimum extraction conditions, the linearity ranged from 4 to 1000 ng/mL (vitamin B1) and 20 to 1000 ng/mL (vitamin B6), and the correlation coefficients (R^2) was better than 0.999. The intra-day ($n = 3$) and inter-day precisions ($n = 3$ working days) calculated in the form of percent relative standard deviations (%RSDs) were below 7%. The proposed method was successfully practiced for the analysis of vitamins B1 and B6 in several brands of infant formulas and food supplements.

Keywords: Magnetic solid phase microextraction, Mg/Fe layered double hydroxide, Pyridoxine (vitamin B6), Thiamin (vitamin B1)

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Application of magnetic functionalized carbide in effervesces-assisted DSPE combined with DLLME for several pesticides extraction from fruit juice

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In the present study, magnetic benzamide coated carbide composite was synthesized, characterized and used in a dispersive solid phase extraction (DSPE) procedure. The designed method was used for extraction of 12 mostly used pesticides from fruit juice samples. The extracted pesticides were analysed by gas chromatography-mass spectrometry (GC-MS). As per the knowledge of the authors, no work has been reported on the functionalized carbid sorbents. In recent years, carbid-based nanomaterials have been recognized as a rising star in chemistry due to their outstanding properties [1-3]. In this approach, an effervescent tablet was prepared by pressing mixture of tartaric acid, sodium bicarbonate and the synthesized sorbent. Then the tablet was released into the sample solution and the produced carbon dioxide bubbles were used for dispersion of the sorbent particles into the solution. After extraction, the sorbent was collected by an external magnet. The procedure was followed by dispersive liquid-liquid microextraction (DLLME) to achieve low detection limits. The optimal conditions were obtained as follows: sorbent mass: 25 mg, 0.5 mL acetone as eluent; desorption time: 2 min; 22 µL carbon tetrachloride as extraction solvent and 2.5% w/v sodium chloride solution as aqueous phase in DLLME step. Under the optimal conditions, linear ranges of the method were obtained from 0.1 to 2000 ng mL^{-1}. The detection limits and precision of the method (expressed as relative standard deviations) were in the ranges of 0.02-0.21 ng mL-1 and 3.1-6.4%, respectively. Finally, the method was done on grape, apple, and orange juices. Chlorpyrifos and diniconazole were found in the grape juice at the concentrations of 3.9 ± 0.3 and 1.5 ± 0.1 ng mL^{-1}, respectively.

Keywords: Pesticides, Dispersive solid phase extraction, Gas chromatography-mass spectrometry, Silicon carbide, Dispersive liquid-liquid microextraction, Fruit juice

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Investigation of amino acid profiles for prostate cancer biomarkers using magnetic dispersive solid-phase extraction

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Prostate cancer is the second most common cancer in men and the fourth most common cancer. Prostate cancer is an invasive disease and usually manifests itself in the advanced stage of the disease [1]. The present study aimed to analyze the characteristics of metabolic amino acids as a biomarker identification strategy for early detection and screening of prostate cancer [2]. Biological samples are given to patients in the early and often asymptomatic stages of cancer. What is necessary is the changes observed in the amino acid profiles of these patients. Among several analytical methods, the LC-ESI-MS/MS is a promising tool. In this experimental study, we are dealing with complex biological samples, so a new extraction method of magnetic dispersive solid phase extraction (MDSPE) using layered double hydroxide (LDH) is used to purify and concentrate amino acids [3]. The synthetic magnetic adsorbent and the effective factors of the extraction method are investigated and optimized one by one. This study obtains and analyzes the free amino acid profiles in the plasma of prostate cancer patients and healthy men. Given the contradictory results in changing the amino acid profile in cancers and the high prevalence of prostate cancer in Iran, and the lack of an epidemiological study on plasma amino acid levels in patients with prostate cancer, this study could provide the basis for further studies. Under the optimized experimental conditions, the method provided a linear range of 1 to 500 ng/mL with the correlation coefficients (R^2) of 0.991. The intra-day ($n = 3$) and inter-day precisions ($n = 3$ working days) calculated in the form of percent relative standard deviations (%RSDs) were below 10%. The proposed method was successfully practiced for the analysis of vancomycin in several human plasma samples, with recoveries in the range of 96.0–107.5% for the spiked samples. Determination of amino acid properties using the non-invasive HPLC-Tandem MS method and the new MDSPE method help to easily separate amino acids from the complex medium and determine them rapidly.

Keywords: Amino acid, Biomarker, Magnetic dispersive solid phase extarction

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Development of air agitated dispersive solid-phase extraction in combination with dispersive liquid-liquid microextraction for pesticides extraction before GC-MS analysis

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In the present study, magnetic carbide was prepared using a simple procedure and utilized as an effective sorbent in magnetic dispersive solid phase extraction (DSPE) combined with dispersive liquid-liquid microextraction (DLLME). The developed method was used for extraction and preconcentration of diazinon, ametryn, chlorpyrifos, hexaconazole, diniconazole, tebuconazole, and triticonazole from the aqueous sample.Silicon carbid can be used in analytical chemistry potentially as an adsorbent in extraction methods [1-3]. Determination of extracted pesticides was carryover by gas chromatography-mass spectrometry (GC-MS). In this approach firstly, a few mg of the prepared nanocomposite was added into an aqueous solution containing the analytes and it was contacted with the sample solution by performing aspiration/dispersion cycles. After collection of the nanocomposite particles by an external magnet, the adsorbed analytes were eluted by a water-miscible organic solvent with the aid of vortex and used in the following DLLME step to achieve high sensitivity and enrichment factors. The optimized method was validated using the International Council Research protocol and the results showed a satisfactory linear range of 1.0-1000 ng mL^{-1} whit good precision and linearity ($r^2 \geq 0.992$) and low limits of detection (LOD: 0.06-0.3 ng mL^{-1}) and quantification (LOQ: 0.3-1.0 ng mL^{-1}), high enrichment factor (EF: 600-850), and acceptable extraction recovery (ER: 60-85%). The method was successfully done on different real samples and diazinon and chlorpyrifos were determined in some samples.

Keywords: Pesticide, Dispersive micro solid phase extraction, Gas chromatography, Silicon carbide, Dispersive liquid-liquid microextraction

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HPLC-MS/MS determination of Linagliptin and Empagliflozin after their extraction by LDH/N-doped carbon nitride composite from spiked plasma samples

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Empagliflozin and linaglyptin are new drugs in the treatment of type II diabetes that are used in combination with proper diet and activity to treat type II diabetes [1]. Low levels of linagliptin in biological samples are legal for pharmacokinetic studies and important in toxicology [2]. Therfore, in this research, liquid chromatography with quadrupole ionization source was used to identify and measure ampaglyflozine and linaglyptin in spiked plasma samples. For the preparation and extraction of the desired drugs from plasma tissue, the dispersive solid phase extraction method was used. The adsorbent used in the extraction method was composit of N-riched caron nitrid with layerd double hdroxide. The proposed method is fast, efficient, easy to operate and low detection limit. In this method, 2 mL of the prepared plasma sample was extracted with only 20 mg of adsorbent and after elution, it was injected into the HPLC-MS/MS in the MRM mode. Under optimal conditions, the experimental detection limit of 0.02 ng/mL and the theoretical detection limit of 0.03 ng/mL were obtained. The linear range was obtained in the range of 0.06 to 1000 ng/mL and the correlation coefficient was more than 0.99. The method is accurate enough and the inter- and intra-day repeatibility of the method in 3 different concentrations was below 5 %.

Keywords: Empagliflozin, Linaglyptin, HPLC-MS/MS, Carbon nitride

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Inventing a bacteriocidal porous cryogel for immediate disinfection of contaminated water on site

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According to some estimates, one-third of the world's population does not have access to safe drinking water, and half of the population will live in areas with water crises by 2025. An important challenge in water treatment is its bacterial disinfection [1], because ineffective treatment leads to pathogenic bacteria in the water source, which then leads to the spread of disease. The increase in multidrug-resistant bacteria in recent years has increased the difficulty of fighting these microorganisms [2]. Antibacterial polymers are a group of polymeric materials with antimicrobial properties and can prevent the growth of microorganisms such as bacteria and fungi. These polymers are engineered to behave similarly to antibacterial peptides used by the immune system to kill and fight bacteria. This study reports the development of new polymeric material with excellent intrinsic antimicrobial activity called antimicrobial polymer cryogel. In this study, we synthesize a cryogel with biological scaffold. Cryogel scaffolds are made by cross-linking at -20 ° C to create a structure with interconnected macro cavities with acceptable porosity. Adding different crosslinks to cryogel platforms is done to investigate various purposes such as reducing water reabsorption, reducing inflation rate, and decreasing insolubility [3]. The mechanical properties and rheology of the synthesized cryogel will be examined. While polymers are responsible for bacterial properties by disrupting the cell wall of bacterial membranes as antimicrobial peptides behave, the macro-porous structure of the gel allows it to act like a sponge and absorb bacteria from the solution. Maximum contact between the bacterium and the polymer occurs due to the high level of the internal structure of the gel. The platform technology developed here is not only limited to water disinfection but may also apply to other bacterial inactivation programs.

Keywords: Antibacterial, Cryogel, Water purification

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UiO-66-based metal organic framework for dispersive solid-phase extraction of vanillylmandelic acid from urine before analysis by capillary electrophoresis

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Vanillylmandelic acid (VMA) is the end product of epinephrine and norepinephrine metabolism in the human body [1]. Dispersive solid-phase extraction (DSPE) has been developed as a new approach for the extraction of vanillylmandelic acid (VMA) in urine samples prior to capillary electrophoresis with diode array detection (CE-DAD). In the DSPE, due to the high contact surface between the analyte and the sorbent, the sorption kinetics increase, which increases the extraction efficiency and reduces the extraction time [2]. In the developed method, extraction of VMA by DSPE was carried out by direct addition of 7.5 mg of synthesized amino-functionalized UiO-66 (Zr) metal-organic framework adsorbent into the 5 mL sample solution (pH 4.0), followed by sonication and centrifugation. The supernatant layer was discarded, then the sedimented adsorbent was eluted using borate buffer (75 mM, pH 10). Effective extraction parameters including the amount of adsorbent, sample pH, adsorption and desorption time, type, volume and pH of eluent, and type of adsorbent dispersion method were systematically investigated. Under optimized conditions, the linearity of the method was in the range from 40 to 2000 µg L^{-1} with a correlation coefficient over 0.9948. The method detection and quantification limits were 12 and 40 µg L^{-1}, respectively. The relative standard deviations for intra-and inter-day precision were 2.4 and 2.8 (n = 5), respectively.

Keywords: Dispersive solid-phase extraction, Urine, Biomarker, Biogenic amines, Sorbent

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Study of electrochemical behaviour of salbutamol on electrodes modified with MWCNT

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Salbutamol, 2-(tert-butylamino)-1-[4-hydroxy-3-(hydroxymethyl)phenyl]ethanol, also known as albuterol, is a β2-adrenergic bronchodilator widely used for the treatment of bronchial asthma and management of premature labour [1-3]. Salbutamol (SAL) is also applied as a tocolytic agent in humans as well as in veterinary medicine. High doses of SAL may have lipolytic effect and residues of this compound, which are most abundant in liver and meat, can be toxic to humans [4]. In this work a simple procedure was developed to prepare a glassy carbon electrode (GCE) modified with multi walled carbon nanotubes (MWCNT). The application of this sensor was investigated for determination of Ade. The materials were characterized by field emission scanning electron microscopy, Fourier transform infrared spectroscopy, and the modified electrode was characterized by cyclic voltammetry and differential pulse voltammetry. The modified glassy carbon electrode is shown to display high electrocatalytic activity toward the oxidation and determination of Ade. Linear relationships between peak current and the concentration of Ade was obtained in the range from 2 μM to 45 μM with detection limits of 1.81 μM. Furthermore, the biosensor showed high sensitivity, good selectivity, good reproducibility, and long-term stability to salbutamol detection.

Keywords: Salbutamol, Electrodes modified, Carbon nanotubes

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Development of biodiesel production through electrochemical processes using graphite electrodes modified with carbon quantum dots

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Currently, petroleum is the largest source of energy consumption when compared with other energy sources; today the world faces energy tension. This has caused increased research on alternative fuels and renewable sources of energy. Bio fuels, such as bioethanol and biodiesel, are today's considerable interest for many reasons [1]. The synthesis of high-purity, glycerol-free biodiesel is a concern that has challenged many researchers around the world. The main problem is the cost of biodiesel production compared to the cost of fossil fuels, which is solved by electrochemical methods that reduces the cost of heat required for the reaction and the cost of washing due to the high amounts of sodium hydroxide in the conventional methods [2]. There are three major methods for biodiesel synthesis such as: Microemulsion, Pyrolysis (thermal) and Transesterification [3]. In this research, the electrolysis methods with graphite electrodes modification with carbon quantum dots reduces the applied potential to 4V with less time of production have been used for synthesis of biodiesel from cooking oil as a sustainable feedstock throw out the transesterification method. The effects of methanol/cooking oil ratio and sodium hydroxide concentration as a catalyst on biodiesel conversion were carefully investigated. Under the appropriate transesterification conditions; sodium hydroxide (1 wt% cat /oil ratios) with optimum solvent (methanol) to oil volume ratios (1:6) and water (1.8 wt%) is applied. The obtained product was studied by UV-visible spectroscopy in the range of 200-400 nm wavelength to ensure the synthesis of biodiesel. The results showed that due to the characteristics of the graphite electrode, there was no voltage drop or reduction in reaction rate and the temperature from the beginning to the end of the reaction was constant, which ultimately leads to the production of biodiesel with 99.36% efficiency during 30 min and the amount of glycerol and soap as by-products was very low.

Keywords: Electrochemistry, Biodiesel, Transesterification, Carbon quantum dots.

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Development of new liquid phase microextraction based on the in-situ formation of deep eutectic solvent for extraction of several phthalate esters from hard-shelled drug capsules before GC analysis

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Phthalates are endocrine disruptors widely used as chemical additives in food packaging or polymer carrier for drug delivery [1]. Phthalates cause some adverse effects on human health. It has been evaluated to result in birth defects, organ damage, infertility, type-2 diabetes, endocrine disruptions, and cancer [2]. Therefore the determination of these chemical compounds is very important to assess the health of the body. In this work, a deep eutectic solvent (DES) with a lower density than water has been applied as the extraction solvent for the liquid phase microextraction (LPME) of four ester phthalates (DBP diethyl phthalate; DBP dibutyl phthalate; DIBP diisobutyl phthalate; DIOP diisoctyl phthalate) from powder samples. For the facile collection of DES after LPME, the solidification was performed on the ice bath. Gas chromatography was used as the analytical instrument for the determination of analytes. Real samples including drugs covered by capsules were analyzed by the standard addition method and satisfactory relative recoveries of more than 80% were achieved. The method showed good linearity for all analytes with low limits of detection (LOD) and low limits of quantification(LOQ) in the range of sub ng/mL were obtained. The interday and intraday repeatability (n=5) of the method in 3 different concentrations were less than 6%.

Keywords: Microextraction, Deep eutectic solvent, Phthalate esters, Chromatography

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Mineralization of pirimicarb insecticide and paraquat herbicide in aqueous solution using advanced oxidation processes

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Paraquat is a nonselective contact herbicide and used as the third most widely herbicide in the world [1,2]. The United States Environmental Protection Agency (USEPA), classified paraquat dichloride as a restricted use pesticide due to high acute toxicity to animals and people with the acute oral toxicity of 4,4-bipyridyl with an LD_{50} value of 40-200 mg/kg body weight [3]. Pirimicarb is a selective systemic insecticide that is widely employed against aphids with a contact action. The United States Environmental Protection Agency (USEPA), classified it as a highly toxic substance and carcinogenic to humans and animals due to LD50 =100-200 mg/kg body weight and toxic stimulant effects on lung cell culture in humans and carcinogenic potential high [4]. Nowadays, heterogeneous photocatalytic degradation in the presence of nanostructure catalysts and inorganic oxidants such as $S_2O_8^{2-}$ and IO_3^- as one of the advanced oxidation processes (AOPs) intensively studied as the most environmentally friendly and promising techniques for the degradation of recalcitrant organic pollutants in water by powerful oxidants especially hydroxyl radicals or superoxide radicals [5-8].

In this research, mineralization efficiency of pirimicarb insecticide and paraquat herbicide in aqueous solution using UV-C irradiation/TiO_2 nanophotocalysise(TiO_2NP)/potasium periodate (KPI) process as one of the advanced oxidation processes, have been studied. Resuls of TOC analysis shown that the mineralization efficiency of 400 mL of 30 mgL^{-1} each of the paraquat herbicide (PQ) and the pirimicarb insecticide (PC) solutions under the optimum conditions (PI=[90] mgL^{-1}, [TiO_2NPs]=125 mgL^{-1}, and [pH]in=6 for PQ and PI=[90] mgL^{-1}, [TiO_2NPs]=240 mgL^{-1}, and [pH]in=6 for PC) and UV-C irradiation was about 60 % at 25 °C after 60 min.

Keywords: Paraquat herbicide, Pirimicarb insecticide, Mineralization efficiency, Advanced oxidation processes.

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Development of a simple and inexpensive liquid phase microextraction for spectrophotometric determination of orthophosphate in water samples

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Phosphorus is a nutrient needed for life and plays a major role in the metabolism of plants and animals. Human-induced phosphorus contamination is one of the current main drivers of Eutrophication, so that excessive entry of this nutrient into the aquatic environment is considered as one of the most important environmental problems of human societies today. Phosphates can exist in only three forms: orthophosphates, dense phosphates (pyro, meta, and poly) and organic phosphates. In general, soluble phosphorus is mainly present in the form of orthophosphate [1]. Analytical methods for orthophosphate determination have been reported such as chromatography, electrochemical, fluorescence and spectrophotometric methods. The Environmental Protection Agency has recommended the molybdenum aqueous spectrophotometric method as a standard method for detecting orthophosphate in water samples [2].

In this work, a simple, unexpensive and environmentally friendly liquid – solid microextraction for preconcentration of orthophosphate from water samples has been presented using cetyltrimethylammonium bromide (CTAB) surfactant. At first, ammonium molybdate and ascorbic acid were used in acid medium to form a blue molybdenum phosphate complex with a maximum absorption of 680 nm. The effect of different parameters on the complex formation and the microextraction was investigated and optimized. Under optimal conditions, linear range was obtained 15-150 µg L-1 and 150-950 µg L-1 with a correlation coefficient of 0.985 and 0.988, respectively. Limit of detection was 12.8 µg L-1 . The relative standard deviation for determination of 200 µg L-1 was 6.2 % for five replications. The interference of common cations and anions was investigated. The proposed method was successfully used to determine orthophosphate in different aqueous samples with satisfactory recovery ranged from 91 to 105%.

Keywords: Ortophosphate, Green extraction, Spectrophotometry, Aqueous samples

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3D printed solid phase microextraction scaffolds as novel tool for sample preparation; application in antifungal drugs analysis

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A novel geometry for solid phase microextraction (SPME) adsorbents was developed using 3D printing technology [1], and its application for extraction and determination of three antifungal drugs in human plasma, sewage water and Shampoo by HPLC was introduced. The designed adsorbent was prepared as cubic scaffolds using fused deposition modeling (FDM) 3D printer and a Poly lactic acid (PLA) filament. Scaffold surface was chemically modified using alkaline ammonia solution [2]. Morphology of the modified surface and its chemical changes were studied using FE-SEM and ATR, respectively. The proposed method showed a good linearity in the wide concentration ranges. The limits of detection (LODs) were obtained between 8.59-9.94 and the limits of the quantification (LOQs) were between 26.02-30.11 μgL^{-1}.

Keywords: 3D printing, Antifungal drugs, Poly lactic acid, Solid phase microextraction

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Functional carbon quantum dots from natural materials as an eco-friendly corrosion inhibitor for copper in NaCl 3.5% solution

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Corrosion is the destructive chemical or electrochemical reaction between a common substance, a metal, and its environment that changes the properties of the material [1].Corrosion is a spontaneous phenomenon Which causes huge damage to industries world wide [2,3]. Inhibitors are one of the best methods of corrosion control methods due to its advantages such as cost effectiveness and ease of application in industry which is invested in this article. Most corrosion inhibitors are expensive and environmentally hazardous chemicals, so the research on environmentally friendly inhibitors is a new field of interest. Carbon quantum dots (CQDs) are new class of fluorescent carbon nanoparticles that are usually less than 10 nanometers long [4]. These materials are a new class of zero-dimensional nanomaterials that have many functional groups and good solubility in water [5]. Herein, novel CQDs have been prepared using a facile hydrothermal method. CQDs–adsorption film was formed on copper substrate as a barrier that could prevent transportation of corrosive particles. The relevant anticorrosion mechanism of CQDs was proposed in detail, which could provide powerful guidance to design and synthesis new nanomaterials for metal protection from corrosion. These materials with displacement of corrosion potentials have been able to show the inhibitory effect and be introduced as anti-corrosion materials in NaCl 3.5% as corrosive environment. The inhibition performance of the concerned zero-dimensional nanomaterial for copper inhibition was investigated by electrochemical impedance spectroscopy (EIS) and linear sweep voltammetry (Tafel plots), combining FT-IR methods to investigate the corrosion products. Results indicate that the CQDs were found to be effective in low concentration for long periods of time and high concentration of CQDs shows better results for short time.

Keywords: Corrosion, Copper, Carbon quantum dots, Inhibitors

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Highly selective and sensitive determination of tartrazine in food samples using carbon quantum dots as a fluorescent probe.

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Carbon quantum dots (CQDs) are carbon nanomaterials less than 10 nm in size. In recent years, CQD-based sensors have been used in nutrients owing to their high sensitivity and accuracy, as well as their low cost in detecting hazardous compounds, such as unauthorized additives, heavy metals, and pathogens [1]. Tartrazine is an azo dye that is widely used in the food industry, which can lead to thyroid cancer and allergies and endanger the health of consumers. Therefore, it is essential to control Tartrazine content in nutrients [2]. This study explored the effects of CQD synthesis conditions on their optical properties and system analytical performance. For this purpose, two CQDs, namely CQD1 and CQD2, were synthesized from the same material using the hydrothermal method under different temperatures, times, and concentrations of reagents and then used in optical sensors for the analysis of Tartrazine. In the next step, the synthesized nanoparticles were characterized by fluorescence spectroscopy, transmission electron microscope (TEM), X-ray diffraction (XRD, Elemental Analyzer (CHNS/O), and Fourier transform infrared spectroscopy (FTIR). Maximum emission intensity was obtained when we excited the CQD1 at 340 nm and CQD2 at 400 nm. Tartrazine could selectively decrease the intense fluorescence of carbon quantum dots. Based on this principle, an optical sensor was developed for tartrazine determination. The Limit of Detection (LOD) was also calculated to be 1.4 µM for Sensor 1 and 1.8 µM for Sensor 2. Finally, following the optimization of the conditions, Tartrazine concentrations were measured in real-world samples, including honey and juice. The results indicated that the designed optical sensor could be used to measure Tartrazine sensitivity in real-world samples.

Keywords: Carbon quantum dot, Optical sensor, Tartrazine

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Synthesis of a pH-sensitive Polymer Nanoparticle for Drug Delivery by Aerosol Method

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The severe side effects of systemic high doses of chemotherapy, as well as the development of drug resistance, make anticancer therapy less safe and effective. As a result, novel strategies for improving anticancer medication therapeutic index by targeted administration to tumor locations are constantly being researched and developed. Drug nanocarriers efficiently improve the targeting of diseased areas in the body and can enhance drug efficacy [1]. Among a variety of options, polymer nanoparticles are a potential option because they can be made up of smart materials that respond to environmental influences and change their characteristics appropriately, allowing for targeted drug delivery. Functional nanocarriers combining multi-drug release and other therapeutic strategies for synergistic tumor therapy may be an effective strategy for the accurate and efficient treatment of tumors [2]. This paper reports on a synthesis of a pH-responsive polymers for the controlled release of doxorubicin (DOX) and methylene blue (MB). DOX, and MB drugs were chosen as anticancer drugs and drug treatments for Alzheimer's, respectively. Proposed a pH-responsive polymer nanoparticles consist of chitosan, and alginate, which are natural and biocompatible polymers. To achieve the best performance, the formulation of the pH-responsive polymer nanoparticles was optimized by using aerosol method. Then, the in vitro release of two drugs at neutral and acidic pH was investigated using UV-Vis spectrometer. Under the optimized conditions, the loading amount of DOX, and MB into the polymer nanoparticles was 41.42 mg g^{-1} and 2.28 mg g^{-1}, respectively. In vitro release experiments showed that the release of DOX, and MB from polymer nanoparticles in acidic pH was higher compared to neutral pH. Therefore, DOX, and MB-loaded pH-responsive polymer nanoparticles based on chitosan, and alginate are a promising sustainable delivery system for cancer, and Alzheimer's therapy.

Keywords: Targeted drug delivery, Doxorubicin, Methylene blue, Aerosol method, pH-sensitive polymer

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A novel electrochemical platform based on covalent organic framework integrated with Pt nanoparticles and multiwalled carbon nanotubes for determination of dopamine in human serum

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Covalent organic frameworks (COFs) are a class of crystalline porous polymer that allows the precise integration of organic units into extended structures at an atomic level [1]. The fascinating structures and unique properties such as large surface area, abundant functional group and high chemical stability make COFs attractive materials in the fields of gas adsorption, separation, catalysis, optoelectronic devices and sensors [2, 3]. In this work, a novel electrochemical platform was developed based on facile synthesis of a covalent organic framework (COF) Via in situ growth of Pt nanoparticles (PtNPs) on the surface of COFs and COFs-MWCNTs composites with improved electroactivity. After incorporation of MWCNTs into the composites, the PtNPs@COFs-MWCNTs nanocomposites that possess excellent electrocatalytic activity and unprecedented catalytic performance were formed and utilized for determination of dopamine. Under the optimum conditions, this electrochemical sensor presented excellent electrochemical properties to this biomolecule. The linear ranges for the determination of dopamine was 0.01-40 μmol/L with the correlation coefficients of 0.9905. The detection limits were 7.4 nmol/L ($S/N = 3$). In addition, the modified electrode was also applied to the determination of dopamine in human serum samples and the recovery were varied from 96.5% to 104.8%. Moreover, there are no significant effects from the interferents and The results demonstrated that the modified electrode had the characteristics of high sensitivity, good selectivity and reliability.

Keywords: Covalent organic frameworks, Multiwalled carbon nanotubes; Pt nanoparticles, Electrochemical sensors

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Electrochemical nanosensor based on magnetic nanoparticles for the determination of morphazinamide HCl

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Tuberculosis (TB) is a potentially serious infectious disease that mainly affects the lungs [1]. Pyrazinamide group drugs are unusual anti-tuberculous agents when compared with others that its ability to promote a durable cure and shorten the duration of therapy. Morphazinamide HCl (N- (morpholin-4-ylmethyl)pyrazine-2-carboxamide) (MRA) is a drug that used to treat tuberculosis and it can be very effective in all forms of tuberculosis[2]. In this research, morphazinamide HCl (MRA) was investigated at ultra-trace level in real sample. Iron (III) oxide nanoparticles (Fe_2O_3NPs) were casted on a glassy carbon electrode (GCE) for the determination of MRA. prepared nanosensor was characterized by electrochemical impedance spectroscopy (EIS), scanning electron microscopy (SEM), energy-dispersive X-ray spectroscopy (EDX), transmission electron microscopy(TEM) and cyclic voltammetry (CV). The square wave voltammetry response of the Fe_2O_3NPs/GCE was linear with MRA concentration in the range of 1 µM to 100 µM under optimized conditions (0.1M phosphate buffer solution at pH 3.0; drop casting volume 10 µL; accumulation time 15 s; accumulation potential –0.3 V), with a detection limit of 0.21 nM. Also, the proposed procedure was very efficient for MRA determination from human serum sample with high recoveries.

Keywords: Morphazinamide HCl, Anti-tuberculosis drug, Magnetic nanoparticles, Nanosensor.

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A new approach to synthesis of nano precipitated calcium carbonate based on ion transfer method through liquid membrane

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In the present study, a new synthesis method of nano precipitated calcium carbonate (NPCC) through an ion transfer approach was studied. Precipitated calcium carbonate is one of the most important industrial raw materials widely used in papermaking, polymer composites, constructions and biomedical applications [1, 2]. Due to its various applications of calcium carbonate in the industry, controlled synthesis of this material has been noticed to achieve desirable size and morphology. Recently, liquid membranes have widely been considered in the field of ion transport method owing to their low cost, simplicity in operation, low usage of organic phase, and high mechanical stability [3, 4]. According to the aforementioned points, a new approach based on ion transfer method through liquid membrane was used in this project to synthesize fine particles (in nano size) along with narrow distribution size of calcium carbonate. In this way, in order to find the desired experimental conditions, the effect of influential parameters, such as temperature, time, type of solvent, concentration of surfactant and carrier were investigated which can affect the particle size and morphology of the synthesized nano calcium carbonate. Finally, the successful synthesis of NPCC was confirmed by scanning electron microscopy, energy dispersive X-ray spectroscopy, Fourier-transform infrared spectroscopy, dynamic light scattering, and X-ray powder diffraction. Surprisingly, the results showed that the synthesized calcium carbonate particles by the proposed method are in nano size in very fine dimensions with a narrow distribution size (about 10-25 nm) which leads to more uniformity and applicability of this material in various industrial usages.

Keywords: Ion transfer, Controlled synthesis, Liquid membrane, Nano precipitated calcium carbonate, Narrow distribution size.

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Smartphone-based colorimetric determination of nickel in aqueous samples after air assisted liquid-liquid microextraction technique

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The importance of the determination of heavy metal ions, such as nickel, in environment samples can hardly be overemphasized because they have undoubtedly a serious potential hazard to the human organism [1]. Several analytical techniques are used for determination of nickel such as flame atomic absorption spectrometry (FAAS), inductively coupled plasma optical emission spectrometry (ICP-OES), UV–Vis spectrophotometry. However, these expensive facilities are not always available and it is often desirable to conduct measurements directly in the field. Therefore, simple, fast, inexpensive, portable, and sensitive methods for determination of Ni are in high demand. Recently, a method has been used for rapid and simple determinations in analytical chemistry called digital-image-based colorimetry (DIC). DIC could be examined as a novel and low-cost technique which uses digital images. As the most crucial step in the analytical procedure, sample preparation is mainly aimed to enrich the analytes of interest and purify the extracts before instrumental analyses. air-assisted liquid–liquid microextraction (AALLME) is a disperser solvent free extraction method [2]. In this study, potential of a novel method based on AALLME and digital image analysis has been evaluated for preconcentration, determination and speciation of nickel in different aqueous samples. data was extracted from the digital image of the extraction phase using a free app. In order to achieve high extraction efficiency, the influence of different parameters was investigated. In this work, AALLME coupled with digital image analysis was successfully applied for the determination of nickel species in different water samples. The limits of detection (LOD), the correlation coefficients (R^2) and relative standard deviations (RSD %) were found as 13.5 µg L^{-1}, 0.98 and 4.8 respectively.

Keywords: Image analysis, Air-assisted liquid-liquid microextraction, Smartphone

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Trace measuring of parabens in maternal milk samples via µSPE based on LDH modified graphene oxide nanomaterial as an impressive sorbent

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Parabens, which are esters of p-hydroxybenzoic acid, are a commonly used preservative in several products such as cosmetics, foods, beverages, and pharmaceuticals. The usage of parabens is expanding over recent years because of their many advantages [1]. Frequent evidences proved that parabens present in human biological fluids like maternal milk. Hence, they can enters the body of babies and subsequently cause negative effects on their bodies especially on their developmental processes. In addition, parabens have adverse effects such as perturbations of the endocrine system, being genotoxic, and increasing the risk of breast cancer and male infertility [1, 2]. Thus, determination of trace amounts of parabens in complex matrices like maternal milk samples is accompanied by some serious problems. In this case, sample preparation methods play a vital role to overcome these obstacles. Recently, layered double hydroxide (LDH) materials have received considerable attention as an outstanding sorbent due to their unique properties including supreme anion-exchange capability, large surface area, excellent thermal stability, highly tunable interior architecture, water-resistant structure, variable size of the interlayers and low cost [3]. Combining of Graphene oxide and LDHs can be a proper idea since it takes advantage of both of them. In the present study, a magnesium-aluminum LDH coated on graphene oxide nanosheets was synthesized. It was successfully applied as an efficient medium for determination of the parabens in maternal milk samples using micro solid phase extraction by packed sorbent (in spinal syringe format) followed by HPLC-UV. Influential parameters were optimized by central composite design. Under the optimal conditions, figures of merit of the developed method were obtained in which the limits of detection were found between 3.0 and 5.0 µg L^{-1}. The calibration plots were linear in the range of 10–1000 µg L^{-1}. Intra- and inter-day RSD% (n = 3) at two concentration levels of 25 and 250 µg L^{-1} varied between 4.2 and 9.5%. The relative recovery values for the spiked maternal milk samples were in the acceptable range of 87.2–104.4%. Finally, the introduced method exhibits appropriate repeatability, good sensitivity, and acceptable applicability for the determination of parabens in complex biological matrices.

Keywords: Maternal milk sample, Parabens, Graphene oxide, Layered double hydroxide, nanomaterial

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Aminoacid-intercalated layered double hydroxide as highly selective and efficient sorbent for mercury extraction from water and real samples

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Mercury as the toxic heavy metal has the highest environmental risk. It is a global pollutant that could be found in electrical devices, lamps, batteries, dental amalgam, many industrial wastes, mineral deposits, and agricultural applications [1]. The ability of Hg to accumulate in biological tissues might influence the entire food chain and causes hazardous cumulative effects in humans; like respiratory failure, hypertension, nervous system disorders, maladjustment in hormone secretion of the organism, cardiovascular collapse, acute renal failure, gastrointestinal disorders, and even genotoxicity to some extent [2-3]. This metal is so volatile that can easily be exposed to human environment. Therefore, determination of mercury in ultra-trace levels is very important in environmental and toxicological studies. The maximum elemental intake per day is up to 1.2 grams of mercury. In the Codex standard, the permissible levels of inorganic mercury in table salt, green tea, drinking water, and mineral water are 0.05 $\mu g\ g^{-1}$, 0.05 $\mu g\ g^{-1}$, 6.0 $\mu g\ L^{-1}$, and 1.0 $\mu g\ L^{-1}$, respectively. In this study, magnetic calcined layered double hydroxide modified with aminoacid (Ni/Al CLDH@Fe_3O_4@AA) was synthesized through co-precipitation procedure. The synthesized magnetic CLDH was used as biomagnetic sorbent for mercury removal from the polluted water. Infrared spectroscopy, X-ray diffraction and field emission scanning electron microscopy were confirm the synthesis of the sorbent and modification. The adsorption and desorption time, pH, the adsorbent amount, kind and volume of desorbent were optimized as the effective parameters on the Hg adsorption. The absorption behaviors of Hg on the synthesized sorbent were checked by Langmuir and Freundlich isotherms and the Langmuir isotherm with higher R^2 value were matched well with the obtained results. The obtained values for q_m and R_L were 189 mg g^{-1} and 0.96 to 0.99, respectively, indicating the favorable mercury sorption on the synthesized sorbent. The kinetics studies were fitted well with the linear pseudo-first-order model with higher R^2 (0.965) at sorption process. The obtained results from real samples confirmed that the synthesized biomagnetic sorbent has the excellent Hg sorption capacity in comparison with other sorbents. Therefore, CLDH@Fe_3O_4@AA sorbent can be applied as a new suitable sorbent for removal of Hg from the polluted water.

Keywords: Magnetic Nanoparticles, Layered Double Hydroxides, Aminoacid, Kinetic studies.

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Magnetic layered double hydroxide sorbent in dispersive solid phase extraction for microextraction of chromium in water and leather samples

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Heavy metals get distinguished from other toxic pollutants which, due to their non-biodegradability can accumulate in living tissues, and cause severe physiological or neurological damage to the human body. Chromium ions are one of the most toxic metal ions that are applied in chrome plating, manufacturing of dyes and pigments, leather tanning process and wood preservation. Two stable oxidation states of hexavalent chromium are Cr (VI) and trivalent chromium, Cr (III) [1]. Cr (VI) can cause numerous cancer diseases due to its rapid penetration across biological membranes and subsequent interaction with intracellular proteins and nucleic acids [2]. People can be exposed to chromium through breathing, eating or drinking and through skin contact with chromium or chromium compounds. Chromium concentration in drinking water is generally less than 2 μg L^{-1} [3]. The World Health Organization (WHO) states that the guideline values of 50 μg L^{-1} Cr(VI) are considered to be too high as compared to its genotoxicity, and the national health and nutrition examination survey (NHANES) claims normal chromium levels found in blood are 0.1-1.7 μg L^{-1} and 0.24-1.8 μg L^{-1} in urine [4]. So, determination of this analyte in real samples is critical step in analysis process. In this study, a novel adsorbent based on Zn/Fe/Al LDH@Fe_3O_4 was synthesized and used for extraction of Cr (VI) from water and leather samples. This magnetic adsorbent was characterized by FT-IR, field emission scanning electron microscopy and X-ray diffraction. Optimization of extraction method was done to obtain the highest extraction recovery and reliability. Main parameters such as solution pH, adsorption and desorption time, salt addition, kind and volume of desorption solvent were optimized. Under optimal conditions, the linearity range was obtained in Cr(IV) concentration in the range of 25-1000 ppb, with determination coefficient $R^2 = 0.992$. The limit of detection and quantification was calculated to be 10 μg L^{-1} for water and 25 μg L^{-1} for leather samples. This method presented a short extraction time (within 10 min) for application in real samples. The obtained adsorbent was successfully applied to the identification and determination of Cr(VI) in water and leather samples with good recoveries.

Keywords: Layer double hydroxide, Magnetic adsorbent, Leather samples.

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Decolorization of methylene blue by a heterogeneous sono-Fenton process using $FeMnO_3$ nanocatalyst

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Dyes are a wide group of pollutants. Many industries such as textiles, paints, paper, plastics, leather, food and cosmetics often use dyes and pigments for their color products. Dyes can affect the food and water cycle and can also cause allergies and skin allergies. In addition, these dyes can be toxic and dangerous and can inactivate microorganisms [1-2].
Thus removal of these materials from waste water is more important. Fenton process is an advanced oxidation process that is used for degradation of organic pollutants, especially for dyes [3]. Both of Fenton process and Ultrasonic waves are used as separate method for degradation of the pollutants [4]. Hence, in this research, the decolorization property of the $FeMnO_3$ nanocomposite was investigated. So $FeMnO_3$ magnetic nanocomposite was synthesized by hydrothermal method. The synthesized catalyst was identified using methods such as Fourier transform infrared spectroscopy(FTIR), X-ray diffraction(XRD), energy dispersive X-ray spectroscopy (EDS), Field emission scanning electron microscopy (FESEM), Transmission Electron Microscopy (TEM), and visible-ultraviolet spectroscopy, and the results confirmed the catalyst structure. Influence of some parameters as the concentration of reactants and pH of the solution has been studied. The results indicate the high efficiency of this catalyst in degradation of methylene blue. Therefore using this technique and process was recommended for dye pollutants degradation from aqueous environments.

Keywords**:** Decolorization, Methylene blue, Magnetic nanocomposite,

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Ultrasonic assisted liquid–liquid microextraction method based on deep eutectic solvent for preconcentration/ separation of Sulfonamides in drinks

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Sulfonamides (SAs) are a class of synthetic antibiotics which are widely used in human health and aquaculture. However, their metabolites are often found in aquatic environments, which may be caused by improper treatment of human and animal excretions. Excretions are accumulated in the environment (soil, ground and surface water), causing the emergence of antibiotic resistance [1]. On the other hand, SAs degrade slowly in the environment and have a long residual time. After long-term accumulation and bio-chain transfer, they will be enriched in animals, plants and humans to reach higher concentrations and eaily transfer to fod samles. Therefore application of a potent sample pretreatment method as a separation technique is inevitable. Solid phase microextraction (SPME) and liquid–liquid microextraction (LLME), are miniaturized sample pre-treatment technologies that have the advantages of simple and rapidly, high recovery, low cost and low consumption of organic solvents [2]. In recent years green solvent such as deep eutectic solvents (DESs) are proper replacemnt of organic solvents wich are ecofreindly and biodegradable [3]. In this research study, a sensitive facile ultrasonic assisted liquid–liquid microextraction based a novel deep eutectic solvent was applied for preconcentration and separation of sulfadiazine, sulfathiazole, sulfamethazine in some drinks prior to HPLC analysis. Influential parameters including pH, sonication time, DES volume, ionic strength, and sample volume were investigated. At optimum conditions Limit of detection (LOD) of 0.19, 0.18, and 0.21 were obtained for sulfadiazine, sulfathiazole, sulfamethazine respectively. Linear range of 0.5-200 µg L^{-1} and precision of ≤3.6% were also achieved. The proposed method was successfully applied for analysis of drinking water, milk.

Keywords: Ultrasonic assisted technique, Liquid–liquid microextraction, Sulfamides, Deep eutectic solvent

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Air-assisted liquid-liquid microextraction based on solidification of floating deep eutectic solvent for the analysis of antibiotics

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High-performance liquid chromatography (HPLC) plays an important role in the determination of antibacterial drugs in body fluids. The detection of the infection in its early stages could help achieve better outcomes, and therefore, it is extremely important not only to determine changes within the body, but also to find biomarkers that characterize a given individual or population [1,2]. In this work, a new air-assisted liquid-liquid microextraction based on solidification of floating deep eutectic solvent (AA-LLME-SFDES), coupled with a high performance liquid chromatography (HPLC) method was developed. some types of fatty acid-based hydrophobic deep eutectic solvents (DESs) with low viscosity, low-density, and melting point close to room temperature were prepared and employed as extraction solvents. This air assisted liquid-liquid microextraction was carried out in a glass centrifuge tube. Subsequently, the glass tube was introduced into ice-water bath and held for 4 min, during which the upper DES phase was solidified. The water phase was easily extracted using a syringe equipped with a long needle, and later, the glass tube was removed from ice-water bath. The solidified DES phase was immediately melted at room temperature and used for HPLC analysis. The response surface methodology was employed to optimize some influencing parameters such as the volume of the extraction solvent, the pH value of sample solution, the number of extraction cycles, and the addition of salt. A quadratic model, namely a central composite design, was used to replace the conventional single factor analysis.

Keywords: Antibiotic, Solidification, Air assisted, HPLC-UV

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Pd-NHC-MIL-101(Cr) Nanocomposite as a Novel and High Throughput Electrocatalyst towards Ethanol Oxidation

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Currently, designing and preparing low-cost and high-efficiency electrocatalysts remains a huge impediment for direct ethanol fuel cells [1,2]. In the present work, Pd-NHC-MIL-101(Cr) Nanocomposite was synthesized and characterized by SEM, TEM and XRD analysis. The electrocatalytic properties and stabilities of Pd-NHC-MIL-101(Cr) modified carbon paste electrode (CPE) towards ethanol oxidation reaction (EOR) was investigated using cyclic voltammetry (Fig. 1.) and chronoamperometry. Pd-NHC-MIL-101(Cr) exhibited favorable electrocatalytic performance with higher EOR activity and superior stability compared to Pd/C for ethanol oxidation reaction. Also, the results showed that the poisoning effect of Pd-NHC-MIL-101(Cr) was less than that of Pd/C. The current density for Pd-NHC-MIL-101(Cr) in a KOH (3.0 M) containing ethanol (3.0 M) was 124.7 mA/cm^2 and higher than that of Pd/C (45.83 mA/cm^2).

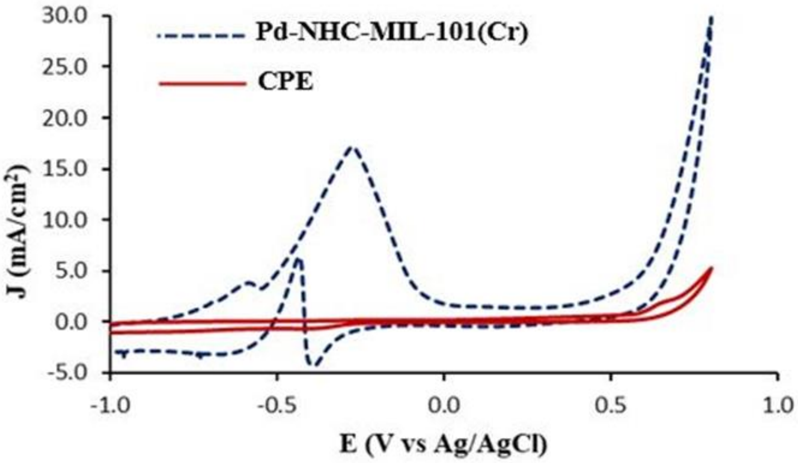

Fig. 1. CVs of bare CPE and Pd-NHC-MIL-101(Cr) in KOH solution in the presence of ethanol at 50 mV.S^{-1}

Keywords: Electrocatalyst, Alcohol oxdation, Fuel cell, MOF, rGO

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Deep eutectic solvent-based liquid phase microextraction Sudan IV prior to UV-Vis spectrophotometric determination

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Sudan dyes are a group of azo dyes that have significant toxic effects on human organs due to their azoic structure and aromatic rings. Sudan dyes are prohibited for use because they are classified as Group 3 carcinogens by the International Agency for Research on Cancer. Therefore, effective and reliable methods are of great importance for the rapid detection of Sudan dyes in the samples [1]. In recent years, green analytical chemistry has been one of the key steps in developing extraction and sample preparation methods. The main goals of green analytical chemistry are to reduce the use of expensive and hazardous chemicals, to minimize time and energy consumption and to increase safety in the laboratory. In this context, deep eutectic solvents (DESs) are introduced as a new generation solvents that has all the qualities as mention above. DESs can be easily prepared by simply mixing two or more compounds classified as hydrogen bond donors and acceptors to obtain a eutectic mixture using basic laboratory equipment. Deep eutectic solvents (DESs) appear to be successfully used as a new generation solvent system that is effective, safe, inexpensive, non-toxic, biodegradable and biocompatible for important analytical and other chemical applications [2,3].

In this study, a deep eutectic solvent was prepared and used as an extraction solvent for the deep eutectic solvent-based liquid phase microextraction, separation and preconcentration of Sudan IV. After the preconcentration step; accurate and precise determination of Sudan IV analyte in the extraction phase was performed using UV-Vis spectrophotometer. Important analytical factors that affect the extraction efficiency of DESs such as pH of the solution, mole ratio of DES components, DES volume and sample volume were determıned and optimized. Quantitative recovery values of Sudan IV were determined at pH 4.0. The validity of the developed method has been proven by applying addition-recovery tests to environmental water and food samples under optimum conditions.

Keywords: Sudan IV, Deep eutectic solvent, UV-Vis spectrophotometer

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Patent Blue V Impregnated Magnetic Activated Carbon Cloth Magnetic Solid Phase Extraction of Ni(II) From Environmental Samples Prior to Flame Atomic Absorption Spectrometric Determinations

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The positive and negative effects of trace species on human health and the environment have attracted more attention in recent years. Nickel, especially from inorganic species, has toxic effects when exposed to hıgher concentration than the limit values determined WHO. For this reason, reliable, accurate and sensitive analysis of Ni(II) has gained more importance with the developing industry. Although the developing industry brings analytical devices, it often does not allow the analysis of trace species [1,2]. For this purpose, separation and preconcentration methods are needed. Therefore, the magnetic solid phase extraction method has been developed, which is simple, environmentally friendly, fast, using minimal equipment and chemicals. Analytical parameters are optimized for sensitive and sensitive Ni (II) separation and preconcentration from environmental samples with synthesized patent blue V impregnated magnetic activated carbon cloth. The parameters affecting the extraction efficiency like pH of the solution, amount of adsorbent, sample volume, desorption solvent and also the ratio of dye and magnetic activated carbon fabric were investigated. FAAS was used for the determination of concentrations of Ni(II) in all the model solution. Analytical parameters such as LOD, LOQ, PF and RSD were calculated under optimized experimental conditions. Validation of the developed method was tasted by applying the method to certified reference materials for trace metal analysis and environmental samples using standard addition method.

Keywords: Nickel, Separation-Preconcentration, Atomic absorption spectroscopy, Solid phase extraction

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Fabrication of monolithic MOF-808 as a novel coating for solid-phase microextraction of phthalate esters

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Phthalate esters (PhEs) are high production volume chemicals and are widely used as additives in the plastics industry. Since they are not chemically bound to the plastics, they can easily leach into the environment. Therefore, determination trace amounts of these compounds is very important. So far several analytical methods were introduced for the analysis of these compounds in various matrices [1]. Solid-phase microextraction (SPME) is a green sample pretreatment technique for extraction trace amounts of the analytes from various complicated matrices. Headspace SPME mode (HS-SPME) is one of the most suitable methods for extracting analytes from complex matrices [2]. In the present study, a novel metal-organic framework-808 composite, (poly styrene-MOF-808-divinylbenzene) was synthesized on the surface of a steel stainless wire by a facile in-situ polymerization. The synthesized adsorbent has excellent mechanical and thermal stability. The prepared fiber was applied as an adsorbent for the headspace solid-phase microextraction of phthalate esters in water samples. The effective parameters on the extraction efficiency including extraction and desorption times, extraction and desorption temperatures, and salt concentration were optimized by experimental design approaches. Response surface methodology (RSM) is a statistical technique to display the coherency between variables, reduction of experiments number, materials, time, and costs. RSM based on an orthogonal central composite design (CCD) in five levels was employed to optimize the quantitative factors. Due to a large number of experiments, they were divided into 2 blocks and carried out on 2 different days. A good detection limit and linear range were obtained under optimal conditions. The proposed method was successfully applied for the fast and sensitive determination of phthalate esters in water samples followed by GC-MS. The results showed that the synthesized fiber has high outstanding stability and repeatability.

Keywords: Metal-organic framework, Composite, Gas chromatography, Trace analysis

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Application of ZIF-67 coated by N-doped carbon dots to extraction of pesticides from fruit juice before chromatographic analysis

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Zeolitic imidazolate frameworks (ZIFs), made of tetrahedral metal cations M (M=Zn or Co) and imidazolate (Im) ligands are a unique and intriguing subclass of porous metal-organic frameworks (MOFs) [1]. In this study, an extraction method was developed for pesticides preconcentration and cleanup. 5 mL of a standard or real sample aqueous solution was used and then an appropriate amount of ZIF67-carbon dot (CD) as sorbent was dispersed into the sample using a vortex. After that, the sorbent is collected and the supernatant solution was discarded. Then a suitable volume of green and water-soluble solvent was added to the sorbent as the elution solvent in dispersive solid phase extraction (DSPE) and the dispersant solvent in the dispersive liquid-liquid extraction (DLLME). After desorption, the supernatant solvent was poured into the conical test tube and a few microliters of extraction solvent were added to it. Then, this mixture was quickly dispersed into the 5 mL of distilled water. The resulting cloudy mixture was centrifuged and the sediment phase was collected at the bottom of the test tube and 1 μL of it was injected into the analysis system. By a combination of the optimized DSPE with DLLME before GC, a sensitive method for the determination of pesticides was developed. At the optimum conditions, the figure of merits of the method was obtained as follows: linear range of (0.1-2000 ng mL^{-1}) and extraction recovery of (>62%).

***Keywords**:* Extraction, Pesticides, Chromatography, Nanocomposite, Carbon dot, Metal-organic framework

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Biosynthesis of nanoemulsion containing Origanum vulgare L. essential oil and zinc oxide nanoparticles and evaluation of its antibacterial activity

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In the present study, we synthesized a nanoemulsion containing *Origanum vulgare L.* essential oil and zinc oxide nanoparticles (EO/ZnO Emu.) by a spontaneous emulsification method [1]. Firstly, Zinc oxide nanoparticles (ZnONPs) were synthesized *via* a green method [2] and these particles were then used as the aqueous phase of the nanoemulsion.

The Origanum vulgare essential oil (EO) exhibits a broad-spectrum antimicrobial activity against antibiotic resistant species [3] so it was used as growth inhibitor for Methicillin-resistant Staphylococcus aureus (MRSA) and it was used as the organic phase in preparing the nanoemulsion. Scanning electron microscopy (SEM), X-ray diffraction spectroscopy (XRD) and UV-vis spectroscopy confirmed the formation of ZnONPs and dynamic light scattering (DLS) was used to measuring the size of nanoparticles and the nanoemulsion droplets. Finally, we investigated the antibacterial activity of EO/ZnO Emu. against MRSA *via* inhibition zone method.

Our results showed that zinc oxide nanoparticles have no inhibitory properties at 0.25-4 mM for MRSA. The *Origanum vulgare L.* EO (100%) had a great antibacterial activity against the pathogen, but its antibacterial activity was drastically decreased at 12.5% which was the concentration used in the nanoemulsion. As expected, EO/ZnO nanoemulsion showed greater inhibition zones than its active components ZnONPs(1.00 mM) and EO 12.5% in which produced the largest MRSA inhibition zone (13.00 mm) within all the compounds ($P<0.01$).

Keywords: Nanoemulsion, Zinc oxide nanoparticles, Origanum vulgare L., Green synthesis, Antibacterial activity

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Development and validation of a new high performance liquid chromatography method for the simultaneous determination of two anticancer drugs in pharmaceutical samples

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At present, a new core-shell nanomagnetic sorbent was synthesized based on reduced graphene oxide nanosheets decorated with gold-palladium bimetallic alloy nanoparticles supported on carbon nanotubes (Fe_3O_4/Au-Pd@CNT@rGO). A magnetic solid phase extraction (MSPE) as a simple and effective preconcentration method coupled to high performance liquid chromatography-mass spectrometry (HPLC–MS) was applied for simultaneous analysis of two vital anticancer drugs (Erlotinib, Nilotinib) in biological samples. Erlotinib and nilotinib are two potent and highly specific tyrosine kinase inhibitors which prevents growing of cancer cells. The combination therapy using these two drugs significantly increases the therapeutic efficacy. The magnetic property of the sorbent, helped with the quick separation of drugs from biological samples after their interaction with the sorbent surface [1]. Acetonitrile, as an effective eluent was used for desorption of the drugs from the sorbent prior to their quantification by HPLC-MS detection. The chemical and morphological characteristics of the synthesized Fe_3O_4/Au-Pd@CNT@rGO were studied by FE-SEM, EDX, elemental mapping, TEM, and XRD analytical techniques. The effects of key parameters including amount of extraction and desorption solvent, extraction and desorption time, and pH of the solution were optimized and good precision and sensitivity were achieved. Under the optimum conditions, the limits of detection were obtained 10 µg L^{-1} for erlotinib and 0.15 mg L^{-1} for nilotinib in aqueous solutions. The relative standard deviations (RSD%) range for samples varied from 0.8% to 8.1% (n = 3). The relative recoveries varied from 66.0% to 110.4%. Finally, the method was successfully applied for the simultaneous determination of three anticancer drugs in human serum and urine samples with good recoveries. This validated method can provide support for clinical therapeutic drug monitoring and pharmacokinetic investigations.

Keywords: Erlotinib, Nilotinib, Extraction, High performance liquid chromatography, Tyrosine kinase inhibitors

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PMMA based nanofiber mats containing carbon quantum dots for the sensitive detection of metal ions: The role of different polymer compositions

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Electrospun nanofibers have utilized at different applications including biomedical application, environmental protection, electrical usage, protective clothing and sensors. Nanofiber-based sensors have attracted a great attention due to their simple fabrication method, large surface area and increasing the surface detection sites [1, 2].

This study describes the influence of different PMMA-based polymer compositions for the preparation of nanofiber mats for sensor application. In this regards, the effect of applied voltage, solvent, polymer concentration and distance were studied and four different compositions were attempted including: 1) Poly(methyl methacrylate)/Acrylamide, 2) Poly(methyl methacrylate)/Acrylic acid/Trimethylolpropane triacrylate, 3) Poly(methyl methacrylate)/Polyethylene glycol acrylate and 4) Poly(methyl methacrylate)/Polyurethane acrylate. The morphology of nanofibers was surveyed using scanning electron microscope. The best morphology with the lowest amount of beads were obtained for the composition of poly(methyl methacrylate) (PMMA) and polyurethane acrylate (PUA). Afterwards, nanofiber-based probe were prepared using carbon quantum dotes (CQDs) and the fluorescent nanofibers were prepared for metal ion detection. Decrease in fluorescence of nanofiber probe was investigated against different metal ions [3, 4]. The results indicated that the PMMA/PUA nanofiber mats could be an excellent candidates for the fabrication of nanofiber-based probe for the selective and sensitive detection of heavy metal ions.

***Keywords**: PMMA, Metal ion detection, Nanofiber, CQDs, Sensor*

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Solid Phase Extraction Method for the Speciation of Chromium Using Activated Charcoal@$MoSe_2$@Fe_3O_4 Composite Prior to its Determination by Flame Atomic Absorption Spectrometry

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Heavy metal pollution has become a big problem with the development of industry. According to the literature, chromium is a heavy metals having toxic and non-toxic properties for humans and other organisms at different oxidation levels. Cr (VI) is considered to be toxic having carcinogenic effects, while Cr(III) is nontoxic and required for metabolism depending on the exposure concentrations. Due to this importance of chromium species, accurate and precise detection is of great importance, especially in natural sciences [1-4]. In the present study, a simple and sensitive magnetic solid phase extraction method was developed for the separation-preconcentration and speciation of Cr(III) and Cr(VI) in real samples. The methdos is based on solid phase extraction of Cr(VI)-ammonium pyrrolidinedithiocarbamate (APDC) complex on the synthesized activated charcoal@$MoSe_2$@Fe_3O_4 composite. Cr (VI) was calculated as the difference between the total Cr content and the Cr(III) content. For quantitative recoveries, the effects of various parameters such as solution pH, sorbent amount, ligand volume, elution type and volume and effect of foreign ions were investigated. The procedure was applied for the determination and speciation of chromium in water samples. The presented procedure was validated with certified reference material and the obtained results were in good agreement with the certified values.

Keywords: Chromium, Speciation, Atomic absorption spectroscopy, Solid phase extraction

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Deep Eutectic Solvent Functionalized Metal Organic Framework Nanocomposite for Solid Phase Extraction of Rhodamine 6G

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Most of the dyestuffs, which are organic pollutants that cause environmental pollution, have a toxic effect even in very low concentrations in water. Therefore, the analysis of dyestuff pollution, which adversely affects both the ecosystem and human health through direct contact, is kept up-to-date with high accuracy, sensitive and innovative and environmentally friendly adsorbents. Rhodamine 6G (Rh 6G), a reactive azo dyestuff, was chosen as a model dye in this study. Rh 6G one of the oldest and most well-known Xanthan dye groups, and its derivatives are widely used in the textile, agriculture, cosmetics, food, pharmaceutical, paper, plastic and printing industries, fluorescent labeling sectors due to their intense pink color fastness and low production costs [1,2]. NH_2-MIL-53 (Al)-DES (MOF-DES) nanocomposite was synthesized by the impregnation method for the extraction and determination of Rh 6G from environmental samples. DES was prepared by mixing choline chloride and urea in a molar ratio of 1:2. MOF-DES nanocomposite was synthesized using impregnation method at a ratio of 60:40 (w/w). The characterization of the structure was performed using SEM-EDX, FT-IR, XRD, XPS, TGA, and BET analyses. For the extraction and determination of Rh 6G from water, the solid phase extraction method was used in real water samples under optimum conditions after the optimization of solid phase extraction parameters. All analyzes were performed using UV-Vis Spectrophotometer and HPLC-FLD system was used to verify the real sample applications. The obtained results showed that the synthesized MOF-DES nanocomposite is a suitable adsorbent for the determination of Rhodamine 6G in water.

Keywords: Rhodamine 6G, MOF-DES, Solid phase extraction, UV-Vis spectrophotometer, HPLC-FLD

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A co-precipitation method for Ziram at trace levels prior to its indirect determination by flame atomic absorption spectrometry

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Ziram (zinc bis(dimethyldithiocarbamate) dithiocarbamate (DTC) fungicide is used for controlling disease of vegetables and fruits. This fungicide is applied to the leaves, seeds and soil of plants against many different fungi. Although Ziram is used to treat plants, it causes eye inflammation and skin allergy in direct exposure. It is known that it causes changes in the cardiovascular system in long-term exposure. For these and similar reasons, it is important to determine the trace level of Ziram [1-2]. In this study, a new co-precipitation method was developed for the separation-enrichment and determination of trace-level Ziram fungicide from food samples. Zinc content of Ziram was determined by flame atomic absorption spectrometry (FAAS). Ziram content of the samples was calculated with the stoichiometric ratio between Ziram and Zinc. Magnesium (II) concentration, hydroxide concentration and interference matrix effects are optimized. This method was validated by the addition recovery tests in various food samples.

Keywords: Ziram, Pesticides, Dithiocarbamate, Seperation, Co-precipitation.

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Combination of a dispersive solid phase extraction method based on octadecylamine modified magnetic nanoparticles with dispersive liquid–liquid microextraction for the extraction and preconcentration of pesticides

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Pesticides have been an integral part of the agricultural process by preventing or reducing losses and unquestionably will continue to play an important role in most areas of crop production [1]. However, there is overwhelming evidence of both direct and indirect dangers involved in the use of these chemicals [2]. Based on these facts there is an increasing need for constant monitoring to determine the concentration of pesticides in extensively consumed food stuff including fruits and fruit juices [3]. In this research, a highly-effective and reliable method based on octadecylamine@Fe_3O_4 was proposed in magnetic dispersive solid phase extraction (MDSPE) procedure. The MDSPE method was followed by dispersive liquid-liquid microextraction and employed for the extraction and preconcentration of some widely-used pesticides (haloxyfop–R–methyl, clodinafop–propargyl, oxadiazon, chlorpyrifos, diniconazole, fenpropathrin, and fenoxaprop–P–ethyl) from fruit juices prior to their analysis with gas chromatography–flame ionization detection. In MDSPE step, the analytes were adsorbed onto the sorbent from aqueous solution containing Na_2SO_4 by vortexing and then the sorbent was separated by an external magnetic field. The analytes were eluted by ACN from the sorbent surface. The eluent obtained was mixed with chloroform and injected into deionized water containing dissolved NaCl. After the final centrifugation, the sedimented phase was collected and an aliquant of it was injected into the separation system. Satisfying analytical figures of merit including high enrichment factors (353-443) and extraction recoveries (70-88%), wide linear ranges of the calibration curves, and low limits of detection (0.23-0.41 $\mu g\ L^{-1}$) and quantification (0.81-1.3 $\mu g\ L^{-1}$) were achieved in the present study.

Keywords: Magnetic dispersive solid phase extraction, Dispersive liquid–liquid microextraction, Gas chromatography, Pesticide, Octadecylamine@Fe_3O_4

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Application of the NiO Catalytic Properties in Chemiluminescence Reactions for Isoniazid Determination in Luminol – Dissolved oxygen Chemiluminescence System

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In this paper, a NiO hollow microspheres-luminol-dissolved oxygen chemiluminescence (CL) system was proposed for determination of isoniazid in tablet and serum samples. The NiO nanoparticles (NiO-NPs) were prepared by a simple hydrothermal method which were characterized by X-ray diffraction (XRD), scanning electron microscope (SEM), and Fourier transform infrared spectroscopy (FT-IR). The NiO-NPs have a catalytic effect on the luminol-dissolved oxygen CL system for measuring isoniazid. The effect of important parameters on determining method efficiency, such as concentration of NaOH, luminol and nanoparticles were investigated. At the optimum conditions, the calibration curve for isoniazid was obtained in the range of 8×10^{-7} to 1×10^{-4} M (R^2=0.99). The detection limit of the method was obtained 2×10^{-7} M. In addition, the proposed method was successfully used to determination of isoniazid commercial tablets and human serum as real samples. The acceptable relative standard deviation (RSD) was obtained for the proposed CL method (2.63%, n=10).

Keywords: Nickel Oxide, Chemiluminescence, Isoniazid, Luminol

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Development of a magnetic dispersive solid phase extraction method with dispersive liquid-liquid microextraction using graphene modified magnetic nanoparticles for the extraction of some pesticides in fruit juices followed by GC-MS

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In agriculture, pesticides are the chemical compounds that are used to prevent pests from spreading and to help farmers produce high-quality products. The environment and human health are harmed by the pesticides used inordinately [1]. It can cause some adverse effects on the health of consumers such as increasing the incidence of cancer, endocrine disorders, neurological disorders, etc. if pesticide residues are present in agricultural products like fruits [2]. As a result, pesticide residues need to be investigated. Various techniques are used to measure pesticide residues in different samples including high performance liquid chromatography, gas chromatography (GC), supercritical fluid chromatography, and ion mobility spectrometry. In this work, graphene magnetic nanoparticles were prepared and used as an effective sorbent in magnetic dispersive solid phase extraction combined with dispersive liquid-liquid microextraction for the extraction of seven pesticides from different fruit juices. Then, their determination was done by gas chromatography–mass spectroscopy. First, the studied pesticides were adsorbed on the sorbent from a solution containing dissolved Na_2SO_4. In the following, the analytes were desorbed from the sorbent by 2-propanol. Then, the eluent containing analytes was separated from the sorbent, mixed with 1,1,2-trichloroethane (at µL level), and quickly injected into a solution containing dissolved NaCl. After centrifuging the formed cloudy solution, an aliquot of the sedimented organic phase was injected into a gas chromatograph equipped with a mass spectrometer. The sorbent was synthesized by a co-precipitation method. The sorbent was characterized by energy dispersive X-ray spectroscopy, scanning electron microscopy, vibrating sample magnetometry, Brunauer–Emmett–Teller nitrogen sorption, Fourier transform infrared spectroscopy, and X-ray diffraction. The developed method exhibited low limits of detection and quantification in the ranges of 0.04-0.06, and 0.13-0.19 ng mL^{-1}, respectively. Extraction recoveries and enrichment factors were obtained in the ranges of 42-76% and 155-362, respectively. The method had good linearities ($r^2 \geq 0.992$).

Keywords: Magnetic dispersive solid phase extraction, Dispersive liquid-liquid microextraction, Gas chromatography, Pesticides, Fruit juice

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Solid phase extraction of Ni(II) from water and food samples on Fe_3O_4@ Diaion HP-2MG

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Heavy metal pollution increasing due to human activities and the problems the problems related with it are increasing gradually. Heavy metals negatively affect the soil, food and water ecosystem and also accumulate in the body through the air, skin or digestive system [1]. Nickel is an essential element for human metabolism at trace level but high amount of nickel toxic effect on human body. Therefore, the analysis of Ni(II) especially in complex matrices is important. Ni(II) concentration in real samples is and cannot be directly determined even by sophisticated analytical devices like FAAS, ICP-MS and X-Ray fluorescence spectroscopy. For this purpose, separation-enrichment methods are needed. In this regard magnetic solid phase extraction method has been developed due to its high enrichment factor, low cost, low reagent consumption, ease of automation and environmental friendly features [2].

In this study, magnetic Diaion HP-2MG resin was synthesized for rapid extraction, enrichment and determination of trace amounts of Ni(II) ions. Diaion HP-2MG polymer with polymethacrylate matrix is relatively hydrophilic. Among the parameters affecting the Ni(II) extraction efficiency like pH, resin amount, matrix effect, sample volume, eluent type and volume were optimized [3]. After optimizing the analytical parameters such as LOD, LOQ, PF and reusability, the accuracy of the developed method was applied to natural water and food samples by using standard addition method. Validation of the method was carried by applying the method to water and food certified reference material having trace Ni(II) content.

Keywords: Nickel, Diaion HP-2MG, Magnetic solid phase microextraction, Separation-preconcentration, FAAS

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Performance evaluation of coated LDH with polymer in the extraction of 12 pesticides in carrot and apple samples before liquid chromatography-tandem mass spectrometry

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To measure small amounts of pesticides in real samples, it is often necessary to perform a pre-concentration and preparation method to clean the sample and concentrate the analytes. The characteristics of an ideal preparation method in analytical chemistry have high speed, ease to use, low cost, environmentally friendly, compatibility with analytical tools and automation capability [1]. In this research, a dispersive solid-phase extraction (DSPE) based on layered double hydroxide (LDH)/polyaniline (PANI) composite as a sorbent was developed to effectively enrich some pesticides prior to high-performance liquid chromatography-tandem mass spectrometry (HPLC-MS/MS). The characterization of the sorbent was carried out in detail. Adsorption and desorption steps have been optimized in detail to obtain efficient phase separation and reliable analytical results. Under optimized conditions, the presented method exhibited a wide working range (0.15-1000 ng mL^{-1}), low detection limits (as low as 0.05 ng mL^{-1}) and acceptable extraction recoveries (70-75%). The precision of the method was evaluated by intraday and interday studies for three different concentrations of studied pesticides. The matrix effect was investigated by the recovery study. Following validation studies, the presented method was successfully applied to the extraction and determination of the studied pesticides from carrot and apple samples.

***Keywords**:* Pesticides, Extraction, Chromatography, High-performance liquid chromatography, Spectrometry

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Pt-Bi-N4/PC Resulting from Reconstructed Bismuth-Based Metal- Organic Framework-redox replacement and investigation of its use as electrocatalyst for ethanol oxidation

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Direct ethanol fuel cells (DEFCs) as clean energy-converting devices, have received considerable attention because of their high energy density, less toxicity of ethanol as fuel, and their potential use in variety of applications. However, the major challenges in these fuel cells are high cost and low poison tolerance of Pt, Pd and their alloy materials as excellent electrocatalyst for ethanol oxidation. Significantly, these problems are overcome by decreasing the amount of precious Pt-group metals via increasing its utilization efficiency through the preparation of highly-dispersed supported metal catalysts and by alloying with the non-precious metals like Bi, Pb, Sn, and Cu, which enhances electrocatalytic activity, minimizes the CO poisoning, and also reduces of the amount of noble metal in the anode of DEFCs [1]. In this study, the bismuth-containing metal-organic frameworks (CAU-17) with hexagonal prisms and fiber morphology have been synthesized through a facile ultrasound-assisted wet-chemical approach at room temperature in methanol solutions of Bi(III) nitrate, 1,3,5-benzenetricarboxylic acid (BTC) ligand and CTAB surfactant. Then, Bi-N4 sites on porous carbon (PC) supports were prepared through decomposition of CAU-17 and dicyandiamide (DCD) for preparing Bi-N4/PC electrocatalyst via post thermal treatment at 400 and 800 °C for 1 h at H_2/N_2 atmosphere [2]. The resulting Bi-N4/PC was used for preparation of Pt-Bi-N4/PC electrocatalyst by redox replacement reaction, which galvanic replacment of Bi atoms with Pt occurs spontaneously. The Pt-Bi-N4/PC electrodes exhbite higher electrocatalytic activity and enhanced poison tolerance for the ethanol oxidation as compared to Pt-Bi/PC, prepared without using of DCD, and commercial Pt/C catalyst. Also, The synthesized electrocatalysts were characterized by transmission electron microscopy, scanning electron microscopy, Raman spectroscopy, Fourier transform infrared spectroscopy, and X-ray diffraction techniques.

Keywords: CAU-17, Electrocatalyst, Direct ethanol fuel cells, Galvanic replacment

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Electrocatalytic Performance of the Ni-MOF/NCB/CC Nanocomposite Decorated with NiNPs for Alkaline Methanol Fuel Cell.

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In recent years, with the development of industry and transportation, the consumption of fossil resources has drastically increased, leading to serious pollution and energy crisis. Thus, the development of renewable energy sources to take the place of gradually depleting fossil resource–based fuel is the most urgently required task to resolve the environment and the energy issues [1]. Direct methanol fuel cells (DMFCs) play an important role in energy conversion and storage. Developing highly-active and low-cost anode catalysts for DMFCs is the main prerequisite for the commercialization of energy conversion systems. Even though Pt is the most widely applied anode catalysts for DMFCs at present, its drawbacks of low electrocatalytic stability, high cost, and the easily poisoned by oxidation intermediates such as CO, have impeded its practical applications. the carbon-based catalysts with porous metalorganic frameworks (MOFs) consisting of metal nodes and organic linkers are a good strategy among many improved methods [2]. Metal-organic frameworks (MOFs) and derived materials have been used in a wide range of fields, e.g. fuel cell, gas storage and separation, batteries and catalysis etc., benefiting from their high specific surface area, tuneable porosity and abundant active metal sites [3].Limited applications of MOFs for electrocatalysis, because of their constrained charge transfer and dejected electrical conductivity, can be overcome by combining them with conductive materials, such as with CNTs, graphene, reduced graphene oxide or metal nanoparticles, transforming them into potential candidates for electrochemical processes, such as direct methanol fuel cells (DMFCs) [4]. In this work, first, carbon black nanoparticles (CBNPs) were integrated into a carbon ceramic electrode (CBNPs/CCE) as a renewable electrode for electrocatalytic purposes, and then the nickel MOF/NiNPs nanocomposite was loaded onto the synthesized electrode. The as-synthesized nanocomposite was structurally characterized by means of various techniques. The results showed excellent electrocatalytic activity and outstanding stability towards the electro-oxidation of methanol in alkaline medium. The greater surface area, additional stability and improved electrical conductivity provided by incorporation of Ni nanoparticle into Ni-MOF and use of carbon black (CB) as a substrate, play important roles in enhancing the electrocatalytic activity of synthesized materials.

Keywords: Fuel cells, Nickel metal-organic frameworks, NiNPs, Electrocatalyst, Carbon black.

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MOF-derived Co/C@GS nanocomposites encapsulated by $Ni(OH)_2$ for high performance glucose sensor

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Glucose (Glu) is an important component of human physiological liquid, and its content is related to the normal metabolism of the human body. High levels of glucose can lead to diabetes, posing a serious threat to human health [1,2]. Therefore, the control of its level is of key importance. Nowadays, the glucose sensors that are supported by electrochemical technique have been widely used for detecting glucose, because the electrochemical sensors have advantages of simplicity, rapidness, high sensitivity and low power requirement [3]. In this study, an electrochemical non-enzymatic sensor based on a $Ni(OH)_2$@Co/C@GS nanocomposite was developed for the selective and sensitive determination of glucose. A metal-organic framework (MOF) with high surface area was used for the design of Co/C nanoparticles. The as-synthesized nanocomposite was structurally characterized by Fourier-transform infrared spectroscopy (FT-IR), X-ray diffraction (XRD), field emission scanning electron microscopy (FE-SEM), energy dispersive spectroscopy (EDS), and elemental mapping. The prepared Ni(OH)2@Co/C@GS nanosensor exhibited excellent electro-catalytic activity for glucose oxidation. Moreover, the sensor possessed high sensitivity and selectivity for real-time amperometric detection of glucose. It performed glucose level detection in human serum samples with acceptable reliability and accuracy.

Keywords: Metal-organic frameworks, $Ni(OH)_2$, Glucose, Electrochemical, Non-enzymatic nanosensor.

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Eco-friendly green method for lead ion removal by *Dunalliela Salina algae*

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The environmental pollution of heavy metal ions has become a major global problem due to thoughtful industrial development[1]. Therefore, the removal of heavy metal ions at an acceptable level, because of economic and environmental concerns, is a key issue. Recently, one of the most effective biosorbent is the algal species that has attracted worldwide attention [2], [3]. This study suggests *Dunalilla Salina* (*D. Salina*) as an efficient biosorbent for the removal of lead ion contaminants. Additionally, this species of algae has high growing potential and is easily harvestable. The aim of the present study is to investigate the efficiency of *D. Salina* algae as an effective and eco-freiendly biosorbent for the treatment of lead-contaminated water. Various parameters such as pH, contact time, biosorbent dosage, injection time and initial concentration of lead ions were also optimized using central composite design (CCD) under response surface methodology (RSM) technique. The most amazing results to appear from the data were that all experiments showed the maximum uptake efficiency of 80% - 96%.The results confirmed the effectiveness of treating lead-contaminated water with low cost, high efficiency and the possibility of metal recovery. *D. Salina* biomass surface was analyzed by means of scanning electron microscopy (SEM) and energy dispersive spectrometry (EDS). This study also applied fourier transform infrared (FT-IR) spectroscopy to identify the main functional groups involved in the interaction between algae and metal ions. Hence, *D. Salina* could be used for bioremoval of lead ions from polluted water in an economic and safe manner.

Keywords: *Dunalliela Salina*, Biosorption, Lead ions

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ZIF-7@ZIF-67/ polyether sulfone composites for dispersive solid-phase extraction of Bisphenol A and 2-phenylphenol

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Bisphenol A (BPA) as a typical endocrine disrupting chemicals (EDCs) result in cancer development and reproduction problems [1]. BPA has been widely used in industries as raw materials for epoxy and polycarbonate plastics, such as baby bottles, lining of food cans, dental sealants [2], as a color developer in a thermal paper. 2-phenylphenol (BPh) is as an agricultural fungicide and used for waxing citrus fruits. Sample preparation and pre-treatment is one of the most important and crucial steps for extraction and preconcentration of target analytes from different matrices. Among sample pretreatment methods. Dispersive solid-phase extraction (DSPE) is a type of SPE method and is as an attractive sample pretreatment technique that offers unique advantages, such as simplicity, high speed, and broad applicability. In this work, ZIF-7@ZIF-67/polyether sulfone was used as an adsorbent for the dispersive solid phase extraction (DSPE) of BPA and BPh from soft drink bottle, disposable plastic food container and thermal paper samples followed by their determination with high performance liquid chromatography-ultraviolet detector (HPLC-UV). The extraction factors such as sorbent amount, sample pH, desorption solvent, desorption time, ionic strength, desorption volume and extraction time, breakthrough volume were investigated and optimized. Under the optimum conditions, the calibration curves were constructed and good linearities were achieved with R2: 0.9994 and 0.9979 for BPA and BPh in the concentration range of 2.0–500.0 μg L−1 for both of the analytes. The LOD was calculated based on 3(sd)blank/m and was found to be 0.6 μg L− 1 for both of the analytes. The recoveries of the spiked samples are in the acceptable range of 90-112%, with the RSD values of 1.0-5.0% for BPA and 76-109%, with the RSD values of 0.3-6.1% for BPh indicating the good validity of the method.

Keywords: Dispersive solid-phase extraction, Zeolitic imidazolate framework, Bisphenol A, 2-phenylphenol, High performance liquid chromatography-ultraviolet detector.

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Synthesis and characterization of g-C_3N_4/$CoFe_2O_4$/ZnS photocatalyst for removal of Acid Blue 92 dye under visible light irradiation

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The textile industry contains a massive dose of dyes pollutants, that causes dangerous diseases and environmental problems by discharging toxic and carcinogenic effluents into the environment. In this regard, various methods like adsorption, chemical precipitation, flocculation, electrochemical processes, and photocatalysis have been used by various Scientific societies [1]. Among the various methods, the heterogeneous photocatalytic process is very suitable due to its simplicity, good efficiency, non-toxicity, and non-selectivity of pollutant removal [2]. This article reported the synthesis of a visible-light photocatalytic composed of spinel cobalt ferrite ($CoFe_2O_4$) and zinc sulfide (ZnS), which are integrated into uniform spheres, on graphitic carbon nitride (g-C_3N_4) nanosheets. The as-prepared nanocomposite was characterized by infrared spectroscopy (FT-IR), field emission scanning electron microscopy (FE-SEM), energy-dispersive x-ray spectroscopy (EDS), and X-ray diffraction (XRD) analysis, and Vibrating Sample Magnetometer (VSM). The oxidation ability of the novel photocatalyst was evaluated using Acid Blue92(AB92) as a target pollutant. The photocatalytic activity of g-C_3N_4/$CoFe_2O_4$/ZnS for degradation of Acid Blue 92 under visible light irradiation was increased, to be much higher than that of single g-C_3N_4, clearly demonstrating a synergistic effect between $CoFe_2O_4$, ZnS, and g-C_3N_4. The synergic effect between $CoFe_2O_4$, ZnS, and g-C_3N_4 was found to lead to an improved photo-generated carrier separation [2, 3]. The catalyst dose, initial dye concentration, pH, and time were set as 0.09 gL^{-1}, 20 mgL^{-1}, 3.8, and 100 min, respectively. The high removal efficiency of AB92 dye (99%) was obtained under these conditions. Finally, a reusability test of the nanocomposites revealed a just 9% decrease in their removal efficiency after seven consecutive runs. As a result, the synthesized nanocomposite can be promising to reduce pollution arising from harmful organic dyes.

Keywords: Advanced oxidation processes, Photocatalysis process, Nanotechnology, Organic dye pollutants

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A smartphone-based digital imaging method for trace determination of cadmium in water

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Health risks of heavy metals (HMs) contribute to advances in diagnosis and treatment of polluted water is an important subject for scientific society [1]. New methods of point of care testing (POCT) include tests in which samples are analyzed at the sampling site [2, 3]. This article describes smartphone-based POCT for cadmium in water. In this study, cadmium quantification was done by a light control box that contains a white light-emitting diode (LED). The dithizone ligand was used to produce a specific dye solution. The results of the free Color Grab application confirm that the cadmium concentration is proportional to the intensity of the red color. The calibration graph was linear range in the range of 0.05–1.0 mg L^{-1} with a limit of detection (LOD) of 0.01 mg L^{-1}, whereas the quantification limit was 0.04 mg L^{-1}. The average recovery rate for cadmium spiked in the water samples was 99.4%. Cadmium was determined in well water, tap water, and commercial water samples. The accuracy of smartphone-based digital imaging method was acceptable compared to atomic absorption spectrophotometric data (paired *t*-test). Smartphone-based POCT tests are cost-effective, accurate, and easy to perform in areas with limited resources. Therefore, they are considered a potential for routine diagnostic tests.

Keywords: Smartphone-based digital imaging, Cadmium, Colorimetry, Water samples

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Amplified Electrochemical Sensor for High Sensitive Analysis of Anti-Tuberculosis Drug Employing Pencil Graphite Electrode Modified with Copper-based Metal-Organic Frameworks Nanocomposite

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Pyridine-4-carboxylic acid hydrazide, isoniazid (INZ), as an antibiotic agent is administered to manage tuberculosis (TB). In addition, the INZ is a common chemotherapy drug to treat pulmonary TB in combination with pyrazinamide, rifampicin, ethambutol, and streptomycin [1]. Several analytical methods based on spectroscopic, chromatographic, and electrochemical techniques are available in the literature for the determination of INZ [2]. the electrooxidation of INZ at the provided modified electrodes always required a high overpotential, and acidic or alkaline supporting electrolyte, which brought great inconvenience to the analytical procedure and was unsuitable for the analysis of the INZ in real biological samples. Hence, it is required imminently for the synthesis of the novel modifiers and construction of the suitably modified electrodes, which could decrease the overpotential of INZ electrooxidation and increases the anodic current to produce high sensitivity, long-term stability, and cost-effective electrochemical sensors for electron detection of INZ in neutral media. This paper reports a series of novel electro-treated pencil graphite electrodes (ETPGE) modified with copper-based metal-organic frameworks (Cu-MOFs)/carbon nitride quantum dots (CNQDs) nanocomposite for the first time for sensing the INZ. The morphology and structure of the composite electrode were characterized via X-ray diffraction (XRD), scanning electron microscopy (SEM) and Fourier transform infrared (FT-IR) spectroscopy. After optimization of the parameters influencing the formation of Cu-MOFs/CNQDs/ETPGE, the composite electrode showed efficient electrocatalytic performance for isoniazid in neutral media. A wide linear concentration range (0.1μM to 65μM), a good sensitivity (1.507 A mol^{-1}Lcm^{-2}), and a low detection limit (0.0675μM) were obtained. Furthermore, the long-term stability and fabrication reproducibility of the electrochemical device has been investigated, as well as its robustness to interferent species. Further, the suggested method was employed successfully for the determination of INZ in drug and biological samples with satisfactory recovery values.

Keywords: Isoniazid, Copper-based metal-organic frameworks, Carbon nitride quantum dots, Pencil graphite electrode

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Rapid and Sensitive Determination of Omeprazole based on New Synthesis of Ferrite/ Functionalized Graphene Oxide Nanosheets Nanocomposite

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Omeprazole (OMP), a substituted benzimidazole compound and prototype antisecretary agent, belongs to a new class of potent and clinically active inhibitors of gastric acid secretion[1]. They mainly act to regulate acid production in the stomach and are used for treating various acid-related disorders such as duodental, gastric, and esophageal ulceration [2]. Therefore, determining of these drugs in pharmaceutical formulations and biological samples is very important. In this research, an effective, selective and accurate method for determining the OMP residues is presented based on glassy carbon electrode (GCE) modified with nickel-copper-zinc ferrite/ carboxymethyl cellulose/ graphene oxide nanosheets ($Ni_{0.4}Cu_{0.2}Zn_{0.4}Fe_2O_4$/CMC/GONs). The morphological properties of the suggested sensor were explored by Scanning electron microscope (SEM), Fourier-transform infrared (FTIR), and X-ray powder diffraction (XRD), techniques as well as its electrochemical characteristics versus OMP were invigilated in detail. The proposed sensor was capable of measuring the OMP in the linear range of 0.24-5 and 5-75 μM with a detection limit of 0.22 μM. The use of the newly designed sensor to determine OMP in real samples such as human plasma and OMP tablets demonstrates its appreciable sensing potential in complex matrices. Most importantly, prepared $Ni_{0.4}Cu_{0.2}Zn_{0.4}Fe_2O_4$/CMC/GONs nanocomposites could certainly be a promising candidate for a wide range of electrochemical and bioassay applications.

Keywords: Omeprazole, Carboxymethyl cellulose, Graphene oxide nanosheets, Ferrite

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Heteroatoms Doped Graphene/Metal–Organic Framework-Based Electrochemical Method for Detection of Anti-Depressant Drug

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Sertraline hydrochloride in pharmaceutical formulation, sold under the brand name (Sidata, Zoloft, Lustral), with the IUPAC name of cis-1S, 4S-N-methyl-4-(3, 4-dichlorophenyl)-1, 2, 3, 4-tetrahydro−1-naphthalenaminehydrochloride, is an anti-depression drug that due to fewer side effects, it is one of the most commonly used drugs for the treatment of depression. However, recent studies have shown that selective serotonin reuptake inhibitors(SSRI) such as sertraline infiltrate the cell membrane and greatly increase the risk of developing cancer [1,2]. Therefore, accurate assay of sertraline and its metabolites in biological samples, such as blood, plasma and urine is necessary. Metal−organic frameworks (MOFs) [3] have been previously investigated as electrode materials for developing electrochemical sensors. They have usually been reported to suffer from poor conductivity and improvement in the conductivity of MOFs is still a great challenge. Here, we reported the fabrication of an electrochemical sensor based on the in situ growth of copper based metal-organic framework (Cu-MOF) on conductive sulfur and nitrogen co-doped graphene (SNDGr) modified pencil graphite electrode (PGE) (Cu-MOF/SNDGr/PGE). The as-fabricated modified electrode was characterized using scanning electron microscopy (SEM), X-ray diffraction (XRD), electrochemical impedance spectroscopy (ESI), and cyclic voltammetry. The voltammetric response of Cu-MOF/SNDGr/PGE toward Sertraline hydrochloride (STLHC), as an anti- depressant drug, is dramatically higher than Cu-MOF/SNDGr/PGE because of the synergic effect of the SNDGr and Cu-MOF. The calibration curve at the Cu-MOF/SNDGr/PGE for STLHC over the concentration range of 0.05 to 2.67, 0.05 to 2.67 μM, with a detection limit of 0.038 μM (38 nM). The content of sertraline in Zoloft tablets was also detected to validate the applicability of proposed modified electrode.

Keywords: Metal−organic framework, Sertraline hydrochloride, Electrochemical sensor, Sulfur and nitrogen co-doped graphene

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α-MnO_2/FeCo LDH composite as an excellent efficient electrocatalyst for water oxidation

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The energy challenge is one of the most important issues facing humanity today, which is why the expansion of cheap, clean, accessible, and environmentally friendly energy sources is important. One of the best ways to get renewable energy is to use water splitting. The water oxidation reaction has slow kinetics, so it is important to use cheap and effective electrocatalysts that reduce the oxidation potential of water [1-3].

In this work, we report the synthesis of α-MnO_2/FeCo LDH by the hydrothermal method. The catalyst of α-MnO_2/FeCo LDH growth on nickel foam demonstrates high electrocatalytic property in oxygen evolution reaction due to its electrical strength and high catalytic activity. Electrochemical measurements were performed in the potential range 0 -1.8 V vs. Ag/AgCl. Linear scanning voltammetry (LSV), chronoamperometry, Electrochemical impedance spectroscopy (EIS) techniques, and Tafel plot were used to investigate the electrocatalytic behavior of synthesized nanostructures. Tafel curves and EIS Method were performed to investigate the kinetics of splitting water reaction. In addition to the high surface area, another advantage of this catalyst is its good stability over time, which was tested by chronoamperometry. For this electrocatalyst, the initial potential for water oxidation reaction is 0.23 mV vs. Ag/AgCl The catalyst synthesized to reach 5 mA cm^2 in oxygen evolution reaction only has 210 mV overpotentials. The electrocatalysts were characterized by XRD, FT-IR, RAMAN, SEM, TEM, EDS, and MAP techniques. The modified electrode has a large exchange current, low overpotential, and a small Tafel slope which indicates the high electrocatalytic performance of the electrode in the water oxidation reaction.

Keywords: Electrocatalysis, Oxygen evolution reaction, Layered double hydroxides, Linear scanning voltammetry

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Investigation of Photocatalytic Properties of Modified Graphitic Carbon Nitride ($g-C_3N_4$) by UV–vis and Fluorescence Spectroscopy

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In this work, graphitic carbon nitride ($g-C_3N_4$) was synthesized and modified with various soft templating such as sodium dodecyl sulfate (SDS) and cetyl trimethyl ammonium bromide (CTAB)[1]. The samples were characterized with FESEM, XRD, FTIR and BET methods. Photodegradation was performed using bulk $g-C_3N_4$ and the modified compounds under visible-light for degradation of rhodamine B as a pollutant. The photodegradation process was studied by UV-visible and fluorescence spectroscopic techniques. The photocatalytic efficiency of $g-C_3N_4$ _SDS (96%) was significantly improved in related to the bulk sample $g-C_3N_4$ (43%). The photodegradation process was optimized by implement of BOX-Behnken design[2]. Results revealed that the photodegradation efficiency was reached to 96% after only 30 min under optimized conditions (pH = 2.73, irradiation time =30 min, dose of catalyst=15 mg and concentration of Rhodamine B= 7 ppm). Results indicated that small amount of rhodamine B is removed in the absence of light (dark). It can be concluded that the optical properties of $g-C_3N_4$ $\_{SDS}$ is improved by enhancing recombination lifetime, and according that the electron and hole are more accessible for the photodegradation process [3].

Keywords: Graphite carbon nitride, Photodegradation, Fluorescence spectroscopy, Soft templating

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A Sensitive Method for Determination Glycolic Acid, Mono- and Di-Chloroacetic Acids in Betaine Media Using Amino-Functionalized SBA-15 as a Sorbent and HPLC Assay

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In this paper, amino-modified nanoporous silica (APS-SBA-15) was synthesized as a new solid-phase sorbent for the extraction of glycolic acid, monochloroacetic acid, and dichloroacetic acid in synthetical betaine products. Octadecyl silica cartridge was used to reduce the concentration of matrix betaine. PS-Ag^+ pre-treatment cartridge was applied to remove high Cl concentration [1,2]. The obtained effluent sample was passed through of the APS-SBA-15 sorbent. The effect of pH, flow rate of sample and eluent, and type and volume of the eluent [3] were investigated and optimized. Chloroacetate and glycolate were eluted with 0.8 $mol.L^{-1}$ solution of HClO4 and measured by HPLC with a UV–VIS detector. At optimum effective parameters, preconcentration factor of 129 was achieved in this method. The limits of detection of mono and dichloroacetic acid and glycolic acid were 13, 3.7, and 8.6 $ng.L^{-1}$, respectively.

Keywords: High performance liquid chromatography, Solid-phase extraction, Amino-modified nanoporous silica, Betaine, Mono-and dichloroacetic acid, Glycolic acid.

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Effect of competitive interferences on the biosorption of lead ions using Artemia Cysts

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Water being an existential element that sustains life on earth, undoubtedly gives rise to the cruciality of dealing with its contamination. Even trace amounts of heavy metal contaminating water impose a detrimental threat to human health [1]. Various biomaterials, have been examined as sorbents to remove heavy metal ions [2]. However, during the treatment process of wastewater, most biosorbents would be saturated with high salt ion concentrations, resulting in loss of chemical stability. Therefor, researchers are persistently investigating the potential use of adsorbents with sufficient capacity for intended ion adsorption in the presence of other competitive ions. Selectivity is argued as one of the essential parameters for successful adsorbent proces [3]. In this study, we propose Artemia cyst as a robust lead ions biosorbent in the presence of high concentration of $Ca^{2+}/Mg^{2+}/Na^{+}/Cd^{2+}/Co^{2+}/Cu^{2+}/Mn^{2+}/Ni^{2+}$ at optimum experimental condition (pH: 5.8, 0.5 g L^{-1} sorbent at 25°C). Results showed Artemia cyst with impressive selectivity and applicability in the presence of common available ions (Ca^{2+}, Mg^{2+} and Na^{+}) in their natural environment. The large selectivity distribution ratio, K_d (mL g^{-1}) for Artemia cyst samples, were verified their excellent selectivity and preferential biosorption performances. Moreover, The interfering heavy metal ion concentrations such as Cd^{2+}, Mn^{2+}, Co^{2+}, $Cu^{2+}$and Ni^{2+}, on lead ion biosorption by Artemia cyst were demonstrated having faintly lower biosorption (73.5%) when compared to single ion biosorption (94.40%). Thermodynamic parameters of the biosorption process calculated. The negative value of change in Gibbs free energy (ΔG) indicated the spontaneous adsorption of lead ion on the biosorbent. The enthalpy change indicated that an exothermic reaction was occurring during the biosorption process in which the ΔH was -28.74 kJ mol^{-1}. The maximum uptake of lead ions was observed at 298 K. Artemia cysts surface was characterized using scanning electron microscopy (SEM), energy dispersive spectrometry (EDS) and X-ray diffraction (XRD) techniques. Results of this study consequentially lead to the recommendation of Artemia cyst with astounding uptake of lead ions as a green approach.

Keywords: Artemia cyst, Selectivity, Biosorption, Heavy metal ions

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Preparation of Zinc Oxide Nanoparticles Reinforced Polyethersolfune Nanocomposite as an Efficient Sorbent for Extraction of Sumatriptan by Thin Film Microextraction and Stir Bar Sorptive Extraction

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In this research, a novel nanocomposite based on incorporation of zinc oxide nanoparticles (ZnO NPs) into polyethersulfone (PES) was prepared by solvent blending method and subsequently it was casted by phase separation method. Additionally, the prepared solvent blending of ZnO NPs/PES was coated on a stir bar substrate through solvent exchange method. The morphology and surface characteristic of PES and ZnO NPs/PES-based thin films and stir bars were investigated using scanning electron microscopy (SEM), X-ray diffraction (XRD) and thermal gravimetric analysis (TGA)[1,2]. The prepared ZnO NPs/PES nanocomposite-based stir bar and thin film was applied for stir bar sorptive extraction (SBSE) and thin film microextraction (TFME) of sumatriptan followed by spectroflourimetry detection. The effect of ZnO NPs doping level into the nanocomposite on the extraction capability of the sorbents was investigated [3,4]. Important factors influencing the extraction and desorption processes including extraction time, salt content, pH, desorption solvent, and desorption time were studied and optimized applying one at a time approach for both techniques. Based on the obtained results, it was revealed that the ZnO NPs doping level of 20 % has lead to the highest extraction efficiency in both techniques. The developed methods has been evaluated in the terms of limit of detection, linearity, precision and accuracy, and their applicability for determination of sumatriptan in real samples was investigated using urine and plasma samples[1,5].

Keywords: Thin film microextraction, Stir bar sorptive extraction, Sumatriptan, Zinc oxide nanoparticles, Nanocomposite

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Smartphone-Based Colorimetric Selective Detection of Propyl Gallate Using Paper-Grafted Molecularly Imprinted Polymer Thin Film Microextraction

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Nowadays, on-site analysis has been considered and has become one of the main goals in analytical chemistry, which has been facilitated by the design of portable analysis devices [1]. Portable devices accompanied by smartphones are the phenomena of modern life and can become an ideal analysis system that acts like common lab analysis instruments [2]. Molecularly imprinted polymers (MIPs) are synthetic polymeric materials synthesized with specific molecular recognition capabilities that have proven to be very interesting mimetic receptors. Selectivity, physicochemistry, stability, ruggedness and sensitivity combined with relatively low cost are some of the benefits of MIP [3]. In this work, the colorimetric test system is based on MIP thin film with synthetic receptor sites that are capable of selective detectin of propyl gallate (PG). The color intensity was measured and converted to red green blue (RGB) values with a smartphone by using a free application (Color Grab). MIP thin film was created on the cellulose paper surface using the surface imprinting method. It was obtained by simultaneous polymerization of a functional monomer with ethylene glycol dimethacrylate (EGDMA) as a crosslinker. The choice of functional monomer, its molar ratio and solvent was based on the results of computational modeling. PG molecules were selectively adsorbed by MIP thin film and after desorption were measured using reaction with Fe(II) ion. The intensity of RGB was analyzed in proportion to the PG concentration in the sample.

Keywords: Thin film microextraction, Molecularly imprinted polymers, Smartphone, RGB, Propyl gallate

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Preparation of a Novel Thin Film Based on Montmorillonite doped chitosan Nanobiocomposite for Microextraction of Triazines

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In this work, a novel analytical method based on thin film microextraction (TFME) [1] technique has been developed to determine triazines in environmental samples. Triazines are used as important herbicides in weed control, and there are growing environmental concerns about these compounds due to their persistence in nature for many years [2]. Concerning the sorbent based microextraction techniques, designing an efficient adsorbent is an important issue in this research area. Nowadays, there is a growing interest in designing various biodegradable, environmental-friendly and cost-effective adsorbents with controlled adsorptive properties. Chitosan (CS) is a promising biopolymer that has attracted more attention in this research field and has been used as an adsorbent to prevent environmental pollution [3]. Herein, montmorillonite (MMT) nanoclay was incorporated into CS by solvent blending method and subsequently it was casted by solvent evaporation. The morphology and surface characteristic of CS and MMT/CS-based thin films were investigated using scanning electron microscopy (SEM), X-ray diffraction (XRD) and thermal gravimetric analysis (TGA). The prepared MMT/CS nanobiocomposite-based thin film was applied for TFME of triazines followed by gas chromatography-flame ionization (GC-FID) detection. The effect of MMT doping level into the nanobiocomposite on the extraction capability of the sorbents was investigated, revealing that 10 % of doping level has led to the highest extraction capability. Important factors influencing the extraction and desorption processes including extraction time, salt content, pH, desorption solvent, and desorption time were studied and optimized applying multivariate optimization approach. The developed method has been evaluated in the terms of limit of detection, linearity, precision and accuracy, and their applicability for analysis of real samples was investigated by determination of the studied triazines into environmental water samples and the obtained relative recoveries have indicated that the developed TFME-GC method can be successfully applied for this purpose [4].

Keywords: Thin film microextraction, Nanobiocomposite, Triazines, Montmorillonite, Chitosan

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Catalytic activity of polyethylene imine based ionic liquids in the reaction of CO_2 and epoxides to produce cyclic carbonates

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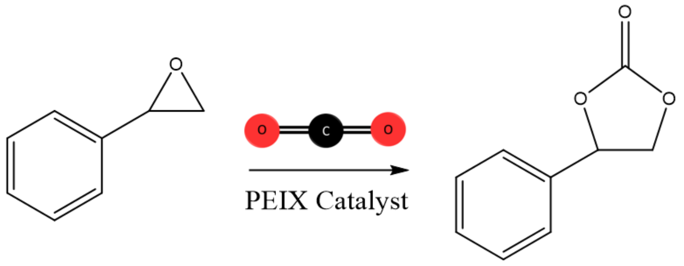
Carbon dioxide is a renewable, inexpensive and non-toxic C_1 building block for the production of valuable chemicals such as methanol, polycarbonates and cyclic carbonates [1]. CO_2 is thermodynamically stable and thus, the required energy for its activation must be provided by different strategies such as reacting it with high free energy substrates. With this regards, using epoxides in the reaction with carbon dioxide is a promising method. The product is cyclic carbonate which has found various industrial applications as polar solvents, precurors for polycarbonate and polyurethane and in the production of fine material [2]. Various homogeneous and heterogeneous catalysts including metal oxides, zeolites, silicates, metal-organic compounds, organic compounds, and ionic liquids have been developed for this reaction [1-4]. However, developing a cost effective catalyst which can give high yield at ambient conditions would be promising. In this study, for the first time we synthesised halogenated polyethylene imines (PEIX, X =I, Br) and characterized them by FT-IR and ^{1}HNMR. PEIXs were evaluated as catalyst in the conversion of carbon dioxide and different epoxides to cyclic carbonates at ambient temperature and pressure. The products of catalytic tests were evaluated by ^{1}HNMR technique. To optimize the catalytic activity of PEIX, reaction condition including reaction time, catalyst loading, and temperature were tuned to get the best yield at CO_2 pressure of 4 atm.



Keywords: Carbon dioxide fixation, CO_2, Epoxide, Cyclic carbonate, Organic catalyst

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Nickel oxide nanoparticles modified with dimethylglyoxime deposited on the surface of filter paper as a thin film for microextraction of tramadol from biological samples

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Tramadol is an opioid, synthetic analog of codeine and has been used for the prevent and treatment of acute or chronic pain [1,2]. Measurement of tramadol is important because of its effects on health and addiction [3]. In order to develop a simple, inexpensive, rapid, and efficient analytical method for the measurement of tramadol, in the present work, a novel thin film based on modification of filter paper surface by deposition of nickel oxide nanoparticles (NiO NPs) adsorbent modified with dimethylglyoxime was used as extracting device for thin film microextraction (TFME) of tramadol combined with high performance liquid chromatography (HPLC-UV) detection. Nanostructured Nickel oxide (NiO) were synthesized by co-precipitation method using Nickel nitrate ($Ni(NO_3)_2$) and sodium hydroxide (NaOH) as initial material on filter paper. After deposition of NiO NPs on the cellulose paper, dimethylglyoxime was grafted onto the surface to increase the extraction efficiency for tramadol determination in biological samples.The morphology and the surface characteristics of the prepared thin films were studied applying scanning electron microscopy (SEM) , X-ray diffraction (XRD), and attenuated total reflection-Furier transform infrared spectroscopy (ATR-FTIR).The effects of important parameters influencing the extraction efficiency including pH, extraction time, desorption solvent, desorption time and ionic strength were optimized.The calibration curve was linear in the concentration range of 5-1000 $\mu g\ L^{-1}$ .The repeatability of the developed method in the terms of intera-day precision, inter-day precision and inter-sorbent precision based on the relative standard deviation percentage (RSD %) were evaluated by performing six replication of extraction from spiked deionized water (1mg L^{-1}), were 6.6 , 8.3 and 6.2 %, respectively.The developed method was applied for determination of tramadol in urine and plasma samples and the obtained relative recovery percentage (RR%) have indicated that the developed TFME-HPLC can be employed for this purpose efficently, with sufficient sensitivity, accuracy and precision.

Keywords: Thin film microextraction, Tramadol, Nickel oxide, Dimethylglyoxime, Filter paper

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Extraction of azole antifungal drugs by solidification of floating organic droplets-liquid-liquid microextraction method

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Fungal infection as mycosis is a disease which is caused by fungi especially in the consumption of immunosuppressive agents in cancer therapy and the frequent use of broad-spectrum antibiotics[1]. Recently, liquid-phase microextraction (LPME) methods, have been appointed as solvent-minimized procedures of LLE due to low utilization of extraction solvents and high preconcentration factors [2,3]. A free dispersive method, air-assisted in situ deep eutectic solvent decomposition followed by the solidification of floating organic droplets liquid–liquid microextraction was indicated in this study. In this research, a quasi-hydrophobic deep eutectic solvent was formed from tetrabutylammonium bromide and 1-dodecanol as an organic solvent. The synthesized deep decomposition in the sample solution caused in situ dispersion of extraction solvent and analytes. Air-assisted enhanced a dispersion condition in the sample solution. 1-dodecanol as a green option was replaced with typical extraction solvents providing the advantages of a suitable freezing point near room temperature and low density. Under these optimal conditions, good linear ranges were attained concentration ranges of 5-500 µg L^{-1}. The limits of detection (LODs) and limits of quantitation (LOQs) determined from blank samples were in the range of 0.5-1.5 µg L^{-1} and 1.5-4.5µg L^{-1}, respectively. The Intra-day and inter-day relative standard deviations (RSD% n=5) were calculated to be 2.9-4.1 % and 5.2-8.9 %, respectivelyThe results represented the effectiveness of the developed method for the extraction and determination of analytes in biological samples.

Keywords: Antifungal drugs, Air-assisted, In situ deep eutectic solvent decomposition.

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Indirect determination of diazinon using a chemiluminescence method based on the peroxidase-like property of molybdenum disulfide/zirconium-based metal-organic framework nanocomposite

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Organophosphate (OP) toxins, as the most familiar agents of neurotoxins, are widely used in public health, agriculture or by animal husbandry [1]. Global depletion of OPs into the environment threatens public health through widespread pollution of food and water [2]. An excess amounts of diazinon can lead to the dimness of vision, nausea, muscle tremors and, difficult breathing [3]. The application of new diagnostic systems to measure organophosphates has been an important issue for researchers. In this research, a sensitive analytical method provided for indirect determination of diazinon based on the peroxidase-like property of molybdenum disulfide/zirconium-based metal-organic framework nanocomposite (MoS_2 @ MIP-202 (Zr)). The inhibitory effect of diazinon on the enzymatic activity of acetylcholinesterase was used to obtain appropriate selectivity. In addition, MoS_2 @MIP-202 (Zr) nanocomposite, has a very effective peroxidase-like activity, and significantly increases the very poor emission resulting from the chemiluminescence reaction of the $NaHCO_3$-H_2O_2 system. In the presence of diazinon and its binding to acetylcholinesterase, the catalysis of acetylcholine to choline decreases and consequently, decreases the concentration of H_2O_2. So, the emission intensity of the chemiluminescence decreases linearly. The proposed system has a high sensitivity in diazinon measurement. The synthesized MoS_2@ MIP-202 (Zr) catalyst could be created a very effective diagnostic system using the green, cost-effective and easy method as well as the easy-to-use chemiluminescence system. A wide linear range of 0.2–200 ppb and the detection limit of 0.04 ppb obtained for the determination of diazinon using the method. The high repeatability of the method was confirmed by its application for environmental samples.

Keywords: Metal-organic frameworks, Optical sensors, Chemiluminescence, Molybdenum disulfide, Diazinon

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Photogenerated Reagent Radicals for Flow Injection Analysis of Ascorbic Acid Using Highly Photoluminescent Carbon Quantum Dots

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Ascorbic acid (AA), a water-soluble vitamin, is an essential for the production of collagen in the body. It helps absorption of iron in plants, and is also a known essential biological antioxidant [1]. The deficiency of ascorbic acid in body can cause the scurvy disease that causes symptoms such as muscle weakness, tooth loss, skin rash, fatigue and joint pain [2]. This vitamin is found naturally in various foods such as fruits and vegetables [3]. Detection of AA in fruits, vegetables, biological samples and supplements should be of importance due to the biological activities of ascorbic acid. In this work, a new hydrothermal method has been established for preparation of N-doped carbon quantum dots (N-CQDs) employing citric acid and 3, 4-diaminobenzoic acid as the major and minor precursors, respectively. N-CQDs were characterized by X-ray diffraction spectroscopy, X-ray photoelectron spectroscopy, field emission scanning electron microscopy, EDX-mapping and EDX-spectroscopy, high resolution transmission electron microscopy and FT-IR spectroscopy. The photoluminescence studies revealed that N-CQDs have a high quantum yield of 0.46. By employing N-CQDs, a novel turn off-on photoluminescence procedure with an exciting strategy was developed for trace determination of ascorbic acid. In a flow injection manner, a mixture of persulfate, N-CQDs and ascorbic acid were irradiated by UV light and the resulting photoluminescence response was measured at 437 nm as a peak. Under UV-irradiation, the photoluminescence of a mixture of N-CQDs in presence of perulfate was drastically decreased, while ascorbic acid, as a strong antioxidant, scavenged the reactive radicals. Therefore, through the competitive mechanism a turn off-on method was born for assay of ascorbic acid in some fruits, vegetables, supplements and water samples. A univariate procedure beside a central composite design (CCD) approach were investigated to optimize the sensing condition. The CCD study showed that the analytical response was dependent as a polynomial on the concentrations of N-CQDs and persulfate, and pH. The intensity of photoluminescence was linear in the range of 0.3-11.5 µmol L^{-1} of ascorbic acid. Also, the limit of detection (LOD) of 0.05 µmol L^{-1} was obtained. The method showed satisfactory selectivity, repeatability and accuracy with the sample throughput of 70 h^{-1}.

Keywords: Photogeneration of reagent radicals, N-doped CQDs, Ascorbic acid, 3, 4-diaminobenzoic acid, Central composite design.

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EXTRACTION AND PRECONCENTRATION OF URANIUM (VI) ONTO CHELATED SORBENT

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Actual tasks of radiochemistry are the concentration of radionuclides from natural aquatic environments and the isolation of actinides and rare earth fission products from nitric acid solutions of spent nuclear fuel reprocessing. Sorption methods have found wide application for the preconcentration of radionuclides. Chelating sorbents are of particular interest as sorption material. More efficient use of modified forms of the copolymer of maleic anhydride with styrene. For example, chelating sorbents, which are matrices on which organic compounds are fixed. Recent publications indicate that the copolymer of maleic anhydride with styrene is a promising matrix for the production of chelating sorbents. The present paper discusses the results of a study on the extraction and concentration of microquantities of uranium(VI) by a polymeric chelating sorbent. During the synthesis of the sorbent, a maleic anhydride- methacrylic acid copolymer matrix was used. The uranium solution was prepared by dissolving an accurate sample of $UO_2(NO_3)_2 \cdot 6H_2O$ in distilled water. Working solutions were obtained by diluting the primary solution. The necessary pH values were maintained with solutions of HCl, NaOH, and ammonium acetate buffer solutions. The ionic strength was created by the calculated amounts of KCl. The acidity of the solution was controlled with a glass electrode on a PHS-25 ion meter. Solution concentrations were measured using a KFK-2 photocalorimeter. The dependence of the sorption capacity on the acidity of the solution was studied. Sorption of uranium(VI) was performed from a volume of 20 ml of the solution. At pH 4, the degree of sorption passes through a maximum. With an increase in the concentration of uranium(VI) in the solution, the amount of sorbed metal increases, and at a concentration of $8 \cdot 10^{-3}$ mol/l it becomes maximum (CE=588 mg/g). It is known that the ionic strength of a solution significantly affects the flexibility of the solid-phase matrix and the state of the functional groups of the analytical reagent. Therefore, the dependence of the analytical signal on the ionic strength in the range of 0.1-1.2 was studied. A negative effect of an increase in the ionic strength of the solution on the properties of the sorbent was noted, which is explained by the screening of the coordination-active groups by electrolyte ions. All further experiments were carried out in solutions with an ionic strength of 0.6 Sorption equilibrium is achieved within 3 hours of contact of the solution with the sorbent. The effect of various mineral acids ($HClO_4$, H_2SO_4, HNO_3, HCl) with the same concentrations on the desorption of uranium(VI) from the sorbent was studied. The experiment showed that the maximum desorption of uranium(VI) occurs in 2M H_2SO_4. After determining the optimal preconcentration conditions, the developed method was successfully applied to determine microquantities of uranium(VI) in sea water with preliminary preconcentration. The correctness of the technique was checked by the "introduced - found" method.

Keywords: Uranium (VI), Copolymer, Chelating sorbent, Sorption, Desorption

Flow Injection Colorimetric Detection of Hypochlorite by Using a New Nitrogen-doped Carbon Quantum Dots as a Coupling Reagent

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Hypochlorite as a reactive oxygen compound cannot be disregarded in our life [1]. It is produced in body of organisms, has antimicrobial effect and regulates some physiological functions [2, 3]. However, excess production of hypochlorite in body causes serious problems [1]. Bleach is frequently applied as a strong oxidizing and decolorizing agent and also as disinfectant in drinking and swimming pool water. Hypochlorite produces chlorate, chlorite and trihalomethanes while applying as a disinfectant. The formed chemicals are harmful and carcinogen [1, 4]. In this study, citric acid was thermalized with 3, 4-diaminobenzoic acid as a dry mixure at 200 ºC and a new type of N-doped carbon quantum dots (N-CQDs) was synthesized. N-CQDs were characterized by various microscopy and spectroscopy techniques. N-CQDs were employed for the analysis of hypochlorite in a flow injection manner when a colorimetric detection was applied. 3-Methyl-2-benzothiazolinone hydrazone (MBTH) was oxidized by hypochlorite in an acidic flowing solution by hypochlorite, and then was coupled with N-CQDs to produce an intense pink-blue colored product. The product was monitored on-line at 515 nm. A univariate optimization method and a central composite design (CCD) approach were employed to optimize the analytical parameters. The condition predicted by CCD approach was selected as the optimum condition due to its more sensitivity. At the optimal condition, Beer's law was obeyed in the range of 4-250 µmol L^{-1} of hypochlorite with a limit of detection of 1.0 µmol L^{-1}. The obtained quantum dots showed a high photoluminescence quantum yield of 62.2%. The presented method was successfully applied for sensing AA in various bleach and water samples.

Keywords: N-CQDs, Colorimetric detection, Central composite design, Hypochlorite

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Design of an Electrochemical Reactor for the Synthesis of Ferrate salts

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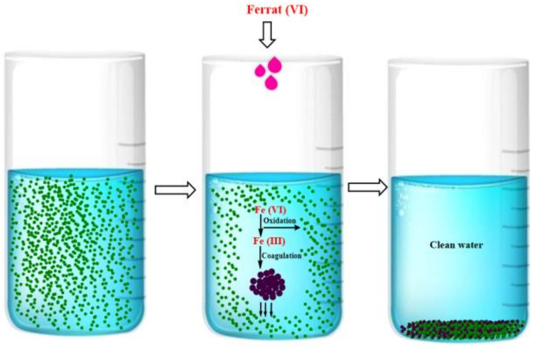
Over the last decades, due to the crisis caused by water shortage and frequent drought in most parts of the world, the provision of suitable approaches for water retention has been converted into an imperative process. As a result, the water treatment processes have been garnered much attention from the community of researchers because of providing various solutions for the conservation of water resources [1]. One of the robust tools for treating various effluents is the use of oxidizing agents for the degradation of organic and inorganic pollutants. In addition, coagulants are also one of the other important types of compounds for the treatment of wastewaters. They can destabilize colloidal impurities, which are reduced to coarse particles by removing or reducing electrical repulsion, which can then be removed by precipitation and filtration [2]. Consequently, the use of Ferrate salts (M_2FeO_4) as both oxidizing and coagulating agents can be a highly efficient and economical method for treating wastewaters [3]. The electrochemical methods have also been recognized as valuable-powerful tools because of developing an environmentally compatible synthetic process, high selectivity, good atom economy, low-energy consumption, and low costs for reagents [4]. In this project, we focused on designing a unique electrochemical reactor to produce ferrate salts at the semi-industrial scale and their in situ injection into the wastewater ponds and tanks. In this way, we have used the constant-current-electrolysis (CCE) as an easily scalable and cost-effective technique for the generation of sodium ferrate solution, and we have also optimized all the effective parameters on the yield and stability of the electrochemically synthesized ferrate.



Keywords: Constant-current-electrolysis, Electrochemical reactor, Environmental Electrochemistry, Ferrate salts, Water treatment.

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Measurement of some annular petroleum compounds (PAHs) in the coastal waters of the Caspian Sea (Gilan region)

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Due to the location of a domestic, industrial and agricultural zone near the Caspian Sea, this water body has long been under pressure and environmental threat. As a result of development of oil production activities in Caspian region, such as oil exploration and extraction in the central and eastern part, a large volume of oil related pollutants is released annually into this important water body. Polycyclic aromatic hydrocarbons (PAHs) are of special ecological importance due to their wide distribution in the environment and potential potential for living organisms [1]. These compounds are a group of stable organic pollutants consisting of two or more interconnected benzene rings[2].In this study, the concentrations of naphthalene, naphthalene, acenaphthane and anthracene in the coastal waters of the Caspian Sea in three study stations (Lisar, Bandar Anzali, Kiashahr) during the two seasons of winter (1399) and Spring 1400) was determined. Samples were prepared after extraction (extraction) by EPA 625 standard method and using mass gas chromatograph (GC/MS) Ultra Trise model of Thermo company. The results showed that in winter the amount of petroleum compounds in the studied samples was higher than the concentration of those in spring so that in winter the concentration of naphthalene at the rate of 157.7 mg/l in Lisar station was the highest. Is Anthracene concentration in winter in Anzali and Kiashahr stations and in spring in Lisar and Kiashahr stations was very low and beyond the measurement of the device.This study showed that Lisar station has the highest oil pollution ($\sum$PHAs =298.4mg/l) And in Kiashahr region the lowest oil pollution was ($\sum$PHAs=26.9mg/l).

***Keywords**:* Petroleum compounds (PAHs), Naphthalene, Bandar Anzali, Caspian Sea

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A green and powerful microextration method: In situ solvent formation microextraction (ISFME) using functionalized ionic liquid for the determination of toxic Cr(VI) in aqueous-saline media

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Chromium is one of the most toxic or hazard heavy metals especially when it is in hexavalent Cr(VI) form. It can hurt human body, so it very important to detection at damaging levels from any environmental sources prior to any elimination actions [1]. There are a number of techniques to determination of Cr(VI) in water and wastewater, such as chemical precipitation, adsorption, membrane filtration, ion exchange, solvent extraction (or liquid-liquid extraction), biosorption and electrochemical treatments [2]. Generally, main disadvantages of the mentioned methods are time consuming, low efficiency, low precision, inflexible and high consumption of chemicals. Recently, one of the new methods at last decade that was used to overcome on those problems is a new mode of liquid–liquid microextraction by use of ionic liquids as green solvents termed *in* situ solvent formation microextraction (ISFME) [3]. Rather than the other microextraction methods such as dispersive liquid-liquid microextraction, solid phase microextraction, liquid-liquid microextraction, liquid-phase microextraction, hollow fibre-liquid phase microextraction and etc. for heavy metal ions, ISFME is faster, simpler, sensitive and is applicable for samples containing higher amounts of salts [4]. In this work, firstly chromium total species converted to the Cr(VI) species and then was complexed with a functionalized ionic liquid namely 3-(3-aminopropyl)-1-octylimidazolium hexafluorophosphate as complexing agent/extractant phase and then chromium complexed was removed from aqueous phase. After phases separation, the extracted enriched phase containing chromium was determined by FAAS. The effect of analytical parameters were investigated and optimized. In the optimum conditions, the limit of detection, relative standard deviation, linear dynamic range and enhancement factor were 1.8 μg L^{-1}, 1.95%, 20-600 μg L^{-1} and 85, respectively. The accuracy and capability of the method was confirmed by analysis of the several real and saline samples.

Keywords: Chromium(VI) determination, ISFME method, Functionalized ionic liquid.

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Investigation and measurement of nitrogen compounds in Glabar reservoir dam water in Zanjan province

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In this study, the electrical conductivity (EC), pH and nutrients including N-NO_2, N-NO_3, NH_4^+,NH_3 and total nitrogen(T.N) in the whole water area of Glabar Dam Lake in four stations seasonally for one year using the method The standard work provided by the American Public Health Association and the methods provided by the Environment Agency as well as the American Water and Wastewater Standard were performed [1].The electrical conductivity (EC) and pH were measured electrometrically with a multi-parameter device from the WTW, model molti 340i.Nitrogen compounds were measured using the absorption method(HACH DR 2800 spectrophotometer).Nitrite was measured by sulfanilamide method, ammonium ion (NH_4^+) was measured by Neesler method and total nitrogen , nitrate (after chemical digestion with persulfate) was measured using a cadmium reduction column.The results show that the difference between the electrical conductivity of surface water and the depth of the lake is very small and the average total electrical conductivity (EC) in the total water area during the sample months was 858.7µs/cm.The average annual concentrations of nitrite, nitrate, ammonium and total nitrogen in the whole water area during the sampling months were measured 0.02, 0.362, 0.428 and 1.23 mg/l, respectively.Based on the results, considering that the lake has been exploited and dewatered in recent years, in terms of nutrients, various nitrogen compounds in the lake water are considered as eutrophic waters, and the pH values of the total water of the lake water area with an average of 8 characteristics It has a good buffer.In the present study, TSI index (trophic index) was used for classification of lake water in terms of atrification and according to the results of calculating TSI index and based on Carson classification, Glabar dam lake is one of the eutrophic and mesotrophic lakes[2].

***Keywords**:* Glabar reservoir dam, Zanjan, TSI index, Nitrogen compounds, Eutrophic

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The role of *Anodonta Cygnea* bivalve in heavy metals absorption (Cu^{+2}, Ni^{+2}, Co^{+2}, Cd^{+2}, Pb^{+2}) Anzali Wetland of Guilan Province (Case Study)

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Anodonta cygnea (linea,1876) is a bentic spicis of Anzali Wetland due to its feading habit on particulate mater and its ability to accumulate heavy metals. This survy were conducted in 2018 to find out the extent of heavy metal accumulation in Anodont and its relation to heavy metal concentration in water and sediment. The Anodont specis were caught from central region of Anzali wetland (Hendkhaleh) the sample first dried powdered and digested by nitric acid[1].The water sample were extracted by liquid-liquid extraction using (MIBK/APDC) [2].The sediment sample owendriev powdered and mineralized by wet digestion method by mixture acid under open reflux[3] and the concentration of seven heavy metals Cu^{+2},Cd^{+2}, Pb^{+2}, Ni^{+2} and Co were determined using flame atomic absorption (FAAS).The concentration of heavy metals Cu^{+2},Cd^{+2},Pb^{+2},Ni^{+2} and Co^{+2} were in *Anodonta cygnea* 5.07±1.42,1.52±0.89,2.78±0.88, 5.42±1.34 and 0.892±0.24µg/g dry weight respectively.The level of Cd^{+2}, Pb^{+2} and Co^{+2} in surficial sediment of Anzali wetland were 1.6 ,1.7 and 1.5 fold higher than thire concentration in *Anodonta cygnea*.The concentration of Cu^{+2} ,Pb^{+2},Co^{+2} and Ni^{+2} in water were 0.384, 0.177, 0.137 and 0.239 mg/l while the level of Cd^{+2} were under the detection limit of FAAS.The concentration of heavy metals in sediment decrease in order of Cu^{+2}>Ni^{+2}>Pb^{+2}>Co^{+2}>Cd^{+2}. According to the high metal concentration in tissuse of A. Cygnea ,this Bivale can be introduced as a bioandicator for Cd^{+2}, Pb^{+2},Ni^{+2} and Co^{+2}.

Keywords: Anzali Wetland, Heavy metal, Anodonta Cygnea, Atomic Absorption

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Quantification of morin and quercetin in tea, vegetable and fruit juice samples by HPLC via development of in-situ produced CO_2 switchable fatty acid microextraction based solidification of floating organic droplet

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Morin and quercetin are two major plant flavonoids which are widely distributed in human foods and herbs, particularly in tea, dark chocolates, onions, and beans [1]. Sample preparations before analysis for determination of morin and quercetin in real samples attracted increasing attention in recent years[2]. In recent years, liquid-phase microextraction (LPME) methods have been applied due to the minimized consumption of extraction solvents, adaptability to different samples, analytes, and almost every analytical instrumentation [3]. In this study, an in-situ produced CO_2 switchable fatty acid microextraction based on solidification of floating organic droplet (In-situ-CO_2-SFA-ME-SFO) was evaluated for microextraction of two antioxidant flavonoids (morin and quercetin) in tea, fruit juice and vegetable samples prior to HPLC-UV. A medium-chain fatty acid (e.g. nonanoic acid) was investigated as switchable hydrophilicity solvents via pH adjustment. Sodium carbonate (Na_2CO_3) was used to solubilize immiscible fatty acid in water as well as, to provide effervescence. The addition of H_2SO_4 into the solution led to the effective dispersion of fatty acid through generated CO_2 and separation of phases. Subsequently, solidification of the fatty acid enabled facile separation without the need for sophisticated equipment. At the optimum conditions, the limits of detection (LOD) and the limits of quantification (LOQ) were found to be 0.5 μg L^{-1} and 1.3 μg L^{-1} and 1.6 μg L^{-1} and 4.3 μg L^{-1} for morin and quercetin respectively. Preconcentration factor was obtained to be 105 while, the precisions (RSDs) of the method for both flavonoids in the samples (n = 6) were <3.5 %. The recoveries of the analytes in tea, vegetable and fruit juice samples were in the range of 95.5% and 98.2%

Keywords: Morin, Quercetin, Medium-chain fatty acid, Switchable-hydrophilicity solvent

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Experimental and theoretical study of properties of opal photonic crystals

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In this work, suspension polymerization is used to synthesize 419 nm Poly(methyl methacrylate) (PMMA) microspheres [1]. Then a vertical evaporation-based method is used to grow opal photonic crystals on a glass substrate and their properties are investigated. The quality and uniformity of PMMA polymer were confirmed by Dynamic Light Scattering (DLS) analysis and scanning electron microscopy images confirm the close-packed face-centered cubic (FCC) lattice of the structure. The maximum absorption is observed at the wavelength of 950 nm. Then, opal photonic crystals were simulated using the FDTD method. In this simulation, a colloidal photonic crystal with 15 layers on a glass substrate has been considered. To simulate the light source, a flat wave in the wavelength range of 0.4-1.05 μm was used and boundary conditions of PML were applied in all three dimensions. The simulation ends automatically after complete field attenuation. The results show that increasing the number of layers in the simulation cause a perfect match of the results with the experimental ones. The opals and their inverse structures (inverse opals) have potential applications in a variety of important fields, including chemical and biological sensors, solar cells, and optical devices [2].

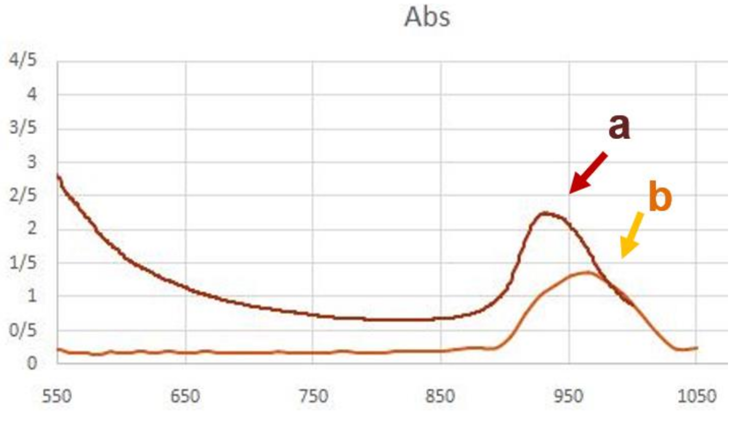

Figure.1.a) Three-dimensional crystal photonic absorption curve and b) Simulation absorption curve.

Keywords: Multilayer, three-dimensional photonic crystal, PMMA, FDTD method

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Experimental and theoretical study of properties of 2D colloidal Crystals

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In this work, a monolayer of poly(methyl methacrylate) (PMMA) microspheres were synthesized using the air-liquid interface deposition method on a glass substrate. Several parameters affect the quality of these 2D colloidal crystals such as the solution concentration, injection rate, the diameter of polymeric spheres, etc. The spheres were arranged in a hexagonal lattice in a close-packed way. Different analysis methods such as UV-Vis spectroscopy, scanning electron microscopy and optical diffraction pattern confirm the formation of close-packed 2D colloidal crystals. Also, using the FDTD method, these structures are simulated and the results well match the experimental ones. The schematic of the simulation and also the SEM image of the structure are shown in Fig.1.

2D colloidal crystals [1] can be used as versatile templates in the colloidal lithography method which is a cheap and easy technique to fabricate various nanostructure arrays. Also, its unique optical properties make it a good candidate for designing optical chemical/biosensors [2].

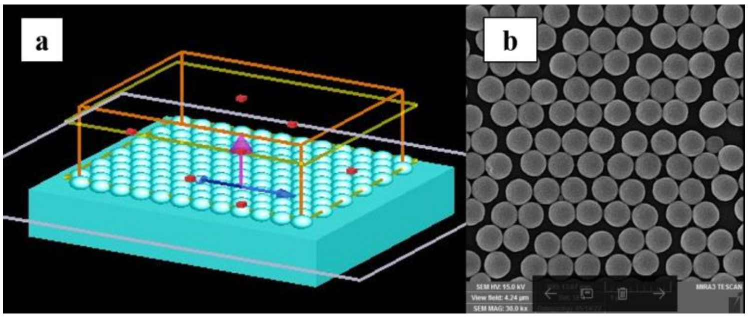

Figure.1.a) The Schematic of the simulation, and b) the SEM image of a 2D colloidal crystal.

Keywords: 2D colloidal crystals, air-liquid interface deposition technique, FDTD simulation method

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Electrochemical Synthesis of Thin Film Metal-Organic Frameworks with Simple Method: Application of Elctrocalytical Oxidation of Amoxicillin

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β-lactam antibiotic especially amoxicillin is one of the world's most important commercial antibiotics due to its high bacterial resistance and large spectrum against a wide variety of microorganisms[1,2]. Many routine and advanced methods for testing this drug in biological media and obtained drug samples show the fact that routine and simple methods such as electrochemical methods are best Tool among other methods. But electrochemical methods need to synthesize electrocatalysts with the best detection and response in the applied potential range to have an acceptable result. Recently a new class of inorganic materials is related to the metal-organic frameworks (MOFs) have used for the investigation of drugs[3]. As respectsfor the design of active catalysts for the measurement of pharmaceutical substances, the best case is for compounds that have been electrochemically deposited as a thin film on conductive substrates. Here, we focus on electrochemical and chemical synthesis as a facile and green method for preparing of zinc metal-organic frameworks cu-(Zn-MOF) on the surface glassy carbon electrode (GCE) to determine amoxicillin in alkaline medium. The Cu/Zn-mMOF/GCE showed high electrocatalytic activity for oxidation of amoxicillin in 0.1 M NaOH solution. Kinetic parameters such as the charge transfer coefficient ($\alpha = 0.31$), catalytic rate constant ($K_{cat} = 3.9 \times 10^5$ $cm^3\ mol^{-1}\ s^{-1}$) and diffusion coefficient ($D = 1.6 \times 10^{-5}$ $cm^2\ s^{-1}$) have found for the AMOX oxidation at the Cu/Zn-mMOF/GCE using cyclic voltammetry and chronoamperometric methods. This electrocatalytic oxidation exhibited a good linear response for amoxicillin concentration over the range of 1.0–205 µM with a detection limit of 0.36 µM. Therefore, this electrocatalytic method was used as a simple, selective and rapid method able to determine amoxicillin used in real samples such as drug and human serum and offered an effective sensing platform for the sensitive determination of amoxicillin with satisfactory recovery values.

Keywords: Amoxicillin, Metal−organic framework, Electrochemical sensor, Kinetic parameters

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Electrocatalytic Oxidation of Methanol on Alternative Nanocomposite based Metal-Organic Frameworks

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Direct methanol fuel cells (DMFCs) are anticipated as a new type of green energy device for the implementation of portable and mobile electronics, which directly converts the chemical energy of liquid methanol fuel into electrical energy [1]. Nevertheless, the tremendous efforts to commercialize DMFCs are still needed to overcome several challenges, including CO poisoning of the catalysts, overflow of methanol to the cathode, and the sluggish oxidation kinetics of methanol. Despite the increasing progress in the development of DMFCs, their commercialization still faces the challenges in developing cheap, highly active, and durable electrocatalysts [2]. The electrochemical methanol oxidation reaction (MOR) has been widely investigatedexperimentally and theoretically. This is driven by two features: MOR is used as a model reaction because of its sensitivity to the composition and structure of the electrode surface [3]. In electrocatalytic oxidation of methanol, electrode materials are obviously an important factor where a highly efficient electrocatalyst is needed. Zinc metal compounds and composites include a lot of flexibility in making catalysts with good electrolytic behavior in fuel cells. Here, Zn-mMOFTFs were synthesized on the glassy carbon electrode via a simple potentiostatic electrochemical method at room temperature. The final modified electrode (Ni/Zn-mMOFTFs/GCE) was fabricated by the incorporation of the Ni species in the pore structure of the Zn-mMOFTFs as a support catalyst for the electrooxidation of methanol. After physicochemical characterization of the fabricated nanocomposite,it wasfound that the Ni/Zn-mMOFTFs/GCE has high electrocatalytic activity toward the oxidation of methanol. The values of catalytic rate constant (k) and the electron transfer coefficient (a) for the electrooxidation of methanol on the Ni/Zn-mMOFTFs/GCE were obtained. Some kinetic parameters such as the transfer coefficient (α) and catalytic rate constant (k) of methanol were calculated. Electrochemical investigation of the introduced electrocatalysts indicated that Ni/Zn-mMOFTFs/GCE has highest activity and stability towards methanol electrooxidation, which highlights its potential use as an anodic material in direct alcohol fuel cells.

Keywords: Direct methanol fuel cells, Metal–organic framework, Kinetic parameters

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CO_2 effervescence assisted dispersive micro solid phase extraction based on magnetic biopolymer nanosorbent for extraction of Bisphenol A prior to high performance liquid chromatographic determination

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Bisphenol A (BPA) is an important industrial chemical that is mainly used in the production of polycarbonate plastics, epoxy resins and polyesters, as well as in other various industrial products. The growing industry and increasing demand for more plastic are becoming more common and consequently becoming more apparent in the environment [1]. Due to the adverse effects of trace concentration of BPA on environmental health also human beings and recognized as one of the endocrine disruptors [2], the development of a new extraction method by minimal consumption of organic solvents and following green chemistry for its analysis has been considered. In the present study, a biosorbent; magnetic zein nanoparticles and dispersive micro solid phase extraction method have been used for the extraction of the BPA from environmental samples. The synthesized adsorbent was characterized by FT-IR, XRD, EDX and SEM. Affecting factors on extraction recovery were investigated and optimized; such as adsorbent dosage, salt addition, type and volume of desorption solvent. The linear range of the method was 25-500 μg L^{-1} and LOD was obtained 8 μg L^{-1}. RSD (n=5) 1.1 % was acceptable and the extraction efficiency of the method was 24.8%. Satisfactory extraction recovery of real samples was obtained 99-103%, which indicates the accuracy of the proposed method.

Keywords: HPLC, μ-solid phase extraction, Effervescence tablet, Biopolymer nanosorbent, Bisphenol A

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Copper Iodide Modified Sol-Gel Derived Carbon-Ceramic Composite Electrode: Application to Electrocatalytic oxidation of Hydroxylamine

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This work presents the results obtained new modified sol-gel electrode.A simple procedure was developed to prepare a sol-gel electrode modified with copper iodide.The CuI-modified sol-gel electrode has been prepared by mixing methyl trimethoxy silan sol-gel precursor and graphite powder with CuI powder, methanol and HCl and then to fix in a plastic tube.After drying the electrode at room temperature it was placed in 0.1 M NaOH and the electrode potential was cycled between -0.25 and 1 V (vs. Ag/AgCl) at a scan rate of 50 mV/s for 5 cycles in a cyclic voltammetry regime until a featureless voltammogram was obtained. The electrocatalytic activity of the modified electrode was examined for the oxidation of hydroxylamine. The electrochemical behavior of hydroxylamine at an CuI-modified sol-gel carbon ceramic electrode has been studied using cyclic voltammetry and amperometric techniques. Compared with the unmodified sol-gel electrode, the modified electrode exhibits good catalytic activity for the oxidation of hydroxylamine. The process is absorption controlled. The effect of the amaunt CuI was studied in the range of 0.05-0.2 gr. The kinetic parameters such as the electron transfer coefficient and the number of electrons involved in the rate-determining step for the oxidation of hydroxylamine were determined utilizing cyclic voltammetry. detection limit of 9.505 μM and %RSD=1.49% was obtained.

***Keywords**:* Copper iodide, Ceramic-carbon composite electrode, Electrocatalytic oxidation, Hydroxylamine, Cyclic voltammetry.

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Colorimetric Ammonia Gas sensors by Mesoporous Silica Core-Shells: Studying the Effects of Various Metallic Species and Different Sensitive Organic Dyes

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This study presents an effective and simple colorimetric probe for sensing ammonia in gas phase based on reaction of a sensitive dye loaded onto the silica based core–shell Nano-structure. A core-shell nanostructure was designed and prepared via a sol-gel approach, and then a very simple impregnation method was employed to enrich it with a sensitive dye (Alizarin). Various analytical tools were used to characterize the structural and textural properties of prepared substrate which all of them proved the presence of a mesoporous system. A series of colorimetric and spectroscopic experiments using diffuse reflectance spectroscope (DRS) were employed to investigate the extent of the changes in dye response. Certain concentrations of ammonia were released into a closed chamber with certain volume via evaporating ammonia solution on a hot plate. Also all responses were detectable with naked eye as long as the ammonia concentration in the air was more than 50 ppm. [1,2].

Keywords: Core-shell, Gas-Sensor, Colorimetric, MCM-41, Ammonia

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Green Synthesis of Carbon Quantum Dots from Heart-of-palm and its Application in Antioxidant Activity, Cell Imaging and Fe Determination

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Carbon quantum dots (CQDs), a new class of carbon nanoparticles, is attracted due to its interesting properties such as biocompatibility, high water solubility, low toxicity and specific physical and chemical properties. Synthesis of the surface modified CQDs has significant applications in many areas including bio-imaging, chemical and biological sensing devices, pollutant remediation [1], drug delivery [2] and etc. In this study, a facile synthesis of carbon dots from a novel natural precursor was developed by hydrothermal treatment. The as-prepared CQDs possess strong blue fluorescence emission, good water dispersibility, and excellent photo stability as well as low toxicity, hence multicolor CQDs could be used as an excellent fluorescent probe for cellular imaging. In addition, the CQD exhibit excellent radical scavenging activities against DPPH radicals. By plotting the inhibition value against the concentration of CQD, a linear relationship ($y=0.184+3.614x$) was obtained for a CQDs concentration ranging from 0 to 500 ppm and the EC50 value of the CQDs towards DPPH was 251.8 µg/ml. It is found that the fluorescence of CQDs can be effectively quenched by Fe^{3+}. Based on this feature, the selective and sensitive detection of Fe^{3+} was performed, showing that a good linear relationship between fluorescence intensity of CQDs and Fe^{3+} was achieved at the concentration from 0 to 900 ppb. The limit of detection and limit of quantification were obtained 23.42 ppb and 78.06 ppb based on a $3\delta/S$ and $10\delta/S$ (δ is the standard deviation of the blank signal and S is the slope of the linear calibration plot), respectively.

Keywords: Carbon quantum dots, Heart-of-palm, Fluorescence, Radical scavenging activity, Fe^{3+} detecting

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Fabrication of a Sensitive Sensor for Determination of Ascorbic Acid by Modifying Over-Oxidized Carbon Paste Electrode with Biowaste

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Ascorbic acid (Vitamin C, AA), as an important water-soluble vitamin, is an essential nutrient for vital activities and plays an extremely important role in the daily lives of humans and animals [1,2]. The development of a quick, selective and sensitive method for determination of AA in real samples is greatly desirable for analytical applications and diagnostic research. In this way, electrochemical techniques are a good alternative and, specially, voltammetric techniques for the detection of AA has attracted great interest due to their rapid response, high sensitivity and miniaturization [3]. Here, chicken feet yellow membrane (CFYM) were preparade by a simple and facile method and used for the modification of over-oxidized carbon paste electrode (OCPE) for the selective determination of ascorbic acid (AA). The various properties of biosynthesised CFYM were investigated using Fourier-transform infrared spectroscopy (FTIR), scanning electron microscope (SEM), X-Ray diffraction (XRD), and cyclic voltammetry, respectively. The electrochemical results demonstrated that the modified electrode shown outstanding performance in the determination of AA with a very low limit of detection (5.95 μM) along with higher stability and repeatability features. The novel AA sensor manifested exceptional sensitivity and selectivity over a wide linear range of concentration from 9.9 –280.5 μM with the coefficient of determination $R^2 = 0.998$. The applicability of the developed sensor was examined in the pharmaceutical samples that contain AA and the sensor selectively detected the AA from multiple ingredients that were present in their formulation with acceptable recovery.

Keywords: Ascorbic acid, Chicken feet yellow membrane, Over-oxidized carbon paste electrode

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Cu–Al LDH/ Biowaste/Graphenized Pencil Graphite Electrode as Efficient Sensing Platform for Determination of Diclofenac in Pharmaceuticals and Biological Samples

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It is known that environmental pollution caused by drug residues has been taken seriously in the past few decades. Diclofenac (DCF), designated as 2-(2-((2,6-dichlorophenyl) amino) phenyl) acetic acid, is one of the most frequently prescribed nonsteroidal anti-inflammatory drugs (NSAIDs) having antipyretic and analgesic properties [1]. However, due to the overuse of DCF, large amounts of DCF residue can cause chronic toxicity and harm human health [2], which was extensively considered a ubiquitous contaminant in water [3]. Several methods have been described in the literature and used for the determination of diclofenac in various types of samples. Electrochemical methods are suitable for determining drugs in real samples (biological fluids and pharmaceutical forms) due to simple yields, effectiveness, reliability, and fast response time, as well as good sensitivity and selectivity. In this research, we successfully designed Cu–Al layered double hydroxide/chicken feet yellow membrane (Cu–Al LDH/CFYM) modified graphenized pencil graphite electrode (GPGE) as a novel electrochemical sensor for the electrocatalytic determination of diclofenac. The composite materials were characterized by SEM and XRD techniques to understand their sensing characteristics. Also, the electroanalytical behaviors of the fabricated sensors were investigated by CV and DPV techniques. The proposed sensor showed an excellent catalytic activity towards the oxidation of diclofenac molecules. The oxidation peak current of DCF was linear in the concentration ranges of 1.99–23.44 µM with a detection limit of 1.91 µM. In the final step, the Cu–Al LDH/CFYM/GPGE was successfully examined for the detection of DCF in real samples.

Keywords: Diclofenac, Chicken feet yellow membrane, Layered double hydroxide, Graphenized pencil graphite electrode

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Synthesis of modified magnetic graphene oxide with mesoporous silica for adsorption and extraction of pharmaceutical compound of quercetin from real samples

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Quercetin (3,5,7,3′,4′-pentahydroxyflavone), which belongs to theclass of bioflavonoids, is an important flavonoid, which is also an indispensable component of the human diet, with fruits, leafy and dried vegetables [1,2]. Ability ofquercetin for scavenging free radicals and binding transition metal ionsallow it to inhibit reducing oxidative stress and associated damages.Therefore, quercetin is often suggested as a main flavonol for antioxidant therapy [3]. Many different analytical methods have been described for the extraction and determination of quercetin. Herein, mesoporous silica–Fe_3O_4–graphene oxide (Fe_3O_4/GO@mSiO_2) adsorbent was synthesized. More importantly, the adsorption ability of Fe_3O_4/GO@mSiO_2 magnetic nanoparticles to extract quercetin from aqueous solutions was investigated. Initially, graphene oxide nanoparticles were synthesized via Hammer method. After that the GO magnetized by $FeCl_{3.6}H_2O$ and $FeCl_{2.4}H_2O$. Furthermore, Modified by mesoporous silica. The magnetic nanoparticles Fe_3O_4/GO@mSiO_2 was used to measure quercetin in four real samples (spinach, green pepper, dill and red onion). Fe_3O_4/GO@mSiO_2 nanoparticles was characterized by Fourier transform infrared (FT_IR), scanning electron microscopy (SEM), X-ray diffraction (EDAX), X-ray diffraction (XRD), vibrating sample magnetometer (VSM) and X-ray photoelectron spectroscopy (XPS). The Fe_3O_4/GO@mSiO_2 strategy revealed a great stability and a superb sensitivity for quercetin measurements, with a suitable linear range 0.8-0.02 ppm and a detection limit 5.24 micrograms per milliliter. The data indicate that Fe_3O_4/GO@mSiO_2 has a specific surface and the maximum adsorption capacity for measuring quercetin.

Keywords: Magnetic graphene oxide, Mesoporous Silica, Quercetin, Spectrophotometer

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Rubber-Fe_3O_4@SiO_2@Mg-Al LDH as a novel magnetic sorbent; application in environmental monitoring of estrogenic hormones

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Steroids belong to a group of substances with a structural core formed by cyclopentane-perhydro-phenanthrene and some of them, such as Estrone (E1), 17-β-estradiol (E2), act as sex hormones, responsible for sexual characteristics and supports for reproduction [1]. The estrogens are reported as highly endocrine-disrupting agents, being recently included in the environmental agencies watch list regarding emerging aquatic pollutants [2]. The main routes of excretion of these compounds are excretion through urine and feces, which is the main source of these compounds in sewage. Layered double hydroxides (LDHs) are a class of layered nanomaterials that form by stacked layers of double hydroxides of trivalent and divalent cations with inherently positive surface charge. LDHs owning some unique features such as large surface areas, high exchange capacity for anions and thermal stability, low cost, and ease of preparation route have been used as sorbents in solid phase extraction [3]. In this work, a magnetic sorbent based on Rubber-Fe_3O_4@SiO_2@Mg-Al LDH was prepared and its application in magnetic dispersive solid phase extraction of E1 and E2 was investigated. The synthesized Rubber-Fe_3O_4@SiO_2@Mg-Al LDH was characterized using various techniques, including X-ray diffraction, Fourier transform infrared spectroscopy, field emission scanning electron microscopy, vibrating sample magnetometry, BET and BJH , EDS-Map, TGA-DSC analyses. Important parameters influencing the extraction efficiency were optimized. Based on the method validation, the calibration curve was linear in the range of 1 to 150 and 1 to 75 μgL^{-1} with a correlation coefficient of 0.9919 and 0.9939 for E1 and E2 , respectively. The limit of detection (LOD) and limit of quantification (LOQ) was estimated to be 0.30 and 1 for both of the analytes, respectively.

Keywords: Mg-Al layered double hydroxide, Estrone (E1) and 17-β-estradiol (E2), Magnetic solid-phase extraction

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The effect of corona COVID-19 vaccination on some plasma metabolites

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COVID-19 is a contagious disease caused by the virus SARS-CoV-2. coronavirus spread around the world in late 2019, leading to the COVID-19 pandemic. Since the publication of the genome sequence of SARS-CoV-2, an endeavor of unprecedented speed and magnitude set out to develop a vaccine against the disease. Several vaccines were developed finally to combat the epidemic and received emergency injection licenses. Metabolomics is a comprehensive assay of small metabolites weighing less than 1,500 Dalton. It has received a lot of attention in recent decades [1]. Metabolomics specifically examines the biochemical changes remained by cellular processes that can reflect metabolic conditions. In the COVID-19, several metabolic pathways are affected, including amino acid metabolism, energy metabolism, and lipid metabolism. Therefore, metabolic analysis of plasma samples and measurement of some important metabolites can be helpful in diagnosing the symptoms of the disease, in the treatment process or in diagnosing subsequent disorders related to the disease. The Covid-19 vaccine is a new vaccine that has been used for the past year. Its goal is to successfully control the COVID-19 epidemic. Because the license to make and inject Corona vaccines is an emergency license, some long-term research on them has been removed due to the corona epidemic and the rescue of humans. Since the need for further study on vaccine interactions in the body seems necessary, in this study, the effect of vaccination on metabolites of human plasma samples has been investigated using HPLC technique. For this purpose, several common vaccines used to control Covid-19 in Iran were selected and their effects on human plasma metabolites were evaluated. According to the primary results, the amount of arginine was significantly different from before vaccination.the dynamic range was 0.10-3100 and its LOD was 0.05 and LOQ was 0.015µM.

Keywords: SARS-CoV2, Metabolomics, HPLC, Human Plasma

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Gas chromatographic detection of phenols from agricultural water samples after a simple and fast preconcentration technique

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A simple and fast pre-concentration technique as solid phase extraction-air assisted-dispersive liquid-liquid micro-extraction coupled with gas chromatography has been developed to determine phenols from agricultural water samples. In this method, a new aniline-activated carbon composite was synthesized and contacted with a solution containing phenol. The adsorbent particles were then separated from the solution by a continuous minicirculation device. The adsorbent particles were transferred into a stripping solution under ultrasonication and air-assisted conditions. Finally, after performing a dispersive liquid-liquid extraction step on resulted solution, microliter volumes of extraction phase were injected to gas chromatography. The effect of several parameters such as extraction solvent type, dispersive solvent type, salt effect, extraction time, adsorbent amount, pH were investigated. Under optimal conditions, the enrichment factor was obtained in the range of 184-146 and the linear dynamic range was from 0.6-200 µg/L. The proposed method is one of the fast methods and it takes less than 20 min to prepare the sample and analytical detection [1,2]. The proposed method was succefully used for determination of phenols in agriculture water samples.

Keywords: Silid-phase extraction, Air assisted, Dispersive liquid-liquid micro-extraction, Aniline-activated carbon composite, Phenol, Gas chromatography

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Accelerating Surface Photoreactions by using MoS_2-FeS_2 Nanoadsorbents: Photoreduction of Cr(VI) to Cr(III) and Photodegradation of Methylene Blue

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Among the conventional methods, semiconductor-based photocatalysis offers a green, sustainable and effective technology for environmental remedy [1-2]. Accordingly, nanocubic MoS_2-FeS_2, as photocatalyst, was synthesized with high catalytic active edges and high specific surface area with capability of absorbing visible light. The results showed that photocatalytic efficiency of nanocubic MoS_2-FeS_2 for adsorption/degradation of methylene blue (MB) as well as the reduction of Cr(VI) was high. The adsorption process was found to follow a kinetic model of pseudo-second-order kind ($Q_{e.cal}$ = 464 mg g^{-1}) along with an isotherm described by Langmuir model with $Q_{e.cal}$ = 340 mg g^{-1}. The photodegradation process was achieved by hole. It was found that the photodegradation rate constant of MB by MoS_2-FeS_2 (0.203 min^{-1}) was about 22 times higher than that of MoS_2 (0.0091 min^{-1}). The percent apparent quantum yield for photoreduction of Cr(VI) to Cr(III) using MoS_2-FeS_2 (5.7%) was about 33 times higher than utilizing MoS_2 (0.1709%). Therefore, the synergistically prolonged visible light harvesting as well as photocarrier diffusion length proved that MoS_2-FeS_2 nanotubes can effectively be utilized in environmental pollutants remediation.

Keywords: MoS_2-FeS_2 nanocubes; Prussian blue analogues; Visible light harvesting; Adsorption, photoreaction.

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Huge emission red-shift of carbon nanodots by azo doping and its applications for red cell imaging and skin wound healing

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Carbon dots (CDs) are an emerging class of fluorescent nanomaterials defined by a feature size of <10 nm and a quasi-spherical morphology [1,2]. In this study, a unique hydrothermal method was applied for the synthesis of red emission CDs, based on azo doping. In this procedure, the reaction of carbon and nitrogen sources under the acidic conditions produced aromatic azo units in the structure of CDs [3]. The CDs exhibited three excitation-independent blue, red, and yellow emission colors under acidic, neutral, and alkaline conditions, respectively. The huge pH-dependent shifts to longer wavelength regions can be related to changes in energy levels due to chromophore doping and the protonation/deprotonation of the surface groups of CDs. At physiological pH, the CDs demonstrated a red emission wavelength at 610 nm. Based on the cytotoxicity result, the red emission CDs showed an outstanding performance in bioimaging (at pH 7) [4]. Moreover, CDs acted as a brilliant candidate for wound healing in rats, due to their high antibacterial activity [5]. It was found that there was a statistically noteworthy difference between the control and sample groups of rats in terms of time required for wound closure. Therefore, we have presented the feasibility of chromophore doping as a promising approach for tuning the optical characteristics of CDs. Finally, we used the attractive properties of CDs for bioimaging and wound healing.

Keywords: Fluorescent nanomaterials, Carbon dots, Red emission, Bioimaging, Wound healing

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Eco-friendly approach for effective extraction and determination of antifungal drugs using electrospun Mg-Al-SDS LDH fibers

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Various fungi are used in the fermentation and food industries, however, fungi can cause disease in a variety of plants as well as local and systemic infections in a variety of animals and even humans [1,2]. This factor has increased the use of imidazole-based fungicides. These drugs have both veterinary and human uses. Although these drugs can be used to treat fungal diseases, they can cause side effects such as redness, blisters, itching, local irritation, irregular heartbeat, and liver toxicity [2,4]. Analysis of drugs in pharmaceutical and biological samples is important to understand the therapeutic effects and toxicity of them [3]. In the present research, fiber in-tube solid-phase microextraction (FIT-SPME) approach coupled with HPLC–UV/Vis was applied for determination of ketoconazole, clotrimazole, and miconazole as antifungal drugs. The SDS intercalated Mg-Al LDH which was synthesized by the urea hydrolysis used as adsorbent. That SDS can interact favorably with the analytes. In the subsequent step, this adsorbent was dispersed in polyvinyl alcohol (PVA) as a biocompatible, safe and green polymer and the resulting solution was electrospinned on stainless steel wires. Due to the high solubility of PVA in the aqueous medium, citric acid and heat treatment were used to increase the stability of PVA. Finally, the obtained fibers were placed in a stainless steel tube to make the extraction media. The solution containing antifungal drugs was passed through the tube using a peristaltic pump and the desorption was performed with a syringe pump and the analytes were separated and measured using HPLC-UV/Vis. The effects of various parameters on the extraction efficiency, including pH, extraction time, extraction flow rate, salt addition, type of eluent, eluent quantity, and desorption time were investigated and optimized. Under the optimum conditions, the method showed good dynamic linearity in the range of 1- 750 µg L^{-1} with LODs of 0.30 µg L^{-1} and coefficient of determinations higher than 0.9913. Intra-day and inter-day RSDs% were obtained 5.0% and 6.2% ,respectively. Finally, RR(%) in the range of 82-115% were obtained for measuring trace amounts of antifungal drugs in tablet, shampoos, and lotions samples.

Keywords: Antifungal drugs, Electrospinning, In-tube solid-phase microextraction, Layered double hydroxides, Polyvinyl alcohol

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Biomass-Inspired Blue-Emissive N, S-Self Codoped Carbon Quantum Dots: An Efficient Fluorophore for Selective and Sensitive Detection of Nitrite Ion in Water with impressive Multi-biological Capabilities

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Selective and sensitive detection of nitrite (NO_2^-) is critically crucial because the water existing concentrations of NO_2^- in these industries are directly connected to public health and environmental security [1]. The World Health Organization (WHO) has ruled the maximum limit of 3.0 mg L-1 (or 65 μM) for NO_2^- in drinking water [2]. This suggests that the development of uncomplicated, rapid and sensitive methods with a relatively low detection limit (<3.0 mg L^{-1} or 65 μM) and high selectivity for NO_2^- detection is considered. Among them, the fluorescence method has been widely employed for the analytical detection of heavy metal ions and harmful anions in the aquatic environment, and the detection performance is highly dependent on the fluorophores utilised [3]. Recently, carbon quantum dots (CQDs) fabricated by different methods have been extensively analysed as fluorophores for sensitive and selective detection of environmental heavy metal ions and anions because of their excellent fluorescent properties, low cost, and easy processing, exhibiting great potential for fluorescence-based analytical detection applications [4]. Based on the fluorescent quenching principle, CQDs as fluorophores for analytical detection of cations (e.g., Cu^{2+}, Hg^{2+}) and anions (e.g., I^-) may be due to the role of CQDs as both electron acceptor and electron donor. More importantly, N and S doping was found to be critically important for improving analytical detection performance owing to N and S doping causing positively charged surface of carbon dots, significantly improving the interaction between carbon dots and I^- [4]. In the present investigation, for the first time, a new biomass as waste with high volume production were chosen and then used as a feedstock for the one-pot synthesis (2h at 300˚C) of novel S, N-codoped CQDs (SN-CQDs). The selectivity and sensitivity of as-synthesized SN-CQDs as a novel fluorescent nanoprobe towards NO_2^- was investigated in detail. Fluorescence quenching of this nanoprobe by NO_2^- confirming its detection ability. Apart from the detection of NO_2^- ions, the SN-CQDs biological activities were explored.

Keyword: Carbon quantum dots, Biomass, Fluorophore, Selective and sensitive detection, Nitrite (NO_2^-).

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Microchip-solid phase extraction device for simultaneous extraction of fluoroquinolones using a new 2D-metal organic framework adsorbent followed by liquid chromatography-tandem mass spectrometry detection

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Herein, an efficient adsorbent for the simultaneous extraction of fluoroquinolones (FQs) from milk samples is introduced based on a two-dimensional metal-organic framework (2D MOF). The high surface area and high porosity of prepared MOF provide a unique adsorbent for solid-phase extraction (SPE). The results showed the great ability of 2D MOF for the retention of ofloxacin (OF), ciprofloxacin (CIP) and norfloxacin (NOR). It was also found that acetic acid (ACA) solution can effectively elute the adsorbed FQs with an acceptable recovery, without any requirement for toxic organic solvents, which are utilized for the common C18 cartridges. A 3D printed microchip containing a microcolumn was also examined for the SPE process using a magnetic composite of 2D MOF, which was fixed inside the column using an external magnet. High-performance liquid chromatography coupled to tandem mass spectrometry (LC-MS/MS) was used as the potent detection system. It was able to detect OF, NOR and CIP in the range of 0.5-1000 ng mL^{-1} in milk samples and the detection limits were 0.012, 0.009, and 0.016 ng mL^{-1}, respectively.

Keywords: 2D metal-organic framework; Solid phase extraction; Fluoroquinolones; Microchip; LC-MS/MS.

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Adsorption properties of chrysosporium sp. fungus-ameliorated carbon nanotubes and their usage for solid phase extraction of cadmium metal ion

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In recent decades, a growing attention has been paid on the high toxicity of heavy metals ions, like cadmium, and exposure to these pollutants has become a major concern for human health. Therefore, removal of these metal ions from wastewaters, as well as accurate and precise determination of trace metal contents different samples. [1,2]. Some yeast species and filamentous fungi have been investigated, after immobilization on various supports including multi-walled carbon nanotubes (MWCNTs) [1], for their adsorption potential towards some heavy metal cations. Therefore, we evaluated here the performance of chrysosporium sp. fungus towards Cd(II) cation after immobilization on MWCNTs and the efficiency of this system for pre-concentration of cadmium ions prior to its determination by an inductively coupled plasma (ICP) instrument. The adsorption properties of chrysosporium *sp.* fungus-ameliorated MWCNTs was checked towards the targeted metal ion, i.e. Cd^{2+} ion, by conducting batch experiments. Then, a mini-column packed with adsorbent was recruited for pre-concentration of the analyte prior to its determination by ICP instrument. Optimal analytical conditions including pH, ionic strength, elution solution, sample and eluent flow rates, and sample volume were determined. Langmuir isotherm fitted with equilibrium data, kinetic studies vouchsafed the obedience of experimental data from pseudo-second-order model, and thermodynamic appraisals revealed the endothermic nature of adsorption process. Also, the new SPE method demonstrated a high performance for the analyte, and its adsorption was not affected by the different co-existing ions. Using the central composite design, the results showed that uranium can be quantitively adsorbed at a sample flow rate lower than 3.0 mL/min and the desorption could be accomplished with 3.0 mL HCL 0.05 M solution. The results vouchsafed low detection limit (0.016 µg/L), high precision (RSD 2.1%), and good accuracy of the proposed procedure. Overall, the results vouchsafed that new adsorbent can be regarded as a suitable adsorbent for preconcentration of the cadmium ion.

keywords: Chrysosporium sp. fungus, MWCNTs, Adsorption, Solid phase extraction, Cadmium ion

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Exploring Structural Requirements of Simple Benzene Derivatives for Adsorption on Carbon Nanotubes: CoMFA, GRIND and HQSAR

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Understanding of organic chemicals-carbon nanotubes interactions is of great importance for exploring the adsorption phenomena. Three quantitative structure–activity relationship (QSAR) methods involving comparative molecular field analysis (CoMFA) and GRid-INdependent Descriptors (GRIND) based 3D-QSAR and hologram QSAR (HQSAR) were evaluated for predicting adsorption coefficients of the simple benzene derivatives on mutiwalled carbon nanotubes (MWCNTs). CoMFA, GRIND and HQSAR models were developed having statistically excellent performance, which also possessed good predictive ability for test set of ten compounds. The contour maps of CoMFA, suggested that the steric hindrance had a significant impact on the adsorption process of substituted benzenes. GRIND studies investigate the important mutual distances between molecular features, which confirmed the role of hydrophobic groups as well as their distances from different steric hot spots in the benzene ring of the molecules. According to HQSAR model and its fragment contribution map, the hydrogen bond donor and acceptor were also found to play an important role in governing adsorption of substituted benzenes on CNTs. The QSAR models facilitate better understanding of the features required for adsorption of benzene derivatives on CNTs and were established to shed light on the structural requirements for high adsorption coefficients.

Keywords: Adsorption coefficient, Benzene derivatives, Carbon nanotubes, HQSAR, CoMFA, GRIND

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Development of dispersive solid-phase extraction based on LDH/chitosan sorbent combined with dispersive liquid-liquid microextraction to extract pesticides before their analysis by GC-NPD

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Agricultural products, including fruits, are used as raw materials for the preparation of fruit juices can be affected by various pesticides during growth. The presence of these toxic compounds is a definite danger to human health and it is necessary to develop effective methods for measuring them in fruits and vegetables [1] . In the present study, a combination of dispersive solid-phase extraction (DSPE) method with dispersive liquid-liquid microextraction (DLLME) was developed for extraction and pre-concentration of pesticide residues from different samples. In this method, for the first time, a simply synthesized composite of double-layer hydroxide/chitosan (Ni-Fe LDH/Chit) was used as an adsorbent to extract pesticides. An appropriate amount of adsorbent was added to an aqueous phase containing analytes. The adsorbent is then separated from the aqueous solution and eluted with acetone. The acetone phase is mixed with chloroform and the mixture was dispersed in deionized water to form a cloudy solution. Finally, after centrifugation, the obtained precipitate phase containing the extracted analytes was injected into gas chromatography equipped with a nitrogen-phosphorus detector (GC-NPD). Under optimal conditions, acceptable linear range (0.036-250 µg/L), low detection limit (0.011-0.032 µg/L) good extraction recovery (ER > 63%), high enrichment factor (315< EF< 380) and good inter-and intra-day repeatability (<5.6%) were obtained. Other advantages of this method are the low consumption of organic solvents, simplicity and cost-effectiveness.

Keywords: Solid phase extraction, Dispersive liquid-liquid microextraction, layered double hydroxide, Chitosan, Fruit juice, Pesticides

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A novel QSPR study on the selectivity coefficients of Lanthanum-selective electrode

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Ion-selective electrodes (ISEs) are electrochemical sensors that respond selectively to the presence of ionic species [1]. The influence of the interfering ions on the response behavior of the ion-selective membrane electrodes is usually described in terms of selectivity coefficients, k_{sel}.In this study, the selectivity coefficients of a Lanthanum-selective electrode were predicted with the novel QSPR model for the first time. The selectivity coefficients of the La(III) membrane sensor based on 8-amino-N-(2-hydroxybenzylidene) naphthylamine (AIP) were efficiently estimated and predicted. The reported electrode was prepared with reference by Ganjali et al. [2]. Quantitative structure-property relationships (QSPR) models were constructed based on calculated molecular descriptors. Since the cations descriptors are limited; we introduce a new strategy for the calculation of descriptors. We optimized the structure of M^{n+}-AIP to calculate structural descriptors of AIP in the presence cations based on DFT (B3LYP functional) with SBKJC basis set. The most important descriptors were selected by genetic algorithm (GA) and stepwise techniques. After the variable selection, multiple linear regression (MLR) was utilized to construct linear QSPR models. The results showed more quality for GA-MLR (R^2= 0.945 and SE= 0.258) than stepwise-MLR modeling (R^2= 0.880 and SE= 0.400). Also, the prediction results of the GA-MLR model illustrated very good agreement with the experimental values. The new strategy in this paper can be developed for other QSPR studies in cation-selective electrodes.

Keywords: Selectivity coefficient; Multiple linear regression (MLR); Genetic algorithm; Molecular descriptors; QSPR

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Supra Molecular Solvent as Novel Liquid Phase in dye removal

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Supra molecular solvents (SUPRAs) have fantastic properties which have been made them very attractive for separation processes [1, 2].

SUPRAs are nanostructured liquids which can be produced from colloidal solutions of amphiphilic compounds such as surfactants and carboxylic acids. The aggregates of amphiphiles in SUPRA are produced by spontaneous, sequential phenomena of self-assembly, and coacervation processes. The nanostructured aggregates in SUPRA can be micelles, reversed micelles, and vesicles of an amphiphile. SUPRA can be an alternative substitute liquid phase instead of toxic organic solvents in extraction processes. SUPRAs possess interesting advantages such as friendly environment, not flammability, and high extraction efficiency in low volumes. Also nanostructured aggregates in SUPRAs have regions of different polarity which have been made them suitable to extract solutes in a wide range of polarity.

In this research, two kinds of supramolecular solvents were prepared [1-3] and used to compare their efficiencies in removal of Direct Black EX 122 and Acid blue, as textile industry dyes, from aqueous samples. The effective parameters on dye extraction, such as: the concentration, volume, temperature, and pH of dye solution, separation time, types of aggregates in SUPRA phase and volume of liquid SUPRA phase, were investigated. Under optimal conditions, interesting and high extraction efficiencies were achieved.

Keywords: SUPRA, nanostructured, aggregates, supramolecular solvent, extraction

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Determination of thermodynamic parameters of lithium titanates

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Alkali metal titanates are of interest for magneto-optical, ion-conducting and spintronic devices, ion batteries, for the creation of new highly efficient catalysts and functional nanoparticles. Li_2TiO_3 is used in the cathode of some lithium-ion batteries together with an aqueous binder and a conductive agent. Li_2 TiO3 is used because it is able to stabilize high-capacity cathode conducting agents; $LiMO_2$ (M = Fe, Mn, Cr, Ni). Li_2TiO_3 and conducting agents ($LiMO_2$) are layered to create a cathode material. These layers allow lithium diffusion. The most stable phase of lithium titanate is β-Li.$_2$TiO$_3$, which belongs to the monoclinic system. The high-temperature cubic phase demonstrating the behavior of a solid solution type is called γ-Li_2TiO_3 and it is known that it reversibly forms at temperatures above 1150-1250°C. The metastable cubic phase, isostructured γ-Li_2TiO_3 is called α-Li_2TiO_3; it is formed at low temperatures and passes into a more stable β-phase at 400°C. Of lithium titanates, thermodynamic data are available only for the Li_2TiO_3 compound [1]. To determine the thermodynamic parameters of titanium lanthanides the EMF of concentration chains was measured:

$$\mathbf{Pt \,|\, Li_2O \,|\, ZrO_2 + 10\ \text{mas.\%}\ Y_2O_3,\ \text{lithium glass} \,|\, (Li_2O)x(TiO_2)_{1-x} \,|\, Pt} \quad (1)$$

Keywords: Lithium titanates, EMF method, Free energies, Enthalpy, Standard entropy

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The determination and modeling of P-T-X phase equilibria in the Ag-Pb-Se and Ag-Pb-Te systems

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P (pressure) -T (temperature) -X (composition) diagrams of ternary systems are necessary to determine the conditions for obtaining a solid phase, crystallization of a liquid alloy and vapor deposition. However, such data for ternary selenide and telluride systems, which are of practical interest for semiconductor technology, were absent before this dissertation work. P-T-X diagrams were determined only for binary chalcogenide systems. This situation is associated with the laboriousness of the experimental determination of the P-T-X phase diagrams of chalcogenide ternary systems containing volatile components, in particular, selenium and tellurium.In the this work, the partial pressures of the saturated vapor of diatomic selenium and tellurium molecules over the crystallization surface of PbSe and PbTe in ternary systems Ag-Pb-Se and Ag-Pb-Te were determined and 3D modeled by experimental and computational methods [1].

Keywords: Selenide and telluride systems, Partial pressure of the saturated vapor, Calculated method.

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Different coordination modes of ambidentate phosphorous ylide ligands in complexation with Pd/Pt-cyclopropa[60]fullerenes; Synthesis and Cytotoxic investigation

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In the past two decades, there has been considerable interest in the synthesis and theoretical study of transition metal complexes of fullerenes, in which the C_{60} cage is attached to metal center to form corresponding organometallic π-complexes [1]. Although there are many reports of metallofullerenes [2], few studies have focused on the Pd/Pt-cyclopropa[60]fullerene complexes bearing phosphorus ligands [3]. Among them, the simple mono- and diphosphines are the most widely used ligands coordinated to C_{60} and neutral Pd(0)/Pt(0) core which form metallacyclopropa[60]fullerene complexes [4]. Versatile functionalized diphosphines, especially α-keto stabilized phosphorus ylides can coordinate to transition metal ions through the terminal PPh_2 group and/or formally negatively charged carbanion [5]. Reaction of C_{60} with $[Pd/Pt(dba)_2]$ (dba= dibenzylideneacetone) and phosphorus ylides $[Ph_2P(CH_2)_nPPh_2C(H)C(O)C_6H_4\text{-}m\text{-}OMe]$ (n=1, (**Y**^{1}); n=2, (**Y**^{2})) gave the new Pd/Pt-[60]fullerene complexes. All complexes were characterized successfully by multinuclear NMR (^1H, ^{13}C and ^{31}P) spectroscopy and other conventional techniques such as IR, elemental analysis and mass spectrometry. Based on the above backgrounds, we have focused on the synthesis and cytotoxicity investigation of the new Pd/Pt-cyclopropa[60]fullerene complexes of phosphorus ylides.

Keywords: Pd/Pt-[60]fullerene complexes, Phosphorus ylide, Cytotoxicity activity, Multinuclear NMR

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New asymmetric palladacycle complexes with P,P- and P,O-bidentate ligands; Synthesis, X-ray structural and catalytic application in Suzuki reaction

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One of the most important research areas in the organometallic chemistry is C-H bond activation in cyclopalladated complexes [1, 2]. Palladacycles have been known over 30 years [3] and have gained great interest due to their applications in many areas including organic synthesis [4]. The interest in cyclopalladated complexes derived from *N*-donor ligands has increased considerably and it is due to their extremely high catalytic activity in a variety of important C–C coupling reactions including Heck reactions and Suzuki coupling [5]. This work reports the preparation of the mononuclear derivatives $[(K^2\text{-}C_6H_4CH_2NH_2)Pd(K^2\text{-}L)](ClO_4)$ (L = dppp and dppmo). The results of these studies including the full characterization of the obtained complexes (performed by elemental analysis, X-ray structural, IR, multinuclear NMR techniques and also application of the new asymmetric cyclopalladated of benzylamine as a catalyst precursor for the Suzuki reaction) is presented and discussed in this paper. The palladacycle complexes proved to be excellent catalysts for the Suzuki reactions of various aryl halides. Therefore, in order to examine the catalytic activity of Pd(II) complexes in the Suzuki reaction, the reaction between bromobenzene with phenylboronic acid in the presence of catalyst Pd was chosen as model reaction. Influences of different parameters such as base, temperature, solvent, and catalyst concentration have examined to obtain the best possible combination.

Keywords: Ortho-palladation, X-ray structure, Benzylamine ligand, Suzuki coupling

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Crystal engineering and investigations on the *N*-oxide effect of isocinchomeronic acid in a new Mn(II) complex

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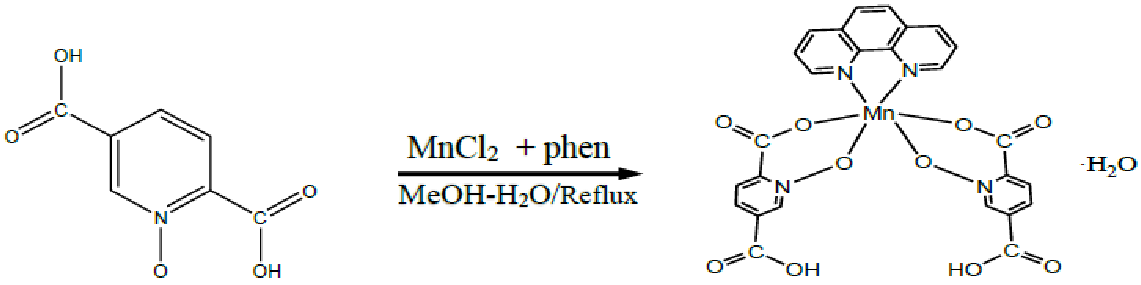
The importance of crystal engineering is highlighted when our purpose is to obtain a compound with desired solid-state properties, understand the stability (or its lack) of given crystalline network, or structural motif, or when we aim to answer this question: “how do crystalline solids self-assemble?”. In fact, the idea of making crystals with design and organization of molecular building blocks into extended architectures with specific dimensionalities and properties is an important goal for scientists in this field and actually it began to flourish. For this purpose, one of the most leading and efficient methods is the use of single-crystal X-ray diffraction for experimental structure determination, and confrontation of the obtained results with the already garnered knowledge by crystal engineers. H_2pydco (isocinchomeronic acid or pyridine-2,5-dicarboxylic acid *N*-oxide) is known as an appropriate candidate for constructing new metal organic compounds. It is well known that Mn complexes containing *N*-oxidation family ligands have been utilized as an anti-HIV agent, gas adsorbent, luminescent agent, etc [1-5].

Keywords: Crystal engineering, Pyridine-2,5-dicarboxylic acid *N*-oxide, 1,10-phenanthroline.



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Investigation of coordination behavior of pyridine-2,5-dicarboxylic acid *N*-oxide and 1,10-phenanthroline toward zinc ion

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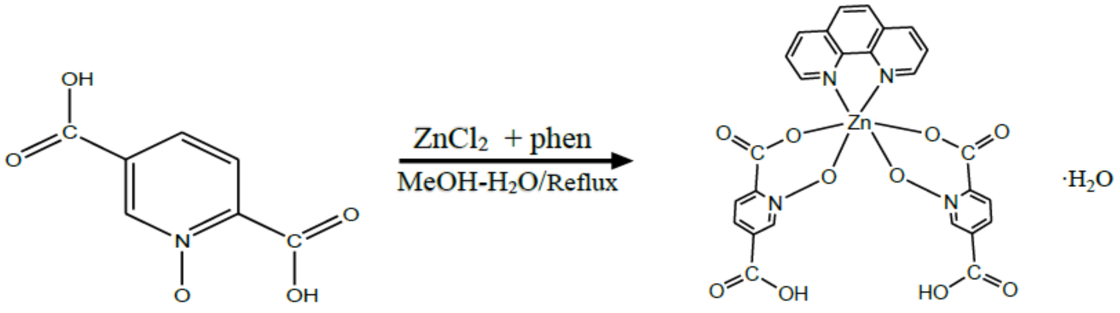
Crystalline solids are formed when molecules arrange in a very orderly fashion by means of many types of intermolecular interactions such as classic and non-classic hydrogen bonding, halogen bonding, π–stacking, ion pairing, van der Waals and donor-acceptor interactions, to name only a few of them. In this work, we select pyridine-2,5-dicarboxyxlic acid *N*-oxide (pydco) as a versatile *O*-donor ligand with two diverge -COOH groups, through covalent bonds with metal ions as well as at the same time can participate in non-covalent interactions (typically π-stacking interactions) that promote the dimensional architectures of the complex. Also, *O*-donor ligands are of particular interest because they have significant medical property specially when they are connected to biologically important metals. Furthermore, heterocyclic *N*-donor π-electron-deficient ligands, with planarity and rigidity have widely used in supramolecular chemistry and/or in the molecular biology as DNA cleaving reagent, *etc* [1-5]. The aim of the present study is to report successful preparation of a new coordination complexe based on H_2pydco, 1,10-phenanthroline (phen) and zinc metal that characterized by physico-chemical approaches such as elemental analysis (CHN) and FT-IR spectroscopy. Based on our obtained data it may be formulated as $[Zn(Hpydco)_2(phen)]\cdot H_2O$.

Keywords: *O*-donor ligands, Pyridine-2,5-dicarboxylic acid *N*-oxide, Intermolecular interactions.



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Grafting and stabilization of manganese complex on kryptofix23 modified Fe3O4@carbon nanosphere: as highly efficient, reusable, and clean nanocatalyst for coupling xanthenes

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Grafting and stabilization of metal complexes for increasing catalytic activity have remained an enormous challenge in the catalytic arena [1-3]. However, designing a catalytic system with complementary properties including high surface area, high loading, and easy separation offers a promising route for efficient utilization of magnetic material for various applications [4,5]. Herein, a novel core-shell nanosphere catalyst (Fe_3O_4@C/KP23@MnCl2) was successfully synthesized with a magnetite core encapsulated in a carbon shell. It was modified using CPTES (3-chloropropyltriethoxysilane) and Kryptofix23 (KP23) ligand in the carbon surface for conversion to Fe_3O_4@C/KP23 support. The Manganese complex was coordinated onto the KP23 ligand decorated Fe_3O_4@C to improve the unusual coupling xanthenes in ethanol. It was found proposed nanocatalyst is greener, recyclable, and more suitable option for large-scale application and provides some new insights into organic transformation.

Keywords: Fe_3O_4 NPs, Nanocatalyst, Kryptofix, Xanthene, Coupling reactions.

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Supramolecular Fe_3O_4@PEG/Murexide@Ni: a magnetic, novel, and reusable nanocatalyst for clean synthesis of benzothiazoles

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As a well-organized system, the nano-magnetic particles are efficient and suitable materials for the synthesis of heterogeneous and homogenous catalysts [1,2]. Magnetite which is well-known as ferrite and/or Fe_3O_4 is identified to use to increase magnetically recyclable and stable heterogeneous nanocatalysts for some metals that have some catalytic activities such as Mn, Ni, Cu, Co, etc. [3] Recently, nanocomposites of inorganic particles and organic materials have the great attention from their wide properties and applications in magnetic information storage media and capacity optical properties [4,5]. Ni@Murexide complex supported on magnetic nanoparticles is successfully synthesized and reported as a novel, heterogenous, reusable, efficient, and green catalyst, modified by using 3-chloropropyltriethoxysilane (CPTES) and Murexide (MX) ligand in the Fe_3O_4@PEG support. The structure of Fe_3O_4@PEG/MX/Ni was characterized by different analyses such as FT-IR, SEM, EDS, TEM, ICP-OES, XRD, VSM, and TGA. For exploring the catalyst activity of Fe_3O_4@PEG/MX@Ni, the catalyst was used for the synthesis of the benzothiazole derivatives through a one-pot process. All reactions were completed in a short time with excellent yield product in presence of the synthesized green catalyst. Moreover, Fe_3O_4@PEG/MX@Ni showed great use for at least five-time with no significant loss of its catalytic activity.

Keywords: Fe_3O_4 NPs, Nanocatalyst, Magnetic nanoparticles, Murexide, Nickel complex.

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Synthesis and Characterization of Zn-Co-Layered Double Hydroxide Intercalated with Vanadate and Molybdate Anions as a More Efficient Electrocatalysts for Oxygen Evolution Reaction

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Electrochemical water splitting has great potential in the storage of intermittent energy from the sun, wind, or other renewable sources for sustainable clean energy applications. However, the anodic oxygen evolution reaction (OER) usually determines the efficiency of practical water electrolysis due to its sluggish four-electron process. Layered double hydroxides (LDHs) have attracted increasing attention as one of the ideal and promising electrocatalysts for water oxidation due to their excellent activity, high stability in basic conditions, as well as their earth-abundant compositions. In the present work, vanadate and molybdate anions were intercalated into Zn–Co layered double hydroxides using the co-precipitation method. The obtained VO_4-LDH and MoO_4–LDH nanohybrids were characterized by Powder X-ray diffraction (XRD), Fourier transform infrared spectroscopy (FT-IR), transmission electron microscopy (TEM), and X-ray energy dispersive spectroscopy (EDS) methods to get information about the structure, composition and morphology. The LDHs were used as an efficient electrocatalyst material for water oxidation in alkali solution. In electrochemical water splitting, the obtained results show that the Zn–Co–MoO_4-LDH exhibits good OER activity, which is expressed as a low onset overpotential, small Tafel slope, and large exchange current density. At the overpotential of 0.42 (V *vs.* SCE), the current density of the Zn–Co–MoO_4-LDH nanosheets is about 188.43 mA cm^{-2}, which is significantly higher than that of the Zn–Co–VO_4–LDH and Zn–Co–NO_3–LDH nanoparticles[1-4].

Keywords: Zn-Co-NO_3-LDH, Intercalation, Vanadate, Molybdate, Water oxidation, Oxygen evolution reaction (OER)

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Synthesis, characterization, and antibacterial application of curcumin-nicotinoyl chloride derivative and its copper complex

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In this research, the chemical structure of curcumin was modified by derivatization reaction. Modification of the curcumin was executed by derivatization with nicotinoyl chloride hydrochloride. The condensation of this molecule with curcumin produced a new compound (Cur-Nic) with a higher solubility and stability than curcumin. After modification of the curcumin structure, the product was characterized by FT-IR, UV-Vis, NMR, XRD, and MS. This ligand was used to synthesis of dinuclear complex of copper. This complex was characterized by FT-IR, UV-Vis, and NMR. Then the antibacterial effect of Cur-Nic and Cu complex on the Escherichia coli (E.coli) bacteria was assessed by the Broth Dilution method. It was found that complexation of Cur-Nic has a positive effect on antibacterial properties [1-3].

Keywords: Curcumin, Nicotinoyl Chloride Hydrochloride, Bioactivity

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Characterization and optical properties of nano-micro structure VO_2/WO_3 composite

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Vanadium has different oxidation states including V_2O_5, V_2O_3, and VO_2, among which vanadium dioxide is considered for its unique properties and is used in various subjects such as catalysts, optical memory, and thermochromic glass [1]. However, controlling the oxidation state of vanadium in synthesis processes is a challenging issue and the properties of the products depend on it [2]. Tungsten is one of the most widely used elements in similar articles to regulate the properties of vanadium dioxide as an oxide composite or as a dopant in structure [3-5]. In this study, WO_3 nanoparticles were synthesized by electrical discharge in water and VO_2 microparticles were synthesized by chemical reduction in ethylene glycol. The samples were characterized by X-ray diffraction spectroscopy (XRD), field emission scanning electron microscopy (FE-SEM), energy dispersive spectroscopy (EDS), and UV-vis spectroscopy. The XRD results showed that component VO_2 has a structure orthorhombic and WO_3 has a tetragonal structure. (FE-SEM) images showed that WO_3 spherical nanoparticles were 27±5 nm in size and composite spherical microparticles were 0.87±0.05 µm in size. The EDS result of the composite sample showed that the atomic ratio of tungsten to vanadium was 2.6%. The optical transmission spectrum obtained from the UV-vis spectrophotometer corresponded to the pattern of the semiconductor material spectrum and the energy gap calculated for samples VO_2 and VO_2/WO_3 composite were 1.9 and 2.1eV, respectively.

Keywords: Optical properties, VO_2/WO_3 composite, Electrical discharge, Chemical reduction

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Template synthesis of a nickel(II)/Schiff base complex: spectral and structural studies

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In this work, a new complex of nickel, $[Ni(L)(NO_3)]$, with 2-(((2-((3-aminoprophyl)amino)ethyl)amino)methyl cyclohexanol (L), was prepared by template synthesis and identified by elemental analysis, FT-IR spectroscopy and single-crystal X-Ray diffraction. As it is shown in Fig. 1, the coordination number of the nickel(II) ion in the compound is four and the nickel atom has NiN_3O environment with square planer geometry. The L unit is a potentially tetradentate ligand that can be bind to metal atoms through three N- and one O-atoms. In this structure the ligand was fully coordinated and forms one six membered and two five membered chelate rings. The phenolic group of ligand was deprotonated during the complexation process to form phenolate group thus the ligand converted to an anionic form. In the crystal network of the complex there is intermolecular N–H···O hydrogen bonds, extending the crystal network into three dimensional[1, 2].

Keywords: Template reaction, Nickel, X-ray diffraction, Schiff base

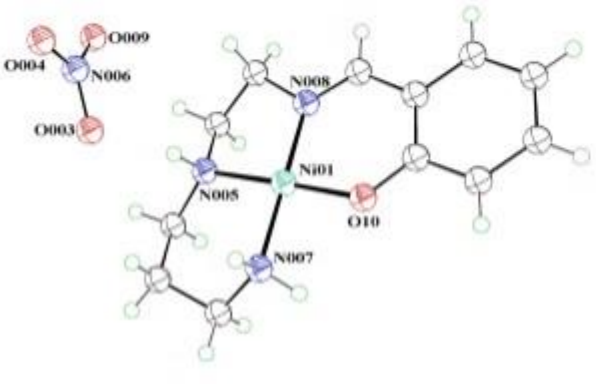

Figure 1. Crystal structure of complex.

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Evaluation of the biological activities of a nickel(II) complex containing a schiff base ligand: docking toward DNA and Proteins

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In this work the biological activity of a nickel(II) complex containing schiff base ligand, [Ni(AEPD)(NO_3)]; AEPD: 2-(((2-((3-aminoprophyl)amino)ethyl)amino)methyl cyclohexanol, was investigated by docking studies. Owing to the expected biological properties of the Schiff base complexes, we performed docking calculations to investigate interaction of L and its nickel complex with ten protein targets [3, 4], including: BRAF kinase, Cathepsin B (CatB), DNA gyrase, Histone deacetylase (HDAC7), recombinant Human albumin (rHA), Ribonucleotide reductases (RNR), Thioredoxin reductase (TrxR), Thymidylate synthase (TS), Topoisomerase II (Top II) along with B-DNA. These proteins were selected either due to their reported roles in cancer growth or as transport agents that affect drug pharmacokinetic properties (e.g., rHA). The DNA gyrase was included to study the possibility of anticancer properties and their activity as antimalarial agents [5]. The knowledge gained from docking on the B-DNA should be useful for the development of potential probes for DNA structure and new therapeutic agents for cancer and other diseases [6]. The docking studies revealed that these compounds might be biologically active and also these compounds can bind to the DNA molecule, thus we suggest that studying anticancer activities of these compounds could bring interesting results.

Keywords: Schiff base, Nickel, Docking study, DNA, Protein

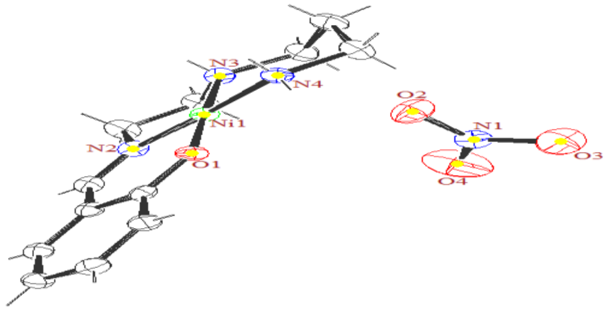

Figure 1. Crystal structure of complex.

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Synthesis, Characterization and Antimicrobial Activity of Some New Benzimidazolyl-phenols Including Halogens and Their Zn(II) and Pd(II) Complexes

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Metal complexes have extensive applications in various fields of human interest on the basis of nature of the metal as well as the type of ligand [1, 2]. Antimicrobial activity of some 2-(1H-benzimidazol-2-yl)-phenol derivatives and their metal complexes were investigated in detail against some microorganisms [3,4]. In this study, four new benzimidazolyl-phenol derivatives (ligands) synthesized and characterized (**HL$_1$** – **HL$_4$**, Figure 1). The complexes of the ligands with $ZnCl_2$ and $PdCl_2$ were prepared and characterized by using common physicochemical data and spectroscopic techniques. The ligands are monodeprotonable chelating agent and showed bidentate characteristic in the complexes. The effect of the halogens was investigated on the ligands and the complexes. In addition, antimicrobial activity of the compounds was tested against some bacteria and fungi. Some of the ligands and complexes showed moderate antimicrobial activity on *S. epidermidis* bacteria and *C. albicans* fungus. It was observed that the complexes are non-electrolyte or 1:1 electrolyte and have 1:1 or 1:2 metal:ligand ratio.

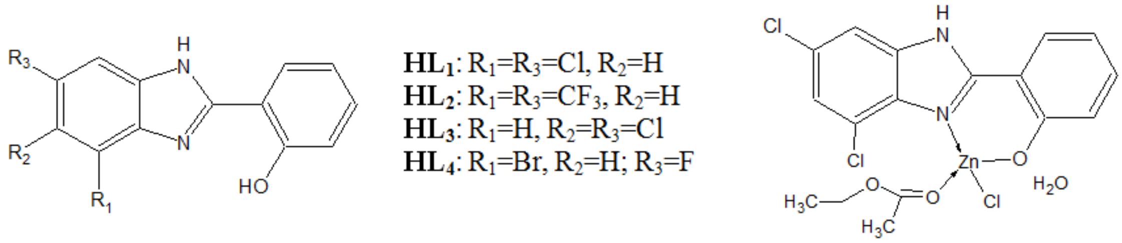

Figure 1: The benzimidazolyl-phenols (left) and the proposed Zn(II) complex of **HL$_1$** (right)

Keywords: Benzimidazole, Phenol, Metal Complex, Antimicrobial

Acknowledgements: This work was supported by Scientific Research Projects Coordination Unit of Istanbul University - Cerrahpasa. Project number: 36467

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Radiochromic Hydrogen-Bonded Organic Frameworks for X-Ray Detection

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Porous materials have been investigated as efficient photochromic platforms for detecting hazardous radiation, while the utilization of hydrogen bonded-organic frameworks (HOFs) in this field has remained intact. Herein, two HOFs were synthesized through self-assembly of tetratopic viologen ligand and formic acid (PFC-25, PFC-26), as a new class of “all-organic” radiochromic smart materials, opening a gate for HOFs in this desired field. PFC-26 is active upon both X-rays and UV light, while PFC-25 is only active upon X-rays. The same building block yet different radiochromic behaviors of PFC-25 and PFC-26 allow us to gain a deep mechanistic understanding of the factors that control the detection specificity. Theoretical and experimental studies reveal that the degree of π-conjugation of viologen ligand is highly related to the threshold energy of triggering a charge transfer, therefore being a vital factor for the particularity of radiochromic materials. Thanks to its convenient processibility, nanoparticle size, and UV silence, PFC-25 can be further fabricated into a portable naked-eye sensor for X-ray detection, which shows obvious color change with the merits of high transmittance contrast, good sensitivity (reproducible dose threshold of 3.5 Gy), and excellent stability. The work exhibits the promising practical potentials of HOF materials in photochromic technology.

Keywords: Sensor, X-ray Detection, Hydrogen-Bonded Organic Frameworks, Radiochromism.

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Preparation and characterization of Chitosan/poly(maleic acid) Membranes as Adsorbents for Water Purification

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In this study, a cross-linked chitosan modified with poly maleic acid were utilized as a possible adsorbent for the elimination of Cu(II) and Cr(VI), Hg(II) and Cd(II) from aqueous solutions[1-3]. The synthesized adsorbent was characterized by Scanning ElectronMicroscopy (SEM) and Fourier Transform Infrared (FTIR) analysis[4-5]. The aim of this study was to prepare a novel modified chitosan nanomaterial with high uptake and selectivity for sorption of Hg^{2+} and Cd^{2+}. The synthesis conditions were optimized.

Keywords: Chitosan, Water purification, Heavy metal ions removal, Maleic acid.

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Oxidative addition of MeI to a Pt(II) complex: kinetic and theoretical elucidation

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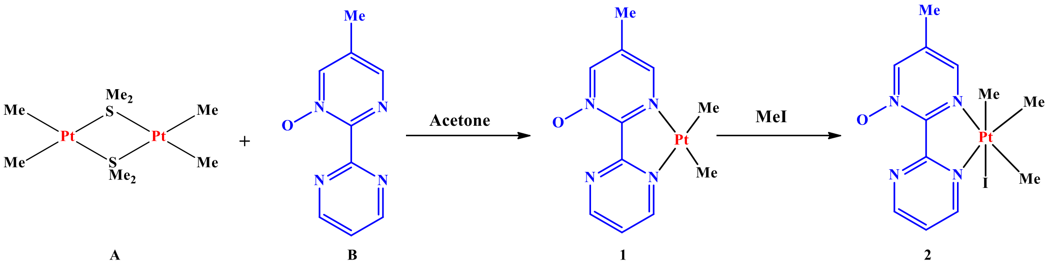
The oxidative addition (OA) reaction plays a vital role in industry and it is one of the most critical reactions in the organometallic research area. Since platinum contains a wide range of stable complexes in organometallic chemistry, the OA in square-planar Pt(II) compounds has been further investigated in recent years [1]. The kinetic of Pt(II) complexes containing N^N (2,2'-bipyridine) [2], N^O (1,10-phenanthroline *N*-oxide) [3] and rollover C^N cyclometalated ligands (2,2'-bipyridine *N*-oxide) [4] with different reagents such as MeI, EtI, $PhCH_2Br$, *etc.* were studied. Additionally, the mechanism of the OA reactions on these platinum complexes were explored. New Pt(II) complexes $[PtMe_2(bpyNO)]$, **1**, bpyNO = 4-methylbipyrimidine-2-*N*-oxide, was synthesized by the reaction of *cis,cis*-$[PtMe_2(\mu\text{-}SMe_2)]_2$, **A**, and bpyNO, **B**, (Scheme 1). MeI reagent was added to a Pt(II) complex **1** and give a corresponding Pt(IV) complex $[PtIMe_3(bpyNO)]$, **2**. Kinetic of this reaction was studied using UV–vis spectroscopy in different temperatures and an S_N2 mechanism was suggested. The reaction followed second-order kinetics, rate = k_2[**1**][MeI] and activation parameters have been determined and large negative values for $\Delta S^{\ddagger}$ were obtained. The results were also supported by theoretical calculations. The computational investigations were used to determine the geometry of the species involved in the suggested mechanism and energy barriers.



Scheme 1: Synthetic route for the preparation of Pt(II) and Pt(IV) complexes.

Keywords: Platinum, Mechanism, Oxidative addition, Theoretical calculations.

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Nanoferrites with Mg-Mn

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Ferrites with a general formula of MFe_2O_4 , where M represents a metal cation, are chemically and thermally stable magnetic materials that have been used for numerous applications. Since their discovery, there has been an exponential increase of interest in ferrites, which is still growing. Their magnetic properties make them beneficial in magnetic resonance imaging (MRI), electronic devices, information storage, and drug delivery[1,3,4,5]. Ferrites, transition metal oxides with spinel structures, are one of the most important MNPs. Ferrites are classified based on their crystal structures and magnetic properties, as spinel (MFe_2O_4 , where M = Mn, Fe, Co, Ni, Co, Zn, etc.), garnet (M_3 Fe_5O_{12}, where M = rare earth cations), hexaferrite ($SrFe_{12}O_{19}$ and $BaFe_{12}O_{19}$), and ortho ferrite (MFeO3 ,M= rare earth cations)[2]. Mg-Mn ferrites are important technological materials. They have electrical and attractive properties. They are utilized for making of nonreciprocal gadgets at microwave frequencies, for example- active components of ferro-fluids circulators, transformer cores, rod antennas and drug delivery[1,3,4]. Properties of Mg-Mn ferrites get influenced by method of preparation. The results of degradation were interpreted depending on the Mg content, particle size and specific surface area[5].Mg-Mn ferrites are important technological materials. They have electrical and attractive properties. The Mg-Mn ferrites are adaptable from the application perspective. The rectangular hysteresis loop of Mg-Mn ferrites shows that they are very appropriate for the utilization in switching circuits and memory of PCs and as stage shifter[3,4,5]. Their interesting chemical and physical properties emerge because of the capacity to distribute cations among the accessible tetrahedral site and octahedral site[4]. Properties of Mg-Mn ferrites get influenced by method of preparation [3]. Ferrites are classified into two families: soft ferrites and hard ferrites[4].

Keywords: Ferrites, Nanoparticles, Mg-Mn ferrites

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Preparation of MCM-41/ammonium salt as an efficient, novel, and reusable nanocatalyst and its catalytic application for clean synthesis of NH-tetrazole derivatives

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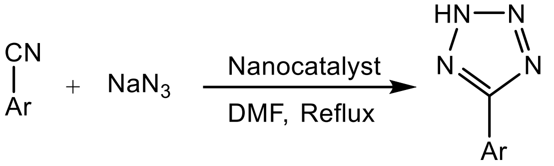
Nanosized materials, besides their special and unique characters, have received a great deal of interest from scientists in recent decades [1]. Among them, heterogenous and homogenous nanocatalysts with a basis of transition metals have gained breakthroughs in the field of green catalysts for chemical processes [2]. A vital parameter for designing heterogeneous catalyst support is the size of a specific surface area. Therefore, there have reported many the using various synthesis process and catalyst materials by researchers recently. One of the efficient supports for catalysts with great thermal stability and a high specific area is the mesoporous MCM-41 [3,4]. NH-tetrazole is a popular organic compound with a vast range of applications such as propellants, explosives, and medicinal chemistry as a ligand. Also, NH-tetrazoles are an excellent replacement for carboxylic acid in drug design [5]. In the present work, we designed and prepared a novel and reusable MCM-41/ammonium salt nanocatalyst and examined its catalytic activity with the synthesis of NH-tetrazole derivatives and characterized by using various techniques such as FT-IR, VSM, BET, EDS, TEM, SEM, and TGA. Also, the synthesized catalyst has shown a great recoverability for 5 rounds of the tetrazole synthesis process.

Keywords: nanocatalyst, MCM-41, NH-tetrazole



Scheme 1. Synthesis of NH-tetrazoles in the presence of new nanocatalyst.

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Synthesis of CH-tetrazole derivatives in the presence of ammonium salt/MCM-41: a novel, efficient, high stable and reusable nanocatalyst

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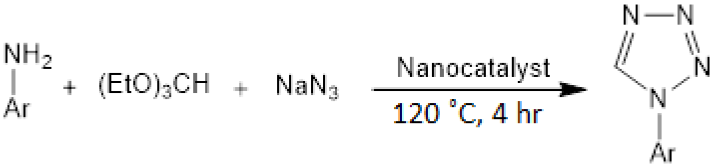
For many years, the procurement of heterogeneous catalysts has been a main field of sub-nanotechnology and remains so nowadays [1-2]. The approach to preparation must be examined in activity and selectivity, which both depend on the atom arrangement at a scale smaller than 0.02 nm. Currently, the synthesis and application of functionalized magnetic particles have caused a high interest. Recently, mesoporous silica such as MCM-41 has received a great fondness in the synthesis of homogenous and heterogeneous catalysts because of their several advantages such as high surface area, easy preparation and functionalization, large pore volumes, easy preparation and functionalization, and recoverability [3,4]. Tetrazole, as a great deal in information recording systems, pharmaceuticals, rocket propellants, and photography, tetrazoles have been studied and used in various medicinal and synthetic applications [5]. In this work, the ammonium salt/MCM-41 are introduced as heterogenous, novel, easy functionalized, and recoverable nanocatalyst. The structure of the catalyst was characterized using various techniques such as TEM, SEM, EDS, BET, TGA, XRD, and FT-IR. This nanocatalyst showed a great function in the synthesis of the CH-tetrazole derivative.

Keywords: MCM-41, CH-tetrazole, nanocatalyst



Scheme 1. Synthesis of CH-tetrazoles in the presence of new nanocatalyst.

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Complexation of a triazine ligand toward the nickel atom: Spectral, structural and docking studies

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A new complex of nickel, $[Ni(L)_2(NO_3)_2]$, with 5-phenyl-3-(pyridin-2-yl)-1,2,4-triazine (L), was prepared and identified by elemental analysis, FT-IR spectroscopy and single-crystal X-Ray diffraction. In the structure (Fig. 1), the nickel atom has NiN_4O_2 environment with octahedral geometry and the triazine ligand acts as N_2-donor through the pyridine and triazine notrogen atoms. Each nitrato ligand acts as monodentate O-donor. The complex has a center of inversion on the nickel atom and C_i symmetry. In the crystal network of the complex there are intermolecular C–H···N and C–H···O hydrogen bonds, extending the crystal network in three dimentions. In addition to these hydrogen bonds, in this network, there are π–π stacking interactions between phenyl and triazine rings on the adjacent molecules. The ability of the complex **1** to interact with biomacromolecules was investigated by docking studies. The results show that the ligand and its nickel comlexes can bind toward the biomacromolrcules and could be biologically active molecules [1-5].

Keywords: Triazine, Nickel, Docking study, X-ray diffraction, Protein

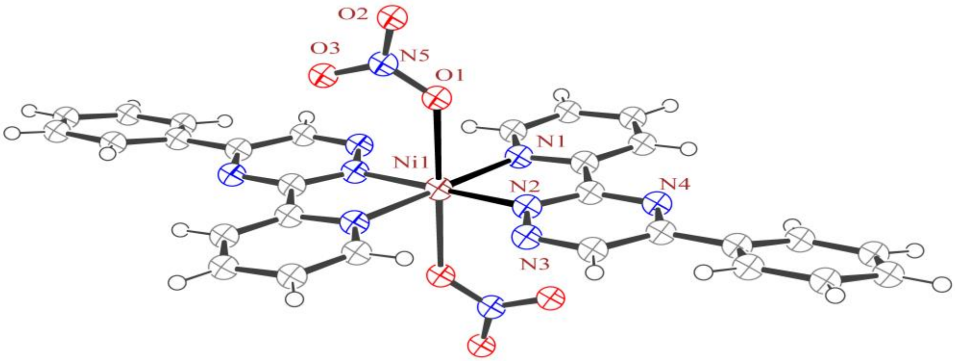

Figure 1. Crystal structure of complex 1.

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The Impact of Phosphine Ligands on the Luminescence Properties of Cyclometalated Pt(II) Complexes: Photophysical and Theoretical Studies

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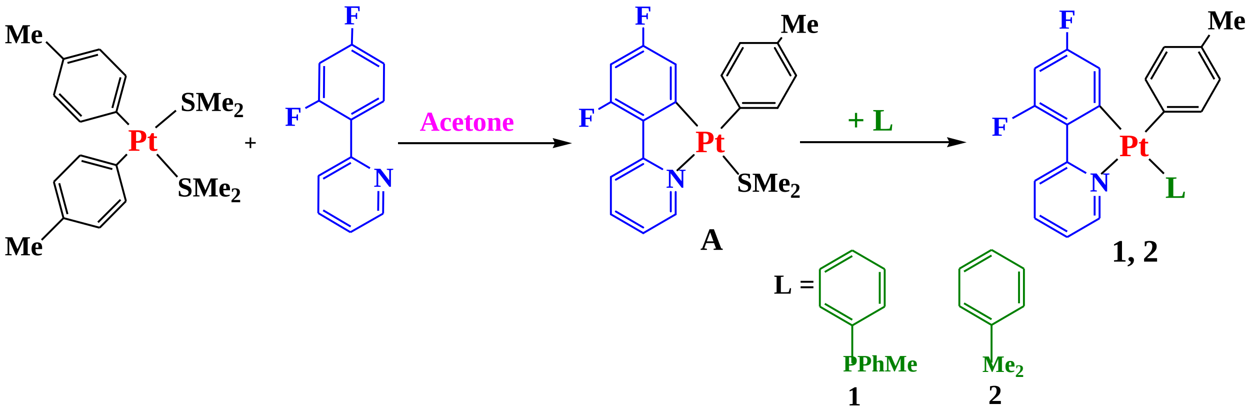
In recent years, cycloplatinated(II) complexes with high emission intensities have attracted a massive amount of attention which refers to their highly efficient triplet harvesting properties[1]. For this reason, they have been frequently evaluated for various applications such as photocatalysts, and chemical or biochemical sensors. In the emissive cycloplatinated(II) complexes, cyclometalated moiety is the key component in determining the emission properties[2]. As demonstrated in Scheme 1, cycloplatinated(II) complexes with general formula of [Pt(pMeC$_6$H$_4$)(dfppy)(L)], dfppy = 2-(2,4-difluorophenyl)pyridinate), L = PPh$_2$Me; **1**, PPhMe$_2$; **2**, were synthesized. These complexes were identified by different techniques and photophysically investigated by means of UV-Vis absorption and photoluminescence spectroscopies. To rationalize the experimental photophysical data, density functional theory (DFT) and (TD-DFT) calculations were employed for both the complexes.



Scheme 1: Synthetic route for the preparation of Pt(II) complexes.

Keywords: Cyclometalated platinum complexes, Luminescence, Photophysical, DFT calculations

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Enhance catalytic performance of SAPO-34 by addition Simultaneous dried seed and PEG in Methanol To Olefins reaction.

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SAPO-34 catalyst has been synthesized via the seed-induced method and addition of polyethylene glycol (PEG) as a soft template through the hydrothermal method and has been characterized by various techniques such as XRD, FESEM, FTIR, BET, and NH3-TPD. In the methanol-to-olefins (MTO) reaction, we studied SAPO-34 as a catalyst in a fixed-bed reactor at 425 C and 1 atm in the methanol-to-olefins (MTO) reaction. The results showed that the simultaneous presence of the soft template and the dried seed improves the performance of the SAPO catalyst in viewpoint of increasing lifetime. An excellent catalytic performance was achieved for the seeding-induced catalyst prepared by PEG template according to its appropriate high acidity and relatively large surface area. Modified SAPO-34 exhibited about 780 min of a lifetime which was 136% higher than the conventional catalyst[1].

Keywords: SAPO-34, Seed, PEG, MTO reaction

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Syntheses, characterization and structural analysis of hetero-metallic trinuclear copper(II)–cadmium(II) complexes derived from a Salen-type ligand: Effect of counteranions on the structure

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Two new trinuclear hetero-metallic copper(II)-cadmium(II) complexes,$[Cu_2(\mu\text{-}L)_2Cd(NO_3)_2]$ (**1**) and $[Cu_2(\mu\text{-}L)_2CdCl_2]$ (**2**), have been synthesized using [CuL] as a so-called ‘‘ligand complex’’ (where L^{2-} = N,N'-bis(salicylidene)-2,2-dimethylpropylenediaminato) and structurally characterized. Crystal structure analyses reveal that two complexes contain a trinuclear moiety in which two [CuL] units are bonded to a central cadmium(II) ion through double phenoxido bridges. The Cd(II) ion in **1**is in a six-coordinate distorted octahedral environment being bonded additionally to two mutually *trans* oxygen atoms of nitrate. Complex **2** contains a heterotrinuclear $[Cu^{II}Cd^{II}Cu^{II}]$ unit in which the central cadmium ion is connected to two copper(II) centers through two doubly bridging phenolate oxygen atoms in addition to a terminal chloride ion. On the other hand, the Cd(II) ions in **1** and **2** adopt distorted octahedral (CdO_6) and square pyramidal (CdO_4Cl) geometries, respectively.

Keywords: Hetero-metallic, trinuclear, Copper, Cadmium, crystal structure.

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Syntheses, characterization and structural determination of hetero-metallic dinuclear copper(II)–mercury(II) complexes derived from a Salen-type ligand

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Three new dinuclear hetero-metallic copper(II)-mercury(II) complexes, $[CuL\{HgCl_2(CH_3OH)\}]$ (**1**), $[CuL\{HgBr_2\}]$ (**2**) and $[CuL\{HgI_2\}]$ (**3**) have been synthesized by reacting [CuL] as a so-called ‘‘ligand complex’’ (where H_2L = N,N′-bis(2-hydroxyphenylidene)-2,2′-dimethyl-1,3-propanediamine) with HgX_2 (X^-= Cl^-, Br^- and I^-). Three complexes have been characterized using elemental analysis, IR spectroscopy and X-ray diffraction. Structural studies on **1**, **2** and **3** reveal the presence of a heterodinuclear $[Cu^{II}Hg^{II}]$ unit in which the central Cu(II) and Hg(II) ions are connected to each other by two phenolate oxygen bridges. In each of the complexes, the Cu(II) ion adopts a distorted square planar (CuN_2O_2) geometry while the Hg(II) ions in **1** adopts distorted square pyramidal (HgO_3Cl_2) but in **2** and **3** adopt tetrahedral (HgO_2Br_2 or HgO_2I_2) geometries.

Keywords: Hetero-metallic, Dinuclear, Copper(II)-Mercury(II), Crystal structure, Salen-type ligand.

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Performance comparison of Ag_2WO_4 and Ag_2MoO_4 based on $CoFe_2O_4$ as visible-light-driven heterogeneous photocatalysts

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Visible-light-driven nanophotocatalysts of Ag/β-Ag_2WO_4 and Ag_2MoO_4 based on $CoFe_2O_4$ magnetic nanoparticles were prepared by the decoration of Ag/β-Ag_2WO_4 and Ag_2MoO_4 nanoparticles on the surface of $CoFe_2O_4$ nanoparticles by a facile in situ coprecipitation method at room temperature [1,2]. The mean crystallite size of Ag/β-Ag_2WO_4/$CoFe_2O_4$ and Ag_2WO_4/$CoFe_2O_4$ was around 43 and 39 nm with flower and grain-like morphology, respectively. The photocatalytic activity of Ag/β-Ag_2WO_4/$CoFe_2O_4$ nanocomposite for the oxidation of benzyl alcohol was enhanced by 85%, while the $CoFe_2O_4$/Ag_2MoO_4 reached 82% under visible light irradiation. This photocatalyst consisting of Ag/β-Ag_2WO_4, Ag_2MoO_4, and $CoFe_2O_4$ nanostructures combines the high photocatalytic activity of Ag/β-Ag_2WO_4 and Ag_2MoO_4 and the stability and magnetism of $CoFe_2O_4$. This photoactivity enhancement was attributed to the impressive separation of electron-hole pairs [3]. The trapping experiments confirm the role of both positive holes (h^+) and hydroxyl radical ($^{\circ}OH$) groups in the proposed mechanism [4]. These robust and high-performance magnetic photocatalysts were recovered easily by a magnet and reused several times without considerable changes in performance [1].

Keywords: Nanomagnetic, Ag/β-Ag_2WO_4, Ag_2MoO_4, $CoFe_2O_4$, Photocatalyst

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Novel Layered Organic-Inorganic Hybrid of Tungsten Oxide as Effective Catalysts in Oxidative Desulfurization of Model Fuel

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The reduction of sulfur compound contents in fuels is an important strategy for the environmental protection. Among different method for desulfurization, oxidative desulfurization (ODS) is suggested as a promising process due to its low-energy consumption [1]. Various catalysts are previously used in the ODS reaction such as W, Mo, V, Ti, and Fe Oxides [2,3]. In this research, the novel layered organic-inorganic materials based on tungsten oxide were synthesized using three amino-carboxylate ligands and their catalytic properties were investigated in oxidative desulfurization of model fuel. On the basis of X-ray diffraction, scanning electron microscopy, thermogravimetry, and infrared results, a possible arrangement of organic ligands in the interlayer space of tungsten oxide has been proposed and the influence of the structural diversity of these hybrid materials on their catalytic performance is discussed. Results display the superior catalytic activity of these hybrids compared to tungsten oxide. Further more, the recycling of catalysts exhibit the good stability of these hybrid catalysts even after five runs.

Keywords: Tungsten oxide, Organic-inorganic hybrid, Oxidative desulfurization.

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Preparation and characterization of MWCNT/$NiFe_2O_4$ nanoparticles in the presence of deep eutectic solvents as a new sorbents: application in extraction of bisphenol A from aqueous samples

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A spinel is a ternary oxide whose general chemical formula is AB_2O_4, where A represents a divalent metal cation that usually occupies a tetrahedral site and B represents trivalent metal cations that normally occupy the octahedral sites of a cubic lattice [1]. Oxide spinels comprise a very large group of structurally related compounds many of which are of considerable technological significance [2]. Among them, nickel ferrites have become one of the best options for usage in different applications such as medical treatment, electronic devices, electromagnetic wave absorption materials and water purification. The popularity of these ferrites is due to their favourable properties such as high permeability, high resistivity and high saturation magnetization, the porosity of the nanostructures limits the adsorption efficiency. For solving this problem, multi-walled carbon nanotubes (MWCNTs) have been integrated into transition metal oxide nanostructures. Hybrid nanostructures show high adsorption capacity due to their increased surface area and can be easily designed.

In this study, a new DESs composed of tetrahexylammonium bromide and hexanol was prepared and it was used to to functionalize the MWCNT/$NiFe_2O_4$ hybrid nanostructures. Materials were identified using Fourier transform infrared spectroscopy, X-ray diffraction, nuclear magnetic resonance spectroscopy and scanning electron microscopy. The prepared CNT/$NiFe_2O_4$ and DES-functionalized MWCNT/ NiFe2O4 were used as adsorbents for bisphenol A (BPA) from aqueous medium. The results showed that BPA adsorption can be significantly improved by functionalizing the surface of MWCNT/$NiFe_2O_4$.

Keywords: Nickel ferrite; Deep eutectic solvent; Bisphenol A, Carbon nanotubes

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Preparation and characterization of MWCNT/cobalt doped $NiFe_2O_4$ nanoparticles functionalized by deep eutectic solvents as a magnetic sorbent; Application in extraction of morphine from urine samples

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Materials with spinel structure of MFe_2O_4 where M is a divalent metal ion such as manganese (Mn^{2+}), nickel (Ni^{2+}), cobalt (Co^{2+}), zinc (Zn^{2+}), copper (Cu^{2+}) or magnesium (Mg^{2+}) etc. are intensively investigated because of their vast applications, mainly due to magnetic properties. Among them, nickel ferrite (NiFe2O4) is very interesting because of its chemical and physical properties. NiFe2O4 has desirable properties such as high thermal stability, high mechanical resistance, low surface acidity, low temperature sinterability, and better diffusion. However, the practically achievable grain size and porosity of the nanostructures limits the surface area of the metal oxides and therefore the contact area with the dye limiting the adsorption efficiency. To increase the surface area and therefore improve the adsorption characteristics, multi-walled carbon nanotubes (MWCNTs) have been integrated into transition metal oxide nanostructures. The resulting hybrid nanostructures exhibit high adsorption capacity due to their enhanced surface area and can be easily tailored. To further improve the adsorption capacity, surface modification can be performed. In recent years deep eutectic solvents (DES) have been proposed for this purpose. DESs are a new generation of solvents which are formed by complexing a hydrogen bond donor with a quaternary ammonium salt. In this study, a new DESs composed of tetrabutylammonium bromide and oleic acid was prepared and it was used to to functionalize the MWCNT/cobalt doped $NiFe_2O_4$ hybrid nanostructures. The prepared materials were characterized using fourier-transform infrared spectroscopy, x-ray diffraction, nuclear-magnetic resonance spectroscopy and scanaing electron microscopy. The prepared CNT/$NiFe_2O_4$ and DES-functionalized MWCNT/$NiFe_2O_4$ were used as adsorbents for morphine (Mo) from urine smaple. The prepared nanoparticles were succsefuuly used for extraction of Mo from urine samples of patients who were suspicious to consumption of MP.

Keywords: Cobalet doped nickel ferrite; Deep eutectic solvent; Morphine, Carbon nanotubes

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Synthesis and characterization of new nano organic-inorganic hybrid (TBA)PWFe and investigation of this catalyst activity in oxidative desulfurization

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Oil pollution is an adverse phenomenon with serious effects on human health. Since the presence of sulfur compounds, especially mercaptans in oil fields, pollutes the environment and causes corrosion in transmission lines and storage tanks, it is necessary to reduce the amount of sulfur and mercaptans in oil fields to international standards [1-3]. Due to the problems of environmental pollution caused by burning high sulfur fuels such as fuel oil and the application of restrictions in this regard, in recent years, much attention has been paid to the development of desulfurization methods [4-5]. In this present work, $((n\text{-}C_4H_9)_4N)_4[PW_{11}Fe(H_2O)O_{39}]$ abbreviated as (TBA)PWFe polyoxymetals were fixed on the surface of polyvinyl alcohol (PVA), and chitosan (CTS) substrates by sol-gel method. The nanocomposite obtained was characterized through FT-IR, UV–vis, XRD, and SEM techniques. The catalytic activity of this hybrid nanocomposite was tested on oxidative desulphurization (ODS) of actual gasoline. (TBA)PWFe supported polyoxymetals are much more active than unsupported polyoxometals catalysts. The advantages of this method is low cost, simplicity and environmentally friendly route.

Keywords: Oxidative desulfurization, Polyoxometalate, Gasoline, Catalyst

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Crystal structure and Hirschfeld surface analysis of a new Dy(III) complex

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The coordination chemistry of hydarazone ligands has attracted considerable attention during last decade. This is related to the wide application of hydrazone complexes in various fields like magnetism, catalyst, medicine, biology and etc. [1]. In addition, hydrazones are suitable hosts for 3d/4f elements. The coordination compounds of 3d/4f metal ions have always been a topic of interest due to their attractive structures. Variety of 3d/4f elements as well as Schiff base ligands can lead to new structures which are inevitable. However, predicting the structure of lanthanide elements with Schiff bases due to their high coordination number is one of the difficulties in the controlled synthesis of this type of materials. In this report, a new Dy(III) complex was synthesized and characterized by elemental analysis and spectroscopic methods. Moreover, the crystal structure of this compound was characterized by single crystal X-ray analysis. Structural studies indicated that this compound is crystallized in monoclinic system and $P2_1/c$ space group. In order to find the intermolecular interactions in the structure of this compound, Hirschfeld surface analysis was also done (see Fig. 1). Hirschfeld surface analysis is one of the newest routes to studying inter-molecular interactions for investigation of crystal structure. This analysis was performed by information obtained from X-ray diffraction analysis in cif file format. In Fig. 1, the blue color represents the interactions that are larger from the sum of the van der Walls radii of atoms in that region. The white and red regions also represent the parts where the interactions are approximately equal and shorter than the sum of the van der Waals radii of the atoms in those regions, respectively [2].

Keywords: Dy(III) complex, Hirschfeld surface analysis, Crystal structure

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Introducing a new N_4-donor oxazolidine/cadmium complex

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The oxazolidine unit is a potentially tridentate ligand that can be bind to metal atoms through one O- and two N- atoms. A survey of the Cambridge Structural Database (CSD) reveals that this unit has two different coordination modes, $N^{py}N^{oxazolidine}$- and $N^{py}O^{oxazolidine}$-donor. The first mode in which two coordinated nitrogen atoms form a five-membered chelate ring is the most common. In this work, a new complex of cadmium, $[Cd(L)Br_2]$ (Fig. 1), was prepared and identified by elemental analysis, FT-IR, ^1H NMR spectroscopy and single-crystal X-Ray diffraction. In this structure (Fig. 1), the cadmium has an CdN_4Br_2 environment with distorted octahedral geometry. The ligand acts as N_4-donor through two pyridine, one imine and one amine nitrogen atoms and forms three five membered chelate rings [1, 2].

Keywords: Cadmium, Oxazolidine, Structural studies, Bromide, X-ray crystallography

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Geometry mismatch strategy for the discovery of a Fe-based MOF for selective oxidation of benzyl alcohol

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Herein, we described the using *geometry mismatch* strategy [1] for the assembly of two building blocks that are not compatibles in their ideal geometry; trigonal prism and hexagon. Combining 6-connected trigonal prism and hexagonal building blocks, seemingly incompatibles since there is no net for their assembly, successfully led to the discovery of a non-interpenetrated, highly porous Fe_3Otrimer-based metal-organic framework (Fe-MOF) with novel (3,3,3,6-c) net topology (Fig. 1). Single crystal and powder XRD, BET, ^{1}HNMR, XPS and FT-IR analysis were applied to characterization of Fe-MOF. Topological studies were carried out using TOPOS.pro software. Owning iron containing cluster, high porosity, large channel dimension, functionality and especially high stability, Fe-MOF can be excellent candidate for selective oxidation of benzyl alcohols. Gas chromatography instrument was used to investigation of catalytic activity of Fe-MOF in aerobic oxidation of benzyl alcohol to benzaldehyde. Interestingly, Fe-MOF showed improved activity in comparison with neat Fe_3O cluster reaching the yield of benzyl alcohol oxidation from 31.86 to 91.89 % toward benzaldehyde which can be attributed to the high surface area and suitable aperture size of 1D channel providing the better bed for oxidation transformation.

Keywords: Metal-organic framework (MOF), Geometry mismatch, Topology, Single crystal X-ray crystallography, aerobic oxidation.

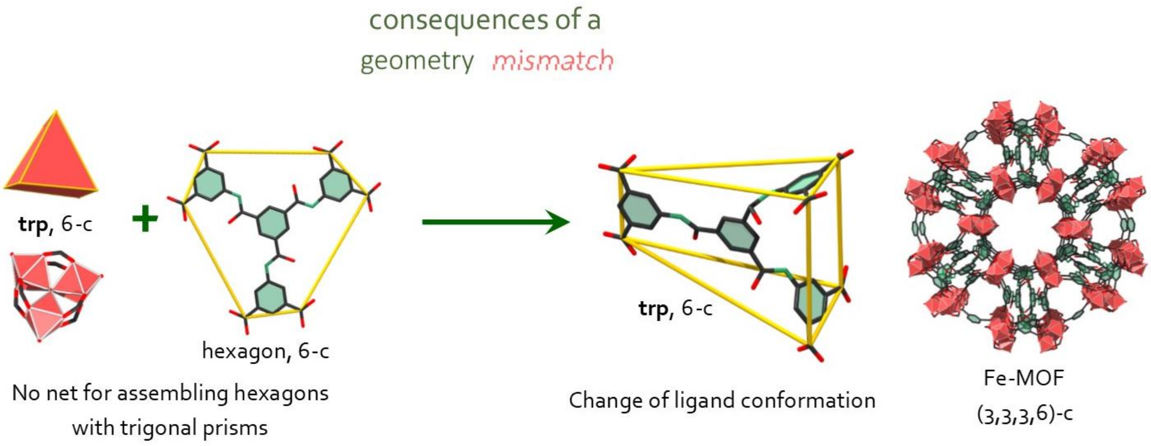

Figure 1. Geometry mismatch of building bloks led to change of ligand conformation to form Fe-MOF.

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Adsorption and photocatalytic Removal of Malachite Green Dye From Aqueous Solutions Using Chitosan/Poly (Maleic Acid) –Zinc Oxide Composite

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In this study, a cross-linked chitosan modified with poly maleic acid were utilized as adsorbent for the removing of Malachite Green Dye from aqueous solutions [1-5]. The synthesized adsorbent was characterized by Scanning Electron Microscopy (SEM) and Fourier Transform Infrared (FTIR) analysis. Malachite green (MG) was the model colorant for the sorption process. Batch adsorption experiments of the dye onto chitosan–ZnO (CS–ZnO) composite was investigated with a UV–Visible photometer. The rate of dye removal was greatly influenced by pH, dye strength, amount of adsorbent and contact time.

Keywords: Photocatalytic activity, Removal of Malachite Green Dye, Chitosan/Poly (Maleic Acid) –Zinc Oxide Composite

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Highly efficient adsorption of iodine by PAN/x%ZIF-8/Fe_3O_4 beads

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The production of some isotopes such as iodine (^{129}I and ^{131}I), ^{99}Tc, and ^{135}Cs is considered the main issue for nuclear technology. Many types of research have been conducted on the successful adsorption of these by-products [1–3]. Polymer nanocomposites consist of metal-organic frameworks (MOFs) developing for various pollutions sorption and separation have attracted much attention. This study reports the fabrication of magnetic polyacrylonitrile (PAN)/zeolitic imidazolate frameworks (ZIF-8) nanocomposites, PAN/ZIF-8(x%)/Fe_3O_4, x=30 and 50, as iodine capture adsorbents. The PAN/ZIF-8(x%)/Fe_3O_4 nanocomposite beads were fabricated via the phase inversion method, and their potential for iodine capture and separation in solution and vapor was investigated through UV-vis and weighing methods, respectively. The as-fabricated compounds were studied by various techniques such as FT-IR (Fourier-transform infrared), XRD (X-ray diffraction), SEM (scanning electron microscope), and EDS (energy-dispersive X-ray spectroscopy) mapping. The iodine capture results showed that the efficiency of nanocomposites is remarkably higher than the pure PAN beads. Additionally, the as-prepared nanocomposite adsorbents displayed higher capture capacities for iodine vapor (1524-4345 mg g^{-1}) than iodine solution (187-295 mg g^{-1}). The as-obtained magnetic nanocomposites can be successfully separated from polluted media by simple filtration or an external magnet, regenerated through washing with ethanol, and reused. Fast capturing, high sorption capacity, rapid separation, and good reusability make the PAN/ZIF-8(x%)/Fe_3O_4 nanocomposites highly effective adsorbents for the separation of iodine from wastewater.

Keywords: ZIF-8; Fe_3O_4; Polyacrylonitrile; Nanocomposite; Iodine capture

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Preparation, characterization, and biocompatibility study of Curcumin/Fe-MOF/PDMS porous scaffolds

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Fabrication of biocompatible scaffolds that can facilitate the mending of damaged tissue has attracted much attention. Recently, MOFs (metal-organic frameworks) are considered promising filler materials to fabricate various composites. These materials exhibited many outstanding features such as high porosity, flexibility in chemical functionality that make them desirable candidates for application in biomedicine, catalysis, sensors, and storage/separation processes [1-3]. In this study, the preparation and structural investigation of a curcumin loaded Fe(II) metal-organic framework/polydimethylsiloxane sponge, Cur/Fe-MOF/PDMS, are reported. Various techniques such as FTIR (Fourier-transform infrared), XRD (X-ray diffraction), SEM (scanning electron microscope), TEM (transmission electron microscope), EDS (energy-dispersive X-ray spectroscopy) mapping, and XPS (X-ray photoelectron spectroscopy) have been used to investigate the as-fabricated materials. Results confirm the successful incorporation of curcumin and Fe-MOF into the PDMS matrix. The obtained SEM images indicate the sponge-like structures of the PDMS and the Fe-MOF/PDMS composite. Indeed, the results from *in vivo* show animals all to be survived without any unusual responses to the transplant. According to macroscopic observation, the Fe-MOF/PDMS and Cur/Fe MOF/PDMS scaffolds seem better confederates than the pure PDMS. H&E staining has confirmed enhanced healing and revascularization in the Cur/Fe-MOF/PDMS than the PDMS and Fe-MOF/PDMS scaffolds. Additionally, a two-stage profile was observed for the release of curcumin into PBS (phosphate-buffered saline) solution. The hydrophilic property of the Fe-MOF resulted in fast release at the first stage. These results exhibit that the Cur/Fe-MOF/PDMS sponge can serve as a 3D porous substrate in the tissue engineering (TE) field.

Keywords: Iron metal-organic framework, Polydimethylsiloxane, Curcumin, Biocompatibility

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Alumina-supported SAPO-34 catalyst for methanol to olefins (MTO) conversion

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In the past decades, methanol-to-olefin (MTO) conversion as a sustainable path for production of lower olefins has drawn considerable interest due to the numerous applications in the chemical and petrochemical industries. Among all silicoaluminophosphate molecular sieves, SAPO-34 has attracted broad attention in the MTO conversion, because of its outstanding shape selectivity, and relatively mild acidity. In this paper, SAPO-34 catalysts were synthesized by in-situ crystallization on the α-Al_2O_3 support. Although the composition of the primary gel was similar in all the samples, the order of precursors addition was different. The effect of such variations on the phase, shape, and composition of synthesized particles was studied. The products were characterized by various techniques, such as SEM, XRD, BET, EDS, and NH_3-TPD. The SEM images showed that various morphologies, including cubic, rectangle, and nanoplates were obtained. It was found that the Si/Al ratio of SAPO-34 particles was directly related to the density of strong acid sites. When silica was added to the bohemite acidic compound, the SAPO-34 phase was rarely formed. However, by adding templates to the compound before adding silica or mixing the template with silica before adding them to the bohemite acidic compound, the crystallinity of SAPO-34 with the crystal structure of chabazite was improved. Moreover, the seed addition during the synthesis process developed the hierarchical structure of SAPO-34 with a higher density of acid sites. Consequently, the catalytic performance of such catalysts (the catalyst selectivity to light olefins and methanol conversion were obtained 89% and 99%, respectively) as well as the catalyst lifetime in the MTO process were extremely enhanced. The SAPO-34 catalyst with the hierarchical structure is expected to serve as a high performance catalyst due to the low mass transfer resistance and the high density of active sites.

Keywords: methanol-to-olefins, SAPO-34, Alumina, Microspherical.

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Synthesis, characterization and nonlinear optical (NLO) properties of N, N-donor pyrazole based ligand and its nickel (II) complex

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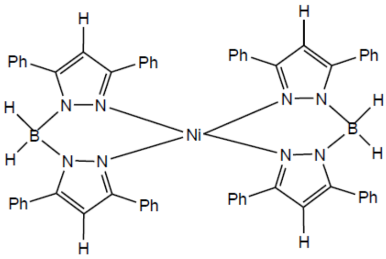
Recently, π-conjugated organic compounds and their coordinated metal complexes have been exposed for extensive investigations as regards their potential applications in nonlinear optical area[1]. Coordination metal based compounds in compartion with organic molecules were attracted significant interest, these inorganic compounds offer a large variety of molecular structures, the possibility of high environmental stability and diversity of electronic properties by the coordinated to metal center[2, 3]. Pyrazolylborate ligands as the π-conjugated system have been suggested to enhance the NLO response[4]. In this research, a type of bis(pyrazolyl)borate derivative and its nickel (II) complex were synthesized and characterized by physico-chemical and spectroscopic methods and nonlinear optical properties of them were investigated by z-scan method. Our findings indicated the synthesized nickel (II) complex have the highest value of the nonlinear absorption and nonlinear refraction parameters in comparison with the free ligand and other similar compounds.



Keywords: Bis(pyrazolyl)borate, Nickel complex, Nonlinear optical properties

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Synthesis, characterization and nonlinear optical properties (NLO) of copper (I) complex with N, S donor indazole based ligand

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Compounds containing sulfur and nitrogen donor ligands are highly regarded due to their biological activity and applications in the optical electronics industry. Transition metal complexes that prepared from these ligands indcated significant nonlinear optical properties, also these compounds have been extensively applied in broad practical fields[1-2] .In the present study, copper (I) complex were prepared with N, S donor indazole based ligand as the main ligand and triphenylphosphine as adjuvant ligand. Various spectral techniques (UV−Vis, IR and ^{31}P NMR) were used to characterization the synthesized complex . The nonlinear optical responses of the synthesized metal complex were investigated under irradiation of 35 mW continuous wave He-Ne (632.8 nm) laser.We used the Z-scan technique for measurement nonlinear absorption (n_2) and nonlinear refraction (β). The results indicate that copper (I) complex have the highest value of the measured (n_2) and (β) in compared with similar samples.

Keywords: N,S donor ligand , Nonlinear optical material , Z-scan technique

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Structural Behaviors of Nicotinamide Complexes of Cd(II) Arylcarboxylates

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Cadmium(II) is compatible with a wide range of stereochemical settings due to its d^{10} electronic structure. Cadmium(II) has four, five, six, seven and eight coordination numbers. In a study comparing the structures of the 200 cadmium(II) complexes with crystal structure, it was found that in 19.8 % of these complexes, coordination numbers of cadmium had four and five. In addition, in 56 % of these complexes, the coordination number of cadmium was reported to be six. In the same study, seven-coordinate cadmium(II) complexes were reported to be less common in the literature [1].

Cadmium(II) complexes with carboxylic acid and carboxyate ligands play an important role in coordination chemistry. In this study, the crystal structures of nicotinamide complexes of cadmium arylcarboxylates were examined. These complexes exhibit different structural properties such as monomeric, dimeric, ionic, polymeric and supramolecular. Six of these complexes, which have eleven different examples in the literature, have a dimeric structure. The coordination number of cadmium in all dimeric complexes is seven, and these dimeric complexes contain the coordinated water molecules. The number of coordination in the monomeric complex containing 2-nitrobenzoate anion is six, while the number of coordination in the monomeric complex containing 2,4,6-trimethylbenzoate anion is seven. The 4-formylbenzoate anion in the ionic complex is located outside the coordination sphere. The main ligand of the polymeric complex is terephthalate anion, and it is the only complex that does not contain a water molecule among the nicotinamide complexes of cadmium arylcarboxylates. The asymmetric unit in the supramolecular complex, which has an interesting structural architecture, contains two different molecules. In the supramolecular structure, 2-hydroxybenzoate ligand is a monodentate coordinate in one molecule and a bidentate coordinate in another. In a study in which dimeric nicotinamide complexes of cadmium 3-fluorobenzoate were synthesized by classical and hydrothermal methods, 3-fluorobenzoate anions form a bridge in the complex synthesized by the classical method, while nicotinamide molecules form a bridge in the complex synthesized by the hydrothermal method. This complex is the only literature example in which the nicotinamide molecule is bidentate coordinated among the nicotinamide complexes of cadmium arylcarboxylates [1, 2].

Keywords: Cadmium complexes, Arylcarboxylate, Nicotinamide, Crystal structure.

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Synthesis and characterization of the complex resulting from the reaction of dimethylpyridine-2,6-dicarboxylate with cadmium, mercury

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In this work, a new complex of cadmium and mercury with dimethyl pyridine-2,6-dicarboxylate(MPC)(L), was prepared and identified by elemental analysis, FT-IR spectroscopy and single-crystal X-Ray diffraction. As it is shown in Fig. 1, the coordination number of the cadmium in the compound is nine. Pyridine dicarboxylic acid derivatives are a kind of important organic ligands, which have rigid conjugated structures and rich coordination forms with the wide application in optical fiber communication system and the time resolution of fluorescence immunoassay deprotonated during the complexation In the crystal network of the complex there is intermolecular hydrogen bonds, extending the crystal network into three dimensional [1-2].

Keywords: X-Ray crystallography, Cadmium, Mercury, Pyridine dicarboxylic acid.

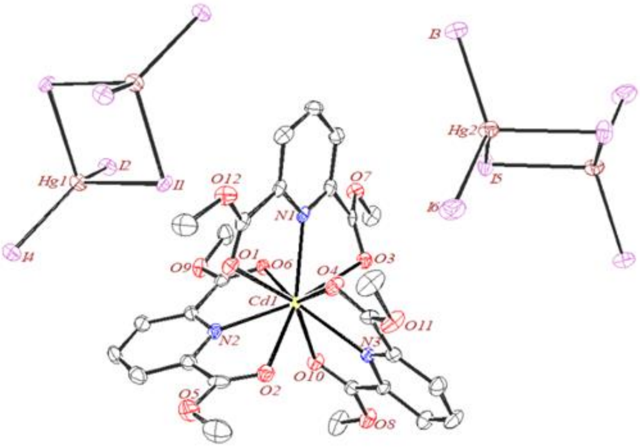

Figure 1. Crystal structure of complex.

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Direct Formation of Persistent Hydrogen-Bonded Organic Framework Radical for Enhanced Photothermal Conversion

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Synthesis of materials with photoresponse in the shortwave near-infrared region (SWIR) is a scientific challenge but highly desired. Herein, we demonstrate creating radical compounds as a convenient and economical solution. In this work, viologen radicals were generated during the self-assembly process and in-situ stabilized into a hydrogen-bonded organic framework (HOF), giving rise to a persistent radical compound (**PFC-26R**) with photoresponse in Ultraviolet-visible and SWIR region. The highly-ordered arrangement guarantees an effective shielding effect to protect radicals from bleaching, therefore **PFC-26R** exhibits outstanding stability in various solvents and ambient conditions for as long as three months. IR thermal camera recorded a drastic temperature rise of **PFC-26R** from 25°C to 214°C in 53s under simulated one-sun irradiation (1 W/cm^2), ranking state-of-art photothermal conversion performance relative to other reported materials. Thanks to the easy processibility of HOFs and the persistent radical nature, a seawater evaporation device based on **Cu@PFC-26R** thin film was fabricated, which presents an effective platform for capturing solar energy to provide freshwater from seawater with excellent salt rejection performance and a high evaporation rate of 2.85 $kg/m^2{\cdot}h$, which is among the top values reported in this field. This research makes an important step toward the direct synthesis of ultra-stable radical materials for safe and efficient solar energy technologies.

Keywords: Hydrogen-Bonded Organic Frameworks, UV–SWIR Absorption, Photothermal Conversion, Persistent Radical, Seawater Desalination.

Selective cupper (II) metal ion detection in water via Yttrium-based MOF; converting MOF approach

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Metal-organic frameworks (MOFs) are coordination polymers extending in 2 or 3 dimentions. As one of post synthetic modification approaches, solvent assisted linker exchange (SALE) is among the most poweful methods to fabricate MOFs [1]. For example, direct synthesis of rare-earth MOFs (RE-MOFs) with *fcu* topology is more complicated based on existing RE-MOFs. [2]. To produce this type of structures one should employ indirect methods, i.e. ligand exchange [3]. In this regard we have successfully exchanged the organic linker of 3,3-biphenyldicarboxylic acid-based RE-MOF (3,3-bpdc-Y) to Yttrium based amino-UiO-66 structure, which is not available by direct synthesis based on our attempts. Upon this modification in addition to changing the network from *bcu* to *fcu*, porosity and rigidity of the structure was also improved. Changing the network of resulting MOF also made the structure luminescent active, which was used to detect Cu^{2+} ion in water medium.

Ligand exchange process and the structure of materials were analyed by ^{1}H-NMR, PXRD, FT-IR, BET and elemental mapping analysis. Sensing performance study was conducted using NH_2UiO-66(Y) dispersed in aquatic solutions of $M^{X+}(NO_3)_x$ (M=Li^+, Na^+, K^+, Mg^{2+}, Sr^{2+}, Ba^{2+}, Mn^{2+}, Co^{2+}, Cd^{2+}, Zn^{2+}, Pb^{2+}, Cu^{2+}, Y^{3+}, Fe^{3+}, Al^{3+}, and Cr^{3+}). Mixture was sonicated and the fluorescence emission was recorded. Among these metal ions, only Cu^{2+} successfully quenched fluorescence emission of MOF. The quenching efficiency was determined >90%. The strong fluorescence intensity of NH_2UiO-66(Y) was moderately reduced via increasing concentration of Cu^{2+} solution. Based on Sterm-Volmer diagram, in low concentration of Cu^{2+}, linear sensing behavior was observed. In summary, a novel UiO-66 structure MOF based on Yttrium metal was obtained via SALE method and successfully used as selective sensor of Cu^{2+} ions. Our results revealed post-snthetic modification methods are versatile tools to constructing rare structures with superior properties.

Keywords: Metal-Organic Framework (MOF), Sensing, Rare-Earth metal.

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The study of electrochemical hydrogen storage behaviour of the zirconium-based metal-organic framework UiO-66

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Hydrogen storage is an important technology for generating hydrogen technology and electrochemical cells in the fields of stable energy, transportation, and portable energy. Hydrogen has the highest specific output of all fuels; however, its low ambient temperature density appears in a lower energy density; thus, it is necessary to create progressive storage methods that have the potential for higher energy densities. The low volumetric density of hydrogen as an alternative fuel cussed a primary limitation to its efficient and economical hydrogen storage [1]. Metal-organic frameworks (MOFs) with prominent features such as large specific surface area and permanent porosity are attractive and suitable for hydrogen storage. Especially the zirconium-based MOFs show the high moisture and thermal stabilities, because of the strong bond between Zirconium and Oxygen ligand. In this work, the hydrogen storage capacity of UiO66 was investigated for the first time using electrochemical hydrogen storage. This process lacks the dissociation of molecular hydrogen into atomic hydrogen, overcoming significant limitations of hydrogen storage [2]. Fig. 1 indicates the discharge capacity curve of the UiO-66 electrode after 15 cycles under 1 mA current. The electrochemical discharge capacity of the UiO-66 increased from 1200 mAh/g (4.51 wt%) to 3500 mAh/g (13.16 wt%) after 15 cycles. The result showed that UiO-66 is a promising candidate for potential application in high-performance hydrogen storage.

Keywords: Volumetric density, Metal-organic framework, Electrochemical hydrogen storage.

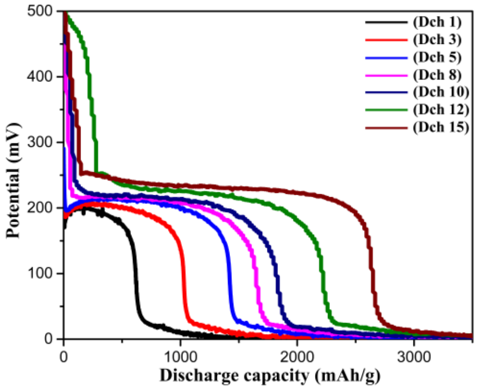

Fig. 1. Discharge curve of the UiO-66 electrode at 1 mA.

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Improving hydrogen storage capacity of graphene oxide using Manganese dioxide nanoparticle

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Hydrogen has proven to be the desirable fuel in the economy based on renewable resources [1]. On the other hand, carbon materials seem to be suitable for hydrogen storage due to their high microporosity and large surface area, which are considered as significant characteristics of hydrogen adsorption. Graphene (GO) layers are designed with metals such as manganese (Mn) to prevent decreasing specific surface areas by Van der Waals forces and the agglomeration of graphene sheets [2]. In addition, embedding Mn metal between GO layers increases the ability to store hydrogen because of an appealing effect called the "spillover effect" [3]. In this study, the hydrogen storage capacity of pure GO and Mn/GO nanocomposite was investigated using the electrochemical method. The discharge capacity curves of the GO and Mn/GO nanocomposite electrodes after 15 cycles under 1mA current, are shown in Fig. 1 (a, b). The discharge capacity of the GO increased from 300 mAh/g (1.12 wt%) to 500 mAh/g (1.88 wt%) after 15 cycles. Also, the hydrogen storage capacity of the 15th cycle of the Mn/GO nanocomposite is 1750 mAh/g (6.58 wt%), which is a significant enhancement of approximately 3.5 times compared to the GO electrode.

Keywords: Hydrogen storage, Renewable resources, Spillover effect, Mn/GO nanocomposite.

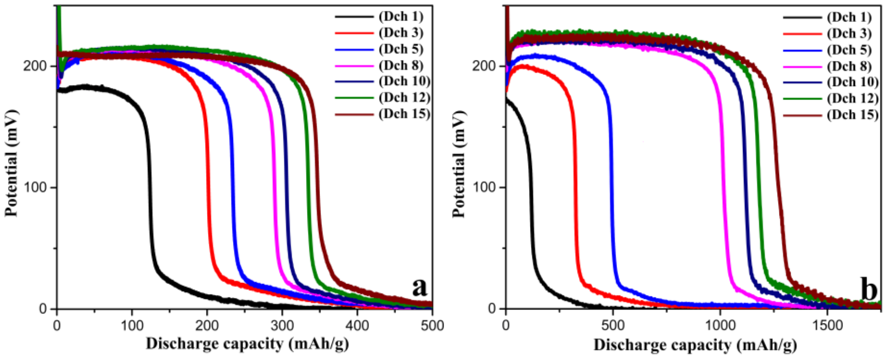

Fig. 1. Discharge curve of the (a) GO (b) Mn/GO nanocomposite electrodes at 1 mA.

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Synthesis and characterization of zeolite A by hydrothermal transformation of kaolin

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Zeolites are crystalline, microporous, hydrated aluminosilicates of alkaline and alkaline earth metals. Their frameworks were made from $(SiO_4)^{4-}$ and $(AlO_4)^{5-}$ tetrahedral. Synthetic zeolite A is characterized by its absorption, adsorption, ion exchange, and catalytic properties due to its unique porous structure. So, there are many applications of zeolite-A in agriculture, water treatment, and oil industries. Many sources have been used to synthesize zeolite-A such as fly ash, kaolin deposits, inorganic wastes, and alumatrane with silatrane precursors [1-3]. In this work, the synthesis of zeolite materials by hydrothermal transformation of kaolin in NaOH solutions was investigated, where kaolin was used as silica and alumina source. The kaolin was converted into metakaolin by a process of calcination. The synthesized zeolites were characterized by X-ray diffraction (XRD), scanning electron microscopy (SEM), EDX, and N_2 adsorption-desorption. A mixture of zeolite A and quartz was obtained. The BET surface area of synthesized zeolite was comparable to that of commercial zeolite A.

Keyword: Aluminosilicate, Metakaolin, Zeolite A, Kaolin

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Preparation and characterization of nano cobalt oxide-zeolite 4A composites and investigation of their photocatalytic properties

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Recently, various photocatalytic methods were used to remove contaminants from water and wastewater. Among them the photocatalytic degradation of pollutants by semiconducting materials has gained more attention [1-3]. In this article, Co_3O_4/zeolite4A photocatalyst was used to remove contaminants. The nano cobalt oxide and Co_3O_4/Zelite4A nanocomposites were synthesized by the co-precipitation method. For synthesis of nano cobalt oxide, cobalt acetate tetra hydrate was used as the raw material and sodium hydroxide as the precipitating agent. To prepare the nanocomposites, the commercial zeolite 4A was added to a solution containing cobalt acetate tetra hydrate salt, and the cobalt oxide was synthesized on the 4A zeolite by co-precipitation method. The products were analyzed by XRD, SEM, and EDX identification techniques. Finally, the photocatalytic properties of the prepared samples in the removal of organic pollutants such as methylene blue were evaluated. The highest removal efficiency was 98% for degradation of methylene blue**.**

Keywords: Nanocomposite, Co-precipitation, Zeolite, Co_3O_4

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The effect of particle size on cytotoxicity properties of some Carbacylamido phosphates

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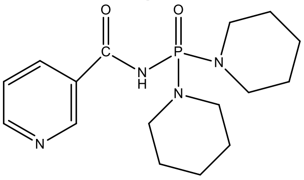
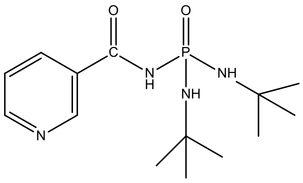
Cancer is an important health issue that can be removed by surgery or has to be treated by chemotherapy in combination with radiotherapy and surgery. One approach to improve the therapeutic effectiveness is through the design of targeted anticancer prodrugs [1]. Due to steric, electronic, and conformational properties, structure of phosphorus derivatives allows them to interact easily with the biopolymers of the living systems. Therefore, they inhibit acetylcholinestrase and butylcholinestrase enzymes and as such are useful for inhibiting of cell proliferation in the treatment of cencer [2]. In this study, two Carbacylamido phosphates with formula $3\text{-}NC_5H_4CONHPO(NC_5H_{10})_2$ (1) and $3\text{-}NC_5H_4CO(NHC_4H_9)_2$ (2) and their nano particles, were prepared according to the literature [3,4].



(1)



(2)

Then, the cytotoxic activities of these compounds were assayed against MCF-7 (breast cancer) cancer cell line by applying the MTT colorimetric assay. The obtained IC_{50} for compounds 1, 2 and their nanoparticles were 14.78, 19.65, 3.73, and 4.76 µM respectively. These values are in a normal range and in good agreement with previous successful reported ones [5] Results showed that when the particle size decreased, the interaction between the compound and the cell membrane was increased and the cell proliferation was decreased. Also, compound 1, with six-membered ring amine had more cytotoxicity than compound 2, against MCF-7 (breast cancer) cancer cell line.

Keywords: Carbacylamidophosphates, Nanoparticle, Anticancer, MCF cell line.

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A Phosphoric triamide Compound as an anticancer agent

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Phosphoric triamide compounds are prominent candidates for the development of new biologically active chemicals. They have good structural properties, such as steric, electronic, and conformational interactions. These properties allow them to interact easily with the biopolymers of the living systems [1,2] In this study, a Phosphoric triamide compound with the formula $C_6H_5CONHPO(NC_4H_9)_2$ (**1**) was prepared according to the procedure, in the literature [3]. Next, it was dissolved in methanol and added to the solution of Nickel chloride in methanol. Then, it was stirred for 9 days and the resulting precipitate (**2**) was separated. After that, the anticancer activities of compounds 1 and 2 were determined against A549 (lung cancer) and MCF-3 (breast cancer) cell lines by applying the MTT colorimetric assay. Results showed that the effective doses of compound (**2**) that inhibited 50% growth (IC_{50}) of A549 and MCF-3 cells were 18.6 and 3.56 μM respectively, while IC_{50} values of (**1**) were 31.7 and 12.8 μM respectively (table 1). This means that the presence of Nickel chloride could increase the anti-cancer activity of the compound (**1**). Such results have been also observed for similar Phosphoric triamides in the presence of other metal ions (table1).

Tabel 1. In vitro cytotoxic activity of some phosphoric tri-amides against cancer cell lines

Compound	Cell line	IC_{50}	Ref.
$4\text{-}NC_5H_4CONHPO(CH_3NCH_2C_6H_5)_2$	MCF-7	3.43 mM	4
$4\text{-}NC_5H_4CONHPO(CH_3NCH_2C_6H_5)_2 + SnCl_2Me_2$	MCF-7	0.099 mM	4
$3\text{-}NC_5H_4CONHPO(NC_6H_{11})_2$	MCF-7	No activity	5
$3\text{-}NC_5H_4CONHPO(NC_6H_{11})_2 + AgNO_3$	MCF-7	7.7 μM	5
$C_6H_5CONHPO(NC_4H_9)_2$	MCF-3	12.8 μM	this work
$C_6H_5CONHPO(NC_4H_9)_{2+} NiCl_2$	MCF-3	3.56 μM	this work
$C_6H_5CONHPO(NC_4H_9)_2$	A549	31.7 μM	this work
$C_6H_5CONHPO(NC_4H_9)_{2+} NiCl_2$	A549	18.6 μM	this work

Keywords: Anticancer, Phosphoric triamide, Nickel chloride

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Leaching of Aghbulagh-Valadyan copper deposit in sulfuric acid medium with sodium chloride additive

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Aghbulagh-Valadyan copper deposit is one of the medium-scale deposits located 30 km away from Khoy city. The results of the XRF analysis of samples obtained from this deposit indicated that the amount of copper is 4.63%. The goal of this study is to maximize the dissolution of this element. According to microscopic and XRD analysis, the Aghbulagh-Valadyan copper deposit contains bornite, chalcocite, malachite, and azurite, which due to the presence of copper sulfide minerals in this deposit, maximum dissolution will not be possible without additive (dissolution aid). Because of the presence of sulfide (S^{2-}) in the composition of these minerals in form of metallic compounds and until it is not transferred to solution in form of sulfate (SO_4^{2-}), copper will not practically be recovered. These conditions increase the need for dissolution aid substances. In this research, to extract the maximum amount of copper, the Taguchi experimental design (mixed surface) has been employed and an attempt has been made to present a method of dissolution maximization of copper from the aforementioned deposit. According to S/N plots, the most optimal dissolution method was considered to take place in the temperature conditions of 70°C, acid molarity of 1M, sodium chloride (additive) amount of 25 g/l, a copper recovery rate of 94.3%, and d80 of 40µm. In the initial experiments without sodium chloride additive, the copper recovery rate was 61.2%. The presence of copper sulfide minerals such as chalcocite and bornite reduces the dissolution rate, and the addition of sodium chloride significantly increases the dissolution rate.

Keywords: Copper dissolution, Sulfide minerals, Experimental design, Sodium chloride

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Synthesis and crystal structure of a new octanuclear Cu(II) cluster

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Synthesis of multinuclear transition metal complexes is one of the attractive research fields in coordination and inorganic chemistry fields. These materials by having several metal ions show interesting properties in various fields [1]. Multinuclear metal complexes are attractive materials for magnetic studies when they have paramagnetic metal ions. Using suitable organic ligands and bridging groups is the most successful method for the synthesis of multinuclear complexes [2]. The hydrazone ligands are one of the most significant groups of flexible and adaptable polydentate ligands that chelate with a wide range of metal ions and can form multinuclear complexes in the presence of suitable bridging groups [3]. In this research, a new octanuclear Cu(II) cluster was synthesized and characterized by the reaction of hydrazone ligand, *bis*-imidazole bridging group and $Cu(NO_3)_2 \cdot 3H_2O$ in methanol. The complex was characterized by elemental analysis (CHN), NMR, FT-IR and UV-Vis analyses. The molecular structure of the complex was also determined by single crystal X-ray analysis which indicated it is crystallized in triclinic system. The copper ions are connected together by a mixture of hydrazone ligand, *bis*-imidazole bridging group and also a hydroxyl ion (see Fig. 1). The OH bridging group has connected three Cu(II) ions together. The Cu···Cu distances through the bridging groups are in the range of 3.1-3.7 Å.

Keywords: Copper, Multinuclear, Transition metal

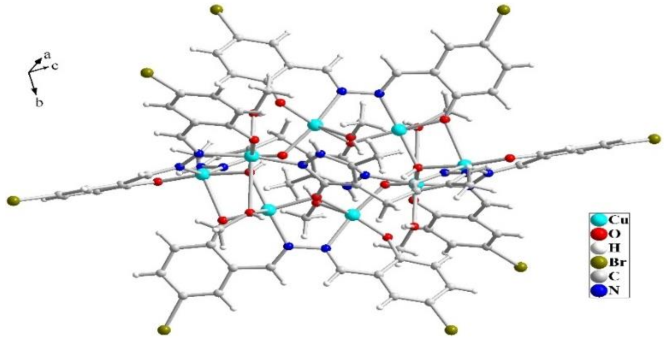

Fig. 1. Molecular structure of octa nuclear Cu(II) cluster

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Oxovanadium (IV) Complexes Containing NNOS Coordination sphere: Synthesis, Characterization and Thermodynamic Studies

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Vanadium coordination chemistry and biochemistry have attracted increasing interest during the last few years. These complexes are known to be therapeutic applications such as the treatment of diabetes and as anti cancer agents [1]. The use of oxovanadium complexes in oxidation and oxo transfer catalysis has been noted [2]. Herein, we describe the synthesis of the newly vanadyl Schiff base complexes derived from the appropriate Schiff base ligand {[1-methyl-2-(2-hydroxy-3, 4-, 5-methoxyphenyl)methylidynen-itrilo]ethyl}amino-1-cyclopentene-dithiocarboxylate and one equivalent of $VO(SO_4)_2$. The synthesized complexes were characterized by analytical and defferent physico-chemical techniques. The IR spectra affirm that coordination takes place through azomethine nitrogen, phenolate oxygen and C=S sulfur.The formation constants and free energies were measured spectrophotometrically, at constant ionic strength 0.1 M ($NaClO_4$), at 25˚C in DMF solvent. The effects of the electronic and steric factors of substituents on the Schiff base ligands on the formation constants and free energy changes were studied.

Keywords: Oxovanadium (IV), Formation constants, Thermodynamics.

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Naked-eye detection of CN^- and AcO^- ions in aqueous medium by a new chromogenic azomethin receptor

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A new azomethine chromogenic receptor, **H_2L**, containing –NH and –OH active sites, has been synthesized and characterized using standard spectroscopic methods (IR, ^1H NMR, UV-Vis) as well as elemental analysis. **H_2L** has been used for qualitative and quantitative detection and colorimetric sensing of CN^- and AcO^- ions in aqueou medium. In the presence of cyanide and acetate ions an obvious change in color was appeared from yellow to orange. As shown in Fig.1, no significant color change was observed upon the addition of other anions such as F^-, Cl^-, Br^-, I^-, N_3^-, SO_4^{2-} , SO_3^{2-}, PO_4^{3-}, $H_2PO_4^-$, HSO_4^-, NO_2^- and NO_3^-. The anions recognition ability of **H_2L** was also evaluated using UV-Vis absorption and ^1H NMR spectroscopy. Job plot data showed that the binding stoichiometry's of **H_2L** with CN^- and AcO^- were 1:2.

Fig1

Keywords: **:** Azomethine, Chemosensore, Anion recognition, Aqueous medium, Chromogenic receptor

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Investigating the Effect of Seed Treatment Temperature to Enhance the Stability and Lifetime of SAPO-34 Catalyst in Methanol to the Light Olefin Conversion process

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The methanol to olefin conversion process is one of the most successful alternative non-petroleum based routes for light olefin production[1-2]. Among numerous synthesized zeolites, SAPO-34 zeolite is the most efficient one in the MTO process[3]. Since seed treatment temperature might have a significant impact on the final size of the seeds to increase the stability and lifetime of the catalyst, the study of seed treatment temperature is a key parameter in the investigation of the MTO process. In this paper, some samples of SAPO-34 were prepared by the addition of treated seeds with TX-100 in a hydrothermal process. The samples were characterized by XRD, FESEM, BET, NH_3-TPD, particle size analysis, and reactor test. Results of these analyses indicate that all the synthesized samples have smaller crystallite/particle sizes, higher surface area, more suitable acidity, and higher mesopore volume. The results of the reactor test revealed that the highest selectivity for olefins belongs to the treated seed at 90˚C. The selectivity of this sample to light olefins and C_2-C_3 is about 93% and 86%, respectively with a 870 min lifetime, which has better catalytic performance and higher stability in the MTO process, compared to conventional SAPO-34 catalyst

Keywords: MTO, SAPO-34, Seed Treatment

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Finding the best solvent for recrystallization of some amino alcoholic complexes by DFT calculations

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In this work, four amino alcoholic complexes including, $[Cd(AEAE)_2][CdI_4]$ (**1**); AEAE: 2-((2-aminoethyl)amino)ethanol, $[Zn(L)Br_2]$ (**2**), $[Cd(L)Br_2]$ (**3**) and $[Cd(L)I_2]$ (**4**); L: 2-(2-(phenyl(pyridin-2-yl)methyleneamino)ethylamino)ethanol were studied by DFT method to find the most suitable solvent for recrystallization of them then the theoretical result were compared with experimental data. Calculation were run for 19 famous solvents including, water, DMSO, nitromethane, acetonitrile, methanol, ethanol, acetone, dichloromethane, dichloroethane, THF, aniline, chlorobenzene, chloroform, diethyl ether, toluene, benzene, CCl_4, cyclohexane and heptane. Based on the calculated ΔG for solvation, the best solvent was selected. The best solvents for complexes of **1**–**4**, are methanol, methanol, methanol and methanol which are in agree with the experimental data. In addition, the solubility order for 19 solvents and the possible effective parameters were presented and discussed for each complexes [1-5].

Keywords: DFT calculations, solvent, amino alcohol, cadmium, zinc

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Finding the best solvent for recrystallization of some Oxazolidine complexes by DFT calculations

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In this work, two oxazolidine complexes including, $[Cd_2(POE)(\mu\text{-}Cl)_2Cl_2]$ (**1**), $[Hg_2(POE)(\mu\text{-}Cl)_2Cl_2]$ (**2**) ; POE: 2-(2-(pyridin-2-yl)oxazolidin-3-yl)ethanol were studied by DFT method to find the most suitable solvent for recrystallization of them then the theoretical result were compared with experimental data. Calculation were run for 19 famous solvents including, water, DMSO, nitromethane, acetonitrile, methanol, ethanol, acetone, dichloromethane, dichloroethane, THF, aniline, chlorobenzene, chloroform, diethyl ether, toluene, benzene, CCl_4, cyclohexane and heptane. Based on the calculated ΔG for solvation, the best solvent was selected. The best solvents for complexes of **1**–**2**, are methanol and methanol which are in agree with the experimental data. In addition, the solubility order for 19 solvents and the possible effective parameters were presented and discussed for each complexes [1-5].

Keywords: DFT calculations, solvent, Oxazolidine complexes, cadmium, zinc

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Preparation and Characterization of Mixed Metal Oxides (MMOs) derived from Layered Double Hydroxides (LDHs) as Photocatalyst for the Photodegradation of Acid Orange 7 dye

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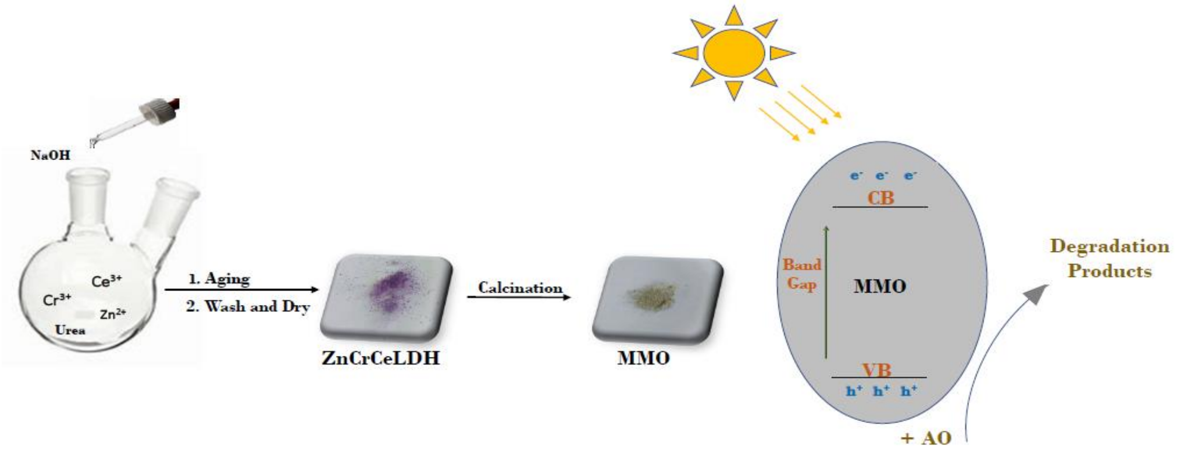
Recently, mixed metal oxide semiconductors have received much attention for heterogeneous photocatalysis due to their layered structure, absorption in the visible region, low manufacturing cost and ease of preparation[1]. The photoactivity of these materials strongly depends on the recombination rate of the electron-hole pairs which are generated upon irradiation of light having an energy equal to or higher than the semiconductor band gap [2]. In this research work, zinc, chromium and cerium layered double hydroxide (ZnCrCe-LDH) was prepared through chemical co-precipitation route and then calcined at specific temperature. The XRD, FT-IR, SEM, EDX and BET analyses were used for the characterization of the synthesized sample. Photocatalytic activity of ZnCrCe-MMO was determined by photodegradation of an azo dye, Acid Orange 7, illuminated with UVC irradiation. The results show that in the presence 0.02 g of ZnCrCe-MMO dose, photodegradation of dye occured in 120 minutes under UVC irradiation with 97% of efficiency, which is about 10 times higher than the photodegradation efficiency of the dye by the pristine LDH.

Keywords: Layered Double Hydroxide, Mixed Metal Oxide, Photodegradation, Photocatalyst, Acid Orange 7 dye



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Green catalytic oxidation of catechol by a new copper(II) complex

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Catechol oxidation is an important reaction in biochemistry. In biological systems, catechol oxidation is performed by copper complexes that are the active catalytic species in catechol oxidation [1]. In recent years, the synthesis of new copper complexes and investigation of their catalytic activity in catechol oxidation and biomimetic studies have become very important in inorganic biochemistry [2]. Oxidation of catechol derivatives is also one of the important reactions in chemical industry because their products have various applications as intermediates and pigments [3]. In this paper, we report the synthesis, characterization and crystal structure of a new Cu(II) complex with ONO-donor Schiff base ligand. The complex was obtained by the reaction of ONO-donor ligand with $CuCl_2\cdot 2H_2O$ in methanol. The structural studies showed the product is a mononuclear Cu(II) complex with general formula of $[CuCl_2(H_2L)]$ where H_2L is the Schiff base ligand. This complex is crystallized in monoclinic system and the copper ion has distorted square pyramidal geometry. There are strong and directed hydrogen bond interactions that stabilize the crystal structure of this compound (see Fig. 1). The obtained copper(II) complex was used as catalyst for oxidation of catechol. Aqueous hydrogen peroxide was used as green oxidant for this oxidation reaction and the reactions were done at room temperature. The results indicate that this complex is active catalyst for oxidation of catechol in the presence of hydrogen peroxide.

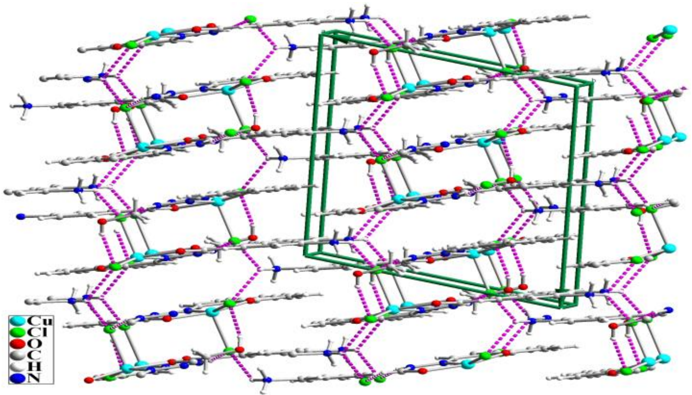

Fig. 1. Hydrogen bond interactions in the crystal of Cu(II) complex shown as pink dashed lines

Keywords: Catechol oxidation, Copper complex, Synthesis, Catalytic oxidation

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Effect of various amount of zirconium on Physicochemical Properties and Catalytic Performance of SAPO-34 catalyst in methanol to olefins conversion

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The nanostructured SAPO-34 catalyst was successfully synthesized with triton X-100 as a mesopore template to create mesopores in the crystals of SAPO-34 via the hydrothermal method. In order to enhance SAPO-34 catalytic performance, it was modified with different Zr contents by the impregnation method, compared to the unmodified catalyst, and then applied for the reaction of methanol to light olefins. The structure of the synthesized catalysts was characterized by various techniques such as XRD, FESEM, BET, FTIR, and NH3-TPD. According to XRD patterns, in samples with low Zr loading, the relative crystallinity increased, and the intact CHA structure was obtained, while further Zr loading significantly reduced the relative crystallinity. Zr impregnation and Zr content have a significant impact on product selectivity and lifetime. Compared to the sample synthesized without metal, product selectivity was prolonged for the samples with low Zr content. Furthur selectivity was reduced when Zr loading was increased[1, 2].

Keywords: SAPO-34, Zirconium, TX-100, MTO reaction

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The Water Diffusion in Modified Silica Membrane with TiO_2 and Magnetic Fe_3O_4, A Molecular Dynamics Simulations Study

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Today, the use of modified silica membrane for the osmosis process has received attention. Titanium dioxide has a significant application in increasing the efficiency of osmotic membranes due to its hydrophilic and non-toxic properties. Magnetic nanoparticles can potentially be used in wastewater treatment as antibacterial agents and nontoxicity.

In this paper, we report the development of a new silica membrane modified in 1, 10^{-2}, 10^{-4} and 10^{-6} mole ratios of titanium dioxide (TiO_2) with a constant number of magnetic nanoparticles Fe_3O_4 for theoretical insights of water molecules diffusion.

In this research, a modified silica membrane is simulated and pure water and Na^+Cl^- solution reservoirs were located at the two sides of membrane. A molecular dynamics (MD) simulations approach is applied to theoretical insights of the diffusion coefficients by performing the Forcite MD calculation at 298.0 K using the Grand Canonical Monte Carlo (GCMC) method. The self-diffusion coefficients (D) of particles in three dimensions are calculated by the slop charts of mean square displacement (MSD) of particles. We believe that the silica membrane containing 0.01 mole ratio of TiO_2 with a constant number of magnetic nanoparticles Fe_3O_4, in addition to having good biological property, with acceptable water diffusion can be applied in water desalination in forward osmosis method.

Keywords: Silica Membrane, TiO_2, Water Diffusion, Molecular Dynamics Simulation, Magnetic Fe_3O_4

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Synthesis of Cobalt Ferrite@$Cu_3(BTC)_2$ Nanocomposite as a Magnetic Metal-Organic Framework (MOF)

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An excellent way with supreme efficiency has been applied to synthesized a magnetic composite material based on metal-organic framework (MOF) like $Cu_3(BTC)_2$ and as well as Cobalt ferrite nanoparticles. This is a new method that presented for the first time. For this goal, via Pechini sol-gel method and using ferric nitrate, ethanol, copper nitrate, and 1,3,5-benzenetricarboxylic acid the composite compound was fabricated. The fabricated magnetic compound, base on its magnetic properties could be a suitable nominate for smart materials [1] , medical [2], sorbent [3] and catalyst[4] applications. the magnetic composite compound was contains both $Cu_3(BTC)_2$ as a MOF and also Cobalt ferrite that characterized and confirmed by different ways like FT-IR, FE-SEM, EDX, XRD, TGA/DTA, BET and VSM. The obtained features in microscopic observations approved that the formation of homogenous nanoparticles are not similar to column-shape-particle of the MOF. Although UV absorption of the composite compound declined, both photoluminescence and specific surface area improved rather than Cobalt ferrite nanoparticles. Such a compound with surface area 491 m^2/g, pore volume 0.69 cm^3/g, and prodigious magnetic response of 23 emu/g seems to be noteworthy enough for more attention.

Keywords: Metal Organic Framework (MOF), Trimesic acid, Magnetic nanoparticles, Cobalt ferrite@$Cu_3(BTC)_2$, HKUST-1

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Synthesis and Spectral Study of a Lead (II) Complex with N_3-Donor Schiff-based Ligand

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In the Article a new complex of Lead(II), $[Pb(L)I_2]$, with 2-((2-((piperidin-2-ylmethyl)amino)ethyl)amino)ethan-1-ol (L) was prepared and identified by elemental analysis, FT-IR, ^{1}H NMR spectroscopy and single-crystal X-Ray diffraction. The spectroscopies data revealed that the ligand acts as N_3-donor mode toward Lead atom and in agree with the structural analysis result. In this structure, the Lead atom has a PbN_3I_2 environment and distorted trigonal bipyramidal geometry. In the crystal network of the complex there are intermolecular C–H···O, Pb–I···Pb and Pb–I···O hydrogen bonds, extending the crystal network in three directions. Schiff base compounds and their metal complexes have been extensively investigated due to their wide range of applications including catalysts[1], medicine [2], organic lightemitting diode (OLEDs) [3], photosensitizers, electrolytes or redox mediators in DSSCs (dye-sensitized solar cells) [4]. and polymer light-emitting diode (PLED) materials [5].

Keywords: Lead(II) iodide, Hydrogen bonds, Single-crystal X-ray, Coordination chemistry

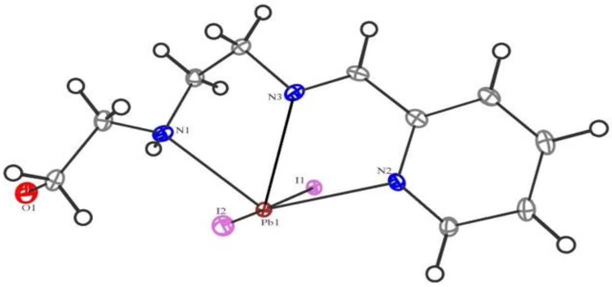

Figure 1. Crystal structure of complex.

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Against to What Observed Up to Now, Formation of Silver Nanostructures with Appropriate Morphologies from Silver Coordination Polymer Precursors by Calcination Rather than Thermal Decomposition in Oleic Acid

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In order to studies the effects of various samples of $[Ag_2(pta)(H_2O)]n$ (1), [H_2pta = phthalic acid] coordination polymer, as new precursors with different morphologies, calcination and thermal decomposing in oleic acid of six samples, which were synthesized previously, were carried out. The obtained radiuses were characterized by X-ray powder diffraction and scanning electron microscopy. Silver nanoparticles, microparticles, microporous spongy structure, thin microporous film, mixture of nanosheets and nanoparticles and agglomerated structures of them were obtained during these processes. For about half of the samples, we observed that calcination is more effective than thermal decomposition in oleic acid.

Keywords: Nano silver, Calcination, Oleic acid, Coordination polymer, Morphology

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Synthesis of Ce Doped Copper Phthalocyanin Intercalated Layered Double Hydroxide Nanohybrid as Photoluminescent Material

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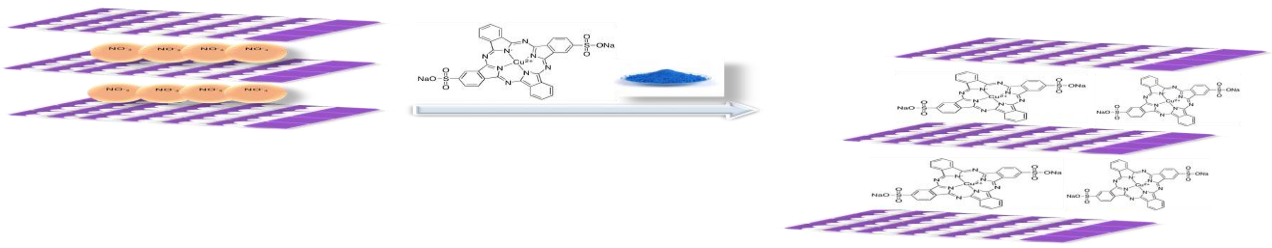
Photoluminescence, where the luminescence is stimulated by UV or visible light, is a widely used materials science technique for characterising dopants and impurities, and finds applications in lighting technologies such as fluorescent and solid state lamps [1] . In this research work, Zinc-Aluminum-Cerium and Magnesium-Aluminum-Cerium layered double hydroxides(Zn/Al/Ce-LDH , Mg/Al/Ce-LDH) was synthesized with chemical co-precipitation method . Then Direct Blue 86 anion was intercalated into the interlayer space of LDHs. The detailed chemical structure of the obtained nanohybrids was characterized by powder X-ray diffraction (PXRD) , Fourier Transform Infrared spectroscopy (FT-IR) , Thermogravimetric analysis (TGA) and Scanning electron microscopy (SEM) . The Photoluminescence analysis and diffuse reflectance spectroscopy (DRS) were used to study the photophysical properties. Resultes show that Direct Blue 86–LDH nonohybrids have a increased emission wavelengths intensity and red shift towards longer wavelengths with the emission wavelength of 420 nm compared with the pristine Direct blue 86 sample due to the nature of the host-guest interaction and existing defects in layered double hydroxides and the photoluminescence property in them .



Keywords: Layered Double Hydroxide, Nanohybrid, Photoluminescence ,Lanthanide element

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The catalytic effect of Zeolitic imidazolate framework (ZIF-8) on thermal decomposition of Ammonium dinitramide ADN

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Ammonium dinitramide (ADN) has attracted attention as a solid rocket propellant or liquid monopropellant oxidizer because it possesses both high oxygen balance and high energy content [1-3]. Combustion products of solid propellants based on ADN are clean and smokeless and they do not release hydrogen chloride gas, which can be an excellent alternative compound as an oxidizer in the solid propellant formulation [4, 5]. Therefore, it is essential to study the thermal decomposition of ADN in the presence of catalysts. In this study, Zeolitic imidazolate framework (ZIF-8) and with 95:5 mass ratios ADN/ZIF-8 by the solvent methods were mixed with ADN. Finally, the catalytic effect of ZIF-8 on the thermal decomposition of ADN by differential scanning calorimetry (DSC). Results showed that adding ZIF-8 reduces the time and temperature decomposition ADN.

Keywords: Ammonium Dinitramide, Thermal Decomposition, Differential Scanning Calorimetry (DSC), Zeolitic imidazolate framework (ZIF-8)

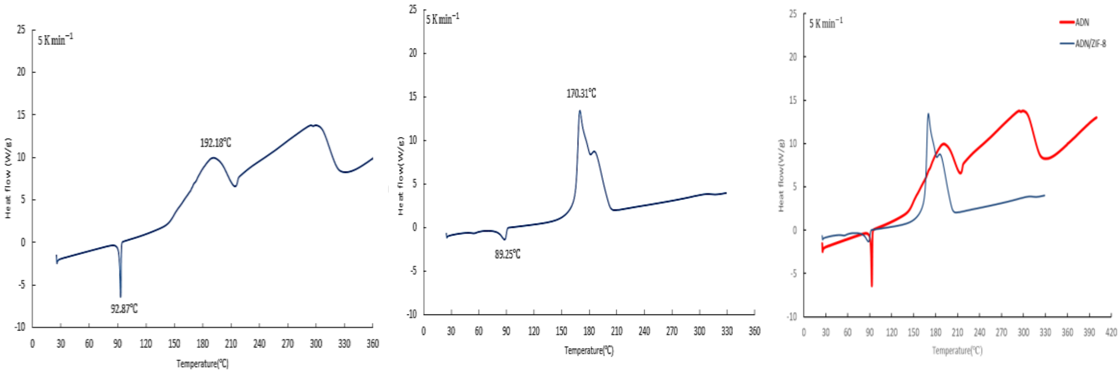

Fig.1. DSC curves of an ADN and b ADN/ZIF-8 (95:5) under Ar atmosphere at heating rate of 5 °C min^{-1}.

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Investigation of control over size and morphology of nanostructures Lanthanide based on carbacylamidophosphate

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Nano-sized materials are widely studied in nanomedicine for their potential use as drug carriers, in imaging, and for diagnostic purposes. Because of their size, they can interact with cells in similar ways as other nano-sized objects, such as proteins, cholesterol particles, and virus particles [1]. Compared to traditional and even newly developed synthetic techniques, the sonochemical approach for the construction of NPs is more simple, convenient and controllable [2]. Morphology and sizes of the nano-structures depend on the concentrations of initial reagents and the power of ultrasound used as well as reaction time [3]. Lanthanide complexes are rising stars as therapeutic agents because their fingerprint luminescence and MRI signals are highly useful for realtime monitoring the drug delivery and therapeutic processes [4]. Carbacylamidophosphates (CAPh), compounds containing –C(O)NHP(O) – are known for their potential biological uses, such as insecticides and enzyme inhibitors [5]. In this work, we report the effect of reducing agents on the size and shape of CAP-La nanocomplex using the sonochemical method. Reactions have been performed in several conditions to find out the role of different factors such as the power and frequency of the reaction in the ultrasonic device and the effect of solvents, time, additives and concentrations of initial reagents, of the Lanthanide complex on the size and morphology of the nanostructures. CAP-La nanocomplex have been characterized by field emission scanning electron microscopy (FE-SEM), powder XRD and FT-IR spectroscopy.

Keywords: Lanthanide complex, Sonochemistry, Carbacylamidophosphate, Nanocomplex

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Synthesis, Crystallography and Antibacterial activities of new Cocrystal Copper-Cerium Based on 1, 10-phenanthroline

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Cocrystals are attractive because the cocrystal solid can be designed to have superior physical properties to either of the pure starting molecules. It has available a range of application areas for physical property manipulation through cocrystal formation. Improvements in solubility, stability, bioavailability, and mechanical properties have been well documented and emerging applications such as pharmaceuticals, agrochemicals and pigments [1]. Copper (II) chelates have been found to interact with biological systems and to exhibit antineoplastic activity and antibacterial, antifungal, and anticancer activity. Some Cu (II) N, S, O/N, N-donor chelators are good anticancer agents due to strong binding ability with DNA base pair [2]. Lanthanide complexes are widely used in optical and magnetic materials, as catalysts as well as they are useful in biomedicine. A survey of the literature reveals that among the different neutral ligands 1, 10-phenanthroline and its derivatives have been the subject of special attention in ternary lanthanide complexes. It is well know that lanthanides behave as typical hard acids and prefer donor atoms with the preference O > N > S and F > Cl. Cerium is one of the cheapest and most abundant rare earths. Cerium nitrate is an effective antibacterial agent [3]. 1, 10-Phenanthroline (phen), a biologically important ligand, and some of its metal complexes have been shown to be effective against various strains of microorganisms [4]. In this study, the novel Cocrystal Copper-Cerium Based on 1, 10-phenanthroline, was synthesized by condensation of $Ce(NO_3)_3.6H_2O$, $Cu(ClO_4)$ and 1, 10-phenanthroline with ethanol solution. The resultant complex was identified *via* IR spectroscopy and X-ray Crystallography. Eventually, the antimicrobial activity against Staphylococcus aureus, Staphylococcus saprophticus and Pseudomonas aeruginosa, were studied by disk-diffusion method.

Keywords: Cocrystal, Crystallography, Antibacterial, phenanthroline

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Ni/Ag_2O nanostructures for efficient hydrogen evolution reaction

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Water-splitting plays an important role in the development of clean and renewable energy production [1-3]. In this project, the Ni/Ag_2O nanostructures were synthezied by co-precipitation method. The obtined nanostructures were characterized using various techniques. The electrocatalytic performance of Ni/Ag_2O nanostructures was investigated for hydrogen evolution reaction (HER) by several electrochemical methods in alkaline solutions. Experiments revealed that $Ni_{0.9}Ag_{0.1}O_x$ nanoparticles exhibit superior activity in alkaline HER cmpared to pure Ag_2O, and only need an overpotential of 104 mV at cdurrent density of 10 mA cm^{-2}.

Keywords: Hydrogen evolution reaction, Electrochemical properties, Metal oxides

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The Investigation of the electrocatalytic activity of Ni-doped and pure Ag_2O nanostructures for water oxidation

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Metal oxides have been good candidates for essential electrocatalytic processes. There are various methods to improve the electro-catalytic activity of metal oxides, for example doping with a guest element can change the electronic and electrocatalytic activity of them [1-3]. In this project, the Ni/Ag_2O nanostructures were synthesized and characterized using several techniques. The electrocatalytic performance of Ni-Ag_2O nanostructures was investigated for Oxygen evolution reaction (OER) by several electrochemical methods. The results showed that the obtained structures significantly decrease the overpotential value for OER compared to pure Ag_2O in alkaline solutions.

Keywords: Oxygen evolution reaction, Electrochemical properties, Metal oxides

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Investigation of water oxidation activity of a Mn (II)-salophen type complex

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Nowadays, the development of environmentally friendly and sustainable energy sources has been received much attention due to the continuous surging demand for energy and depletion of fossil fuels [1,2]. One of the most importants ways to generate energy is water splitting which can be divided into oxygen evolution reaction (OER) and hydrogen evolution reaction (HER). Water oxidation is a slow electrochemical reaction and requires a high overpotential. Therefore, the design of efficient and suitable catalysts to reduce the overpotential of water oxidation reaction is necessary. This reaction can be catalyzed in the presence of heterogeneous and homogeneous catalysts (WOC) [3,4]. Here, we investigated the electrocatalytic activity of a Mn(II)-salophen complex containing methoxy groups for water oxidation in different conditions. The results showed that this complex can catalyze the oxidation of water in alkaline solutions. Electrochemical tests revealed that the carbon paste electrode modified by the complex displays high activity for OER and only requires the overpotential of 270 mV under applied electrochemical conditions in alkaline solutions.

Keywords: Electrocatalytic activity, Oxygen evolution reaction, Mn (II) complexes, Salophen ligands

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Half-Sandwich Cyclometalated Rh^{III} Complexes Bearing Thiolate Ligands: Biomolecular Interactions and In Vitro and In Vivo Evaluations

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A class of cyclometalated RhIII complexes [Cp*Rh(ppy)(SR)] bearing thiolate ligands, Cp* = pentamethylcyclopentadienyl, ppy = 2-phenylpyridinate, and R = pyridyl (Spy, 2), pyrimidyl (SpyN, 3), benzimidazolyl (Sbi, 4), and benzothiazolyl (Sbt, 5), were produced and identified by means of spectroscopic methods. The in vitro cytotoxicity of the RhIII compounds in three different human mortal cancerous cell lines (ovarian, SKOV3; breast, MCF-7; lung, A549) and a normal lung (MRC-5) cell line were evaluated, indicating the selectivity of these cyclometalated RhIII complexes to cancer cells. Complex 5, selected for in vivo experiment, has shown an effective inhibition of tumor growth in SKOV3 xenograft mouse model relative to control (p-values < 0.05 and < 0.01). Importantly, the outcomes of H&E (hematoxylin and eosin) staining and hematological analysis revealed negligible toxicity of 5 compared to cisplatin on a functioning of the main organs of mouse. Molecular docking, UV−vis, and emission spectroscopies (fluorescence, 3D fluorescence, synchronous) techniques were carried out on 1−5 to peruse the mechanism of the anticancer activities of these complexes. The obtained data help to manifest the binding affinity between the rhodium compounds and calf thymus DNA (CT-DNA) through the interaction by DNA minor groove and moderate binding affinity with bovine serum albumin (BSA), particularly with the cavity in the subdomain IIA. It can be concluded that the Rh-thiolate complexes are highly promising leads for the development of novel effective DNA-targeted anticancer drugs [1, 2, 3].

Keywords: Cyclometalated, Anticancer, In vitro, In vivo, DNA interaction, H&E

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Investigation of ability of acid leachate formation from sulfide tailings of Sungun copper mine

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Sulfide tailings and sulfide effluents are important in terms of acidification potential. The results of preliminary studies indicate the possibility of acidic effluent formation and this process has followed an upward trend along with decreasing pH and increasing the concentration of contaminants in the effluent in recent years. Preliminary studies indicate the possibility of lowering the pH in the coming years, in which case it is possible to release large amounts of aluminum ions, iron and other heavy elements. In this study, in order to deal with inventory and future problems, 300 liters of acid drainage reagent sample was prepared in Pakhir valley and a series of mineralization and leaching tests were performed on it. Based on the results of the extraction process of valuable elements along with heavy elements in the above sample and due to the great importance of environmental considerations in the area, while stating the need for additional studies to identify and control future oxidation of mine tailings, the proposed circuit to control and inhibit acid drainage. Wastewater treatment and reconstruction was also provided.

Keywords: Sulfide Tailings, Sulfide Effluents, Wastewater Treatment, Sungun

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HY zeolite functionalized by Organic compounds containing nitrogen atoms: synthesis, characterization and usage for removing of some heavy metals

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The presence of heavy metals in ecosystems has many negative effects on human health and the environment. These ions do not undergo microbial or chemical degradation and their total concentrations in soils tend to persist and thus may cause severe problems for living organisms [1]. Therefore, due to these disadvantages, various techniques such as adsorption, extraction, plant extraction, ultrafiltration, reverse osmosis, electrodialysis, ion exchange and membrane processes for the removal of heavy metals have been proposed [2]. Zeolites are microporous crystalline hydrated alumino-silicates characterized by a three-dimensional network of tetrahedral (Si, Al)O_4 units that form a system of interconnected pores [3]. In this study, HY zeolites are functionalized by organic compounds containing nitrogen atoms and their role in the removal of heavy metals is investigated. The synthesized HY zeolites are detected by powder X-ray diffraction, scanning electron microscopy, nitrogen adsorption isotherms and FTIR spectroscopy [4]. The synthesized HY zeolites structureare is characterized by powder X-ray diffraction, scanning electron microscopy, nitrogen adsorption isotherms and FTIR spectroscopy [5].

Keywords: Heavy metals, HY zeolite, Adsorption, Nitrogenous organic compounds

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Improving water oxidation performance by creating heterointerfaces of ceria and nickel-oxide nanoparticles

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Ceria, CeO_2 plays an important role in catalytic processes due to its special chemical properties. The conductivity of CeO_2 is weak but when interacting with other transition metals its electron-ionic conductivity increases [1-3]. In this project, NiO/CeO_2 nanostructures were synthesized by the co-precipitation method and characterized using the standard method. The electrocatalytic behavior of the synthesized nanoparticles was evaluated for water oxidation by cyclic voltammetry, linear sweep voltammetry, and chronoamperometry technics in 0.1 M KOH solution. Experiments showed the $Ni_{0.95}Ce_{0.05}O_x$ displays high activity for the oxidation of water. This material needs a low overpotential of 423 mV to oxidize water under applied electrochemical conditions, while the pure ceria reveals a weak ability for the reaction.

Keywords: Cerium oxide, Nickel oxide, Water oxidation, Heterogeneous Electrocatalysts.

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Synthesis of nickel–copper–alumina-layered double hydroxide as an excellent electrocatalyst for oxygen evaluation

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Oxygen evolution reaction (OER) play important role in the field of hydrogen energy preparation and pollution treatment [1-3]. The design of high performance, stable and cost-effective electrocatalyst for oxygen evolution is crucial for the H_2 production from electrochemical water splitting [4, 5]. In this work, we successfully synthesize a Cu-doped NiAl- layered double hydroxides (LDH) nanosheets array. The obtained electrocatalyst characterization using X-ray diffraction (XRD) pattern, Field emission- scanning electron microscopy (FE-SEM), Transmission electron microscopy (TEM), and energy-dispersive X-ray (EDX-mapping). The electrochemical water oxidation was investigated using cyclic voltammetry (CV) and linear sweep voltammetry (LSV), and Nyquist plots. The electrochemical results show that the incorporation of Cu into NiAl-LDH could obviously overcome the step of H_2O adsorption during the OER progress. Accordingly, our catalyst affords a low onset potential of 1.0 V (*vs.* reversible hydrogen electrode, RHE) and a stable current density of 6.8 mA cm^{-2} at 0.97 V (*vs.*RHE) for 12 h. The Tafel slope of NiCuAl- LDH is 60.0 mV dec^{-1}, which was smaller than that of reference RuO_2 (68.1 mV dec^{-1}). Therefore, the NiCuAl-LDH electrode exhibits superior OER performance.

Keywords: Oxygen evolution reaction, Layered double hydroxide, Electrocatalyst.

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Ultrasonic-assisted, facile preparation of NiCr-LDH/SWCNT for superior efficiency oxygen evaluation

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Water oxidation to produce oxygen as a means of renewable energy applications has attracted intense interest [1, 2]. However, the oxygen evolution reaction (OER) is still a huge challenge due to its a kinetically slow process requiring high overpotential [3]. Therefore, the design and fabrication of highly active, durable, and cost-effective electrocatalysts are crucial. The present study reported that the NiCr- layered double hydroxide (LDH)/single-walled carbon nanotube (SWCNT) nanocomposite is as a highly stable and superior electrocatalyst for oxygen evaluation reaction (OER). The NiCr-LDH/ SWCNT composites were synthesized using the ultrasonic sound waves. Based on the characterization analyses such as X-ray diffraction (XRD) patterns, Energy dispersive X-ray (EDX) analysis, and field emission scanning electron microscopy (FE-SEM) images, the synthesis of NiCr-LDH/SWCNTs using the ultrasonic method, were confirmed. Next, the NiCr-LDH/SWCNT composites were used as an effective nanomaterials for OER at near neutral media. The obtained data from the linear sweep voltammetry (LSV) process confirm that NiCr-LDH/SWCNT decreases the overpotential to about 120 mV in the pH = 9.5 in comparison with only NiCr-LDH, and RuO_2. The high activity oxygen generation can be attributed to the presence of NiCr-LDH and SWCNT at prepared nanocomposite. The improved water oxidation at NiCr-LDH/SWCNT is due to high electrochemical activity and excellent electrical conductivity from SWCNT and NiCr-LDH, respectively. The stability of the NiCr-LDH/SWCNT was studied during 5 h water oxidation.

Keywords: Water oxidation, Layered double hydroxide, Electrocatayst.

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Preparation and characterization of nano γ-alumina from $Al(OH)_3$ and magnetite-alumina composites

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In the past few years, aluminum oxide attracts more attention due to its strength and corrosion resistance, chemical and thermal stability, and good thermal and electrical insulation properties with high hardness and high melting point. Alumina exists in a variety of stable structures including γ-, η-, δ-, θ-, κ-, and χ-alumina. γ-alumina is one kind of extremely important nanosized material. It is extensively used as a catalyst, catalytic support , adsorbents, planting, and biological basis. Magnetite nanoparticles due to their removal of pollutants, improving the environment, and absorbing various ions are important. Aluminum oxide also plays a very important role as a substrate for composite compounds. Iron oxide nanoparticles due to their inherent magnetic properties are one of the most important nanostructured materials [1]. Aluminum hydroxide and polyethylene glycol were dissolved in deionized water, and the pH of the solution was set to 10. The resulting solution was stirred for 7 days at 70° C. The precipitate was dried at 100° C for 24 hours and after that heated at 900° C for 3 hours to perform calcination. For the synthesis of magnetite nanoparticles, divalent and trivalent irons were added to the deoxygenated double-distilled solution. The resulting solution was also kept at 40° C for 15 minutes and the pH was adjusted to 11 with the ammonia solution. The reaction solution was placed under reflux and nitrogen gas atmosphere for 6 hours at 100° C. The solid diffusion method was used to prepare magnetite-alumina nanocomposites. Nano γ-alumina in ethanol was dispersed by ultrasonic waves. Then different amounts of prepared iron oxide nanoparticles were added to the suspension and stirred at room temperature for 24 hours. Finally, the iron-alumina nanocomposites were prepared with 5, 10, and 30% weight percentages. Alumina peaks were appearance in $2\theta = 67$, 61, 46, 39, 37, 31, 19 of pages 440, 333, 400, 222, 311, 220, 111 (JCPDS card NO. 10-0425). Also, according to the XRD pattern of structure, the prepared alumina has a cubic structure, and the average of particles were 16.51 nm. In XRD patterns of nanocomposites, by increasing the amount of iron oxide in the prepared nanocomposites, the peak intensity of the alumina index decreased. These peaks also indicate the high crystallinity of synthesized iron oxide, which has increased in intensity with increasing the amount of iron oxide in alumina magnetite composites. The peaks that appeared at 580- 832 cm^{-1} are related to the bending and stretching vibrations of aluminum-oxygen metal bonds..

Keywords: Aluminium hydroxide, Alumina, Magnetite, Composite.

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Hydrothermal synthesis of $TiO_2/PbTiO_3$ perovskite nanocomposites for enhanced photocatalytic performance

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Heterostructured photocatalysts based on TiO_2 and perovskite oxides were synthesized by a simple hydrothermal method and the prepared particles were annealed at 600°C.[1]. The $TiO_2/PbTiO_3$ nanocomposites are a group of semiconductor materials that have been widely used in photocatalytic fields due to their suitable band gap and easy synthesis methods. The heterojunction structures can promote the charge separation through favorable band alignments, leading to the reduction of recombination [2], [3]. Successful composite grafting was confirmed by Fourier transform infrared spectroscopy (FTIR), UV-Vis-NIR spectrophotometer, photoluminescence (PL) spectra, field emission scanning electron microscope (FE-SEM) with energy-dispersive X-ray spectroscopy (EDS). The photocatalytic activity of heterostructured $TiO_2/PbTiO_3$ perovskite nanoparticles is utilized for the photocatalytic degradation of methylene blue under UV light (8 Watts Philips UV lamp) irradiation. The $TiO_2/PbTiO_3$ nanocomposite displayed high photocatalytic activity in the degradation of methylene blue, higher than that of pure $PbTiO_3$ under UV light. This high photocatalytic degradation yield may emanate from the effective separation of electron-hole pairs between $PbTiO_3$ and TiO_2. The low peak intensity of the photoluminescence (PL) spectra of the $TiO_2/PbTiO_3$ nanocomposite indicates that a suitable charge separation has been performed by the photocatalyst, which is desirable for the photocatalytic process. The trapping experiments confirm the role of hydroxyl radical (˚OH) in the proposed mechanism. The synthesized photo-catalyst is reusable under several cyclic tests. Thus, $TiO_2/PbTiO_3$ nanocomposites had a certain application value in the field of wastewater treatment

Keywords: Perovskite oxides, Photocatalysis, Lead Titanate ,TiO_2.

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Synthesis of Mn-citric acid modified cysteine complexes and investigation of their antioxidant activity

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Recently, the cause of most diseases are the presence of free radicals. For years, antioxidants have been the focus of many epidemiological studies. Antioxidants are chemical compounds that are capable of preventing the oxidation of other molecules by quenching free radicals. Cysteine is a non-essential amino acid, it contains sulfur in the form of a thiol group at the end of its side chain. The thiol group is responsible for the high reactive capacity of the amino acid and therefore is responsible for many of its biological functions in human beings. Cysteine can be assimilated through different pathways depending on the needs of the cells. The application of this compound in fields related to pharmaceuticals, medicines, and nutraceuticals has been increasing. Cysteine is a compound widely used in the development of numerous drugs so far [1]. With this mind, we prepared Mn-ctric acid modified cysteine (Mn/cys) to investigate their antioxidant activity. To prepare metal-cysteine complexes, a certain amount of cysteine and $MnCl_2.2H_2O$ were dissolved in the citric acid solution. Then the reaction solution was stirred. The resulting solution was dried at 90°C. The disappearance of the thiol and -NH stretching frequency confirmed that the reaction between cysteine and citric acid was successfully carried out. The aqueous solutions of compounds displayed a high-intensity band at 360 nm, ascribed to n-π* transitions. The absorption spectra of manganese-containing CA-Cys exhibited a weak absorption band at 275 nm. To the prepared hydrogels, Tris-HCl buffer was added. After 10 minutes, reaction mixtures were mixed with pyrogallol [2].They showed outstanding activity for superoxide scavenging (> 85%) which was evaluated by a pyrogallol autoxidation method.

Keywords: Cysteine, Mn-CA/cysteine complex, Antioxidant, FTIR.

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Syntheses and characterization of organic-inorganic Nano hybrids of Allura red AC and layered double hydroxides based on Some Transitional elements and study of their photoluminescence properties

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Layer double hydroxides(LDHs) with a nanoscale structure are capable of displacement of their interlayer anions and whit high chemical stability, pH-dependent solubility[1]. LDH nanocomposites used in a Color[2], catalyst[3], drug carriers[4], sensors [5]and so on. In this research work, (Alr) Allura red AC / LDHs Nano hybrids based on Al^{3+} and with different metal M^{2+} ions (nickel, copper, cobalt was synthesized via a conventional co-precipitation method and characterized by x-ray diffraction patterns, FT-IR spectroscopy and elemental analysis. The structure of synthetic Nano hybrids was compared with those of x-ray diffraction patterns of dyestuffs and virgin layered double hydroxides. The displacement of 2θs of (003) and (006) planes to smaller 2θs and reducing of their intensity and broadening, were attributed to the successful placement of guest anions in the interlayer space of LDHs, as well as increasing the amount of spacing between the crystalline planes, replacing the anion pigment with the initial carbonates, nitrates and it even proved interlayer water molecules The TGA analyses was used for evaluating thermal stability and the number of water molecules in the Nano hybrid structure. were then determined by TGA. Also, SEM was used to determine the morphology of the Nano hybrid, and the fluorescence emission spectra were used to detect their photoluminescence properties. By studying the photoluminescence spectrum of synthetic Alr Nano hybrid based on M^{2+} / M^{3+} -Anion Red Anion cations at 437 and 330 nm wavelengths were observed.

Keywords: Anion Intercalation, Photoluminescence, Layered double hydroxides, Allura red A.

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A tris(diimine) Ni(II) complex: Solid-state structure, interaction with biomolecules, molecular modeling, and cytotoxic activity on cancer cells

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Over the last decade bioinorganic chemistry has been a rapidly developing area of pharmaceutical research based on considerable investigation into new metal-based anticancer agents [1,2]. Since DNA is a target molecule for cancer therapy, the study of DNA interaction with suitable pharmaceutical molecules is very important to design of new types of drugs. When the concept of DNA intercalation was first formulated by Lerman in 1961 [3], it has become widely recognized that many compounds of pharmacological interest manifest their biological activities through their ability to interact with DNA. Transition metal complexes with polypyridyl ligands are very interesting compounds due to their biological properties including strong DNA-binding ability, DNA cleavage, and anticancer activity [4,5]. In this paper, we report the synthesis, structural characterization, and biological properties of a new polypyridyl nickel(II) complex, $[Ni(dmb)_3](BF_4)_2$. The molecular structure of the complex was confirmed by single-crystal X-ray crystallography. The interaction of the complex with fish sperm DNA (FS-DNA) was investigated using cyclic voltammetry, emission titration, and UV-Vis spectroscopy in order to evaluate the DNA-binding mode. The results show that the Ni(II) complex interacts with DNA through the electrostatic and minor groove bindings. In addition, the binding of the Ni(II) complex to bovine serum albumin (BSA) was monitored by UV-Vis and fluorescence emission spectroscopy at different temperatures. The mechanism of the complex interaction with BSA was found to be a static quenching. Moreover, the cytotoxic activity of the Ni(II) complex on three human carcinoma cell lines, including MCF-7, A-549, and HT-29, were investigated using MTT assay. The molecular docking method was used to model the interactions of the Ni(II) complex with DNA and BSA.

Keywords: Ni(II) complex, DNA, BSA, Cytotoxicity, Cancer cells.

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Preparation of new bidentate chelates by activation of diols in the presence of $[Os(PQ)_3](PF_6)_2$ for biological applications

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An interesting area of research which has attracted considerable attention from both inorganic and biochemists is the design of new types of pharmaceutical molecules having remarkable applications in many areas of medicine [1]. Transition metal complexes with polypyridyl ligands are very attractive due to their particular optical, magnetic, electrochemical, spectroelectrochemical, and medicinal properties [2,3]. Polypyridyl complexes have efficiently used as the fluorescent probes for nuclear and protein components, DNA photocleavage agents, and electrochemical probes for DNA [4]. They also show good cytotoxicity against cancer cell lines [5]. The investigation of DNA–drug interactions is very important to develop of new therapeutic drugs. DNA molecule is the main target of anticancer drugs owing to its interaction with many transition metal complexes. Therefore, we decided to synthesize the osmium(II) complexes with new derivatives of PQ ligand by activation of different diols, in order to obtain the structural insight into the binding event in biological studies. Herein, we report the synthesis of new polypyridyl Os(II) complexes with different ligands by the metal-assisted effect of $[Os(PQ)_3](PF_6)_2$ complex on the condensation reaction of carbonyl groups of the coordinated PQ ligand with different diols. The tris(chelate) osmium complexes have been characterized by elemental analysis, spectroscopic methods, and single crystal X-ray structure analysis. Their interactions with fish sperm DNA (FS-DNA) under physiological conditions were investigated using UV–Vis spectroscopy, fluorescence spectroscopy, and electrochemical methods.

Keywords: Os(II) complex, DNA binding, Polypyridyl ligands, Metal-assisted effect.

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Synthesis and characterization of novel Cl-CQDs/$NiFe_2O_4$ nanocomposite

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Recently, carbon quantum dots have become the best candidates for photocatalyst activities due to their abundant functional groups, fluorescent properties, and high active sites on their surface. Since quantum dots are homogeneous, they cannot be separated from the reaction solution after the end of the reaction and therefore cannot be reused, which limited their applications [1]. In this work, a new nanocomposite resulting from the coating of Cl-CQDs [2] on the surface of $NiFe_2O_4$ [3] particles, was synthesized by the convenient co-precipitation method [4]. The Cl-CQDs/$NiFe_2O_4$ nanocomposite was characterized by VSM, TGA, EDX, XRD, UV-Vis, FT-IR, and PL techniques. All of them confirm the successful synthesis of this nanocomposite [4]. Decreased value of M_S in Cl-CQDs/$NiFe_2O_4$ versus $NiFe_2O_4$ is mainly due to the presence of Cl-CQDs, which is a non-magnetic substance. In spite of the fact that the value of M_S decreased but the nanocomposite expresses considerable magnetic properties that provide facile separation of catalyst from the reaction solution by an external magnet, which makes it a good candidate as a photocatalyst.

Keywords: Carbon quantum dots, $NiFe_2O_4$, Nanocomposite.

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Synthesis and characterization of a new hexadentate N-donor ligand and related Cu(II), Co(II), and Ni(II) complexes, X-ray crystal structure of Cu(II) complex

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Many studies have been done on the design and synthesis of new polyamines and their metal complexes [1, 2]. In the present work, A new ligand (L) containing two aminophenyl rings as side chains, N1, N2-bis(2-aminobenzyl)-N1,N2-bis(pyridin-2-ylmethyl) propane-1,2diamine, was synthesized. The reaction of this ligand with copper (II), nickel (II), and cobalt (II) metal ions gave complexes with similar structures. The free ligand was characterized using a number of spectroscopic methods such as FT-IR, elemental analysis, mass spectrometry, ^{1}H and ^{13}C-NMR. As well as the synthesized metal complexes were characterized by FT-IR, elemental analysis, and ESI-MS spectroscopy. On the other hand, the structure of the [CuL].2(ClO$_4$).5[H$_2$O] complex has been confirmed by the single-crystal x-ray structural analysis. The crystal structure of [CuL].2(ClO$_4$).5[H$_2$O] showed that the copper atom is in a very distorted square pyramidal environment, coordinated by five of the six nitrogen donor atoms of the potentially hexadentate ligand. Two nitrogen atoms from the pyridine groups and the two tertiary nitrogen atoms form the basal plane with the nitrogen atom from one of the aminophenol groups being in the apical position; the nitrogen from the second aminophenol group is noncoordinating.

Keywords: Hexadentate N-Donor ligand, X-ray crystal structure, Metal complexes.

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The X-ray crystal structure, biological capabilities, and molecular docking studies of the Cu(II) complex with a ligand containing homopiperazine moiety

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[CuL] $(ClO_4)_2$ coordination compound was formed from a reaction of a previously known tetradentate organic ligand containing homopiperazine moiety [1, 2] with Cu(II) ion, and their structure by single-crystal X-ray diffraction was determined. The X-ray structural analysis of [CuL] $(ClO_4)_2$ complex demonstrated that the copper(II) ion is in a slightly distorted square planar environment. metal center coordinated by four nitrogen atoms of the ligand. Molecular docking has become an increasingly important tool for drug discovery [3]. In order to evaluate the biological potential of the tetradentate-free ligand as well as [CuL] $(ClO_4)_2$ their binding behavior with DNA and acetylcholinesterase (AChE) was investigated by a molecular modeling tool. These studies indicated that the copper complex was bound to the major groove of DNA and to polar and apolar residues located in the active-site gorge (binding site of E2020). The molecular docking results and the binding constant values displayed the remarkably high affinity of Cu(II) complex to DNA as well as AChE Compared to the free ligand. Further investigation demonstrated that the synthesized complex [CuL] $(ClO_4)_2$, was capable enough to scavenge DPPH free radicals. Besides, the significant antibacterial activity was recorded against tested pathogenic bacteria, as evidenced by almost 90% inhibition at 1.25 mg/mL and higher concentrations. Moreover, the anticancer activity of the synthesized compounds was assessed by using the MTT test, and the highest activity was observed by [CuL] $(ClO_4)_2$ complex that rendered MCF-7 cells proliferation. Hence, the complex can be considered a potential anticancer drug against breast cancer cells.

Keywords: Molecular docking, Cu(II) complex, Anticancer.

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Crystal structure, the potential of inhibition of acetylcholinesterase (AChE) by molecular docking study, and evaluation of the anti-cancer activity of Ni (II) complex having N-donor ligand

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In recent years, we have extensively attempted to design and synthesize novel ligands that contain the homopiperazine moiety [1,2]. The reaction of N-donor ligand (L), 2,2'-((1,4-diazepane-1,4-diyl) bis(methylene)) dianiline, with Ni(II) metal ions gave a complex with a slightly distorted octahedral coordination environment. The metal complex was characterized using a number of spectroscopic methods including IR and CHNS analysis and mass spectroscopy. The x-ray crystal structure analysis of $[Ni (L) (NCME)_2] (ClO_4)_2$. NCMe complex revealed, that the Ni(II) ion coordinated by four nitrogen atoms of the ligand and two molecules of acetonitrile in the trans configuration coordinated to the nickel ion. Alzheimer's disease (AD) is known as the most common type of dementia. The discovery of acetylcholinesterase inhibitors is an important step in the treatment of this disease. Due to the side effects of known acetylcholinesterase inhibitors, the development of new inhibitors becomes an appealing target for the investigation of novel potential therapeutics [3]. In this study, we investigated the effects of the Ni(II) complex on AChE by molecular docking method for preferable synthetic candidates. In order to evaluate the biological potential of N4-Donor free ligand as well as $[Ni (L) (NCME)_2] (ClO_4)_2$. NCMe their binding behavior with acetylcholinesterase (AChE) was investigated by molecular modeling analysis. The molecular docking results, the binding energy (kcal/mol), and inhibition constant KI (μM) value displayed for Ni(II) complex -9.85, 6.07×10^{-2}, and for L -10.18, 3.46×10^{-2}, respectively. Moreover, the anticancer activity of the synthesized compounds was assessed by using the MTT test. In compression to L and $[Ni (L) (NCME)_2] (ClO_4)_2$. NCMe, metal complex showed greater cytotoxicity effects on cancer cells, although its potential anticancer activity is still less than Cisplatin as the positive control. Hence, the complex can be considered a potential anticancer drug against breast cancer cells.

Keywords: Inhibition of acetylcholinesterase, Ni (II) complex, Molecular docking.

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Investigation of new nitroaromatic ligand and its copper (II) and zinc (II) complexes using molecular docking technique as glutathione reductase inhibitors

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The strong activity of the GR enzyme in cancer cells helps to provide resistance to various chemotherapeutic drugs. This enzyme catalyzes the conversion of oxidized glutathione (GSSG) to reduced glutathione (GSH) using nicotinamide adenine dinucleotide phosphate (NADPH) molecules. High intracellular GSH levels cause tumor cells to survive [1,2]. Therefore, the inhibition of GR is an important target in the treatment of many diseases. As reported in the literature, human GR enzymes are susceptible to NO_2-containing molecules. In this report, docking studies with human GR enzymes were done. The molecular docking of L, $[ZnLBr]ClO_4$, and $[CuL](ClO_4)_2$ with human glutathione reductase (GR) showed that the dominant interactions of these compounds with GR were H-bonding, Vander Waals, and hydrophobic interactions. Indeed, new compounds investigated here showed very effective GR inhibitory activity compared to well-known agents. It was found that the most effective GR inhibitor between free ligand and its metal complexes was $[CuL](ClO_4)_2$ and the placement score equal to -9.46 supported this. These synthesized compounds have the potential to be used as glutathione reductase inhibitors, which are of particular interest due to their possible anticancer capacities, but must be confirmed by in vivo and/or clinical trials for more accurate results.

Keywords: Nitroaromatic compound, Glutathione reductase inhibitors, Molecular docking.

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Investigation of the interaction of $GaInS_3$ and In_2Se_3 crystals with organic molecules

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Layered materials typically exhibit strong in-plane covalent bonds, but weak van der Waals interactions between layers. Due to the unique structural features and physicochemical properties, these materials have been widely studied in recent decades. They are characterized by a wide range of electronic band structures ranging from dielectrics, semiconductors, metals, superconductors to topological insulators. Intercalation is a chemical process aimed at the reversible introduction of alien species (atoms, ions or molecules) into a crystal gap. The most well-known electrochemical energy device using intercalation is the lithium ion battery, in which Li ions are reversibly intercalated in graphite van der Waals gaps for charging and discharging [1]. Intercalation can change the band filling state and the Fermi level, resulting in many physical phenomena. This report presents the results of interactions of $GaInS_3$ and In_2Se_3 crystals with organic molecules. As a result of the interaction of $GaInS_3$ crystals with 4-aminopyridinium (4-AP) molecules, a new intercalated compound with the composition $GaInS_3{\cdot}0.5$ (4-AP) was obtained [2]. The formation of this intercalate preceded naturally, without any special difficulties and with the preservation of the single crystallinity of the final product. Attempts to prepare analogous compounds with more symmetrical analogs of 4-AP, such as phenyldiamine, pyrazine, and also ethylenediamine, were unsuccessful. That is, the intercalation process is highly selective. Interactions of the same molecules with preliminarily intercalated $GaInS_3{\cdot}0.5$ (4-AP) crystals were also studied [3]. In_2Se_3 crystals are also layered and have a black color. As a result of their interaction with 4-AP, a yellow polycrystalline product was obtained. The report will present the structural characteristics of the resulting new compound.

Keywords: Intercalation, $GaInS_3$, In_2Se_3, Crystallinity.

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Reduction of pollution in Landfill leachate of Urmia city by using pozzolan

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Due to high pollution, the water produced in Landfill requires chemical and biological treatment methods. In general, landfill leachate contains organic pollutants, ammonium, halogenated hydrocarbons, heavy metals and inorganic salts, and one of the methods of leachate treatment is the use of silicate-based materials. The purpose of this study is to reduce the contamination of Landfill leachate in Urmia city by using pozzolan mineral. In this regard, experiments were performed using pozzolan in 500 ml balloons and the test conditions consisted of a reaction temperature equal to the ambient temperature of 600 rpm. The minute distribution of pozzolan granulation was 45 microns and 500 nm with a solid weight of 10%. The results of the experiments show that in the granulation of 500 nm, better results have been obtained. Thus, the amount of ammonium in the tap water is reduced by 93% and the contamination is due to the presence of microbes, which before decontamination was 81 in a dilution of 10-18 It was reduced to 46 in a 3-10 dilution.

Keywords: Leachate, Landfill, Urmia, Reduction.

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Synthesis and characterization of magnetic-mesoporous $CoFe_2O_4/mSiO_2/NH_2$/Poly(MAA-co-IA) core/double shells nanomaterial

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In a novel approach, the preparation of $CoFe_2O_4/mSiO_2/NH_2$/Poly(methacrylic acid-co-itaconic acid) (MAA-co-IA) as a magnetic-mesoporous core/double shells (CDS) nanomaterial is reported. Superparamagnetic cobalt-ferrite nanoparticles were synthesized by hydrothermal method (10-18 nm) [1] and then nanoparticles were successfully coated with amine modified mesoporous silica nanoshell through a silanization reaction to prevent the oxidation and agglomeration (15-20 nm) of $CoFe_2O_4$ [2]. The high density of NH_2 groups created on the mesoporous silica surface allows the polymer molecules to bind with the surface. $CoFe_2O_4/mSiO_2/NH_2$ nanostructures were subsequently covered by copolymer molecules, via electrostatic interaction of NH_2 groups of silica surface with COOH groups of copolymer and this led to the formation of $CoFe_2O_4/mSiO_2/NH_2$/Poly(MAA-co-IA) (32-34 nm) nanomaterial [3]. Then, its properties were characterized by XRD, SEM, VSM, BET, TEM and FT-IR techniques. Based on TEM measurement, the diameter of core/double shells was determined to be about 35 nm. The BET showed a specific surface area of 220 $m^2.g^{-1}$ and a pore width of 2.44 nm. In addition, the composite exhibited high magnetization (31.0 emu g^{-1}), thus it is possible for drug targeting under a foreign magnetic field. This nanomaterial have potentials to be used in hyperthermia treatment, selective drug delivery, targeted therapy and water purification, etc [3].

Keywords: Drug delivery, Amine modified silica, Double shells, Targeted therapy.

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Synthesis and characterization of magnetic-luminescent and mesoporous core–shell-structured nanocomposite

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The synthesis and characterization of core–shell structured $ZnFe_2O_4@nSiO_2@mSiO_2@CeF_3(Tb^{3+}, Gd^{3+})$ nanocomposite is reported with magnetic-luminescent and mesoporous properties. The magnetic ($ZnFe_2O_4$) nanoparticles were synthesized by solvothermal route [1] and then core–shell magnetic mesoporous $ZnFe_2O_4@nSiO_2@mSiO_2$ with double-shells structure were synthesized by two-step coating processes of silica on inorganic magnetic core ($ZnFe_2O_4$). The dense inner shell can effectively protect the magnetic core and enhance the stability of the magnetic core to some extent. The porous outer shell can provide high specific surface area and increase the amounts of lanthanide doped fluorides on the surface of the supports [2]. The synthesized adsorbent were characterized using infrared spectrometer (IR), scanning electron microscopy (SEM), vibrating sample magnetometer (VSM), X-ray diffraction (XRD) and spectrofluorometry (analysis of excitation/emission spectra). Based on SEM measurements, the diameters of the cores (≈16 nm) and core/double shells particles (≈31 nm) were determined. The magnetization saturation value (M_s) of the $ZnFe_2O_4@nSiO_2@mSiO_2@CeF_3(Tb^{3+},Gd^{3+})$ nanocomposite was estimated to be 32 $emu.g^{-1}$. The nanomaterial synthesized was exhibited intense green luminescence under UV light irradiation. This nanocomposite can act as a multifunctional nanocarrier in drug delivery systems.

Keywords: Solvothermal synthesis, Mesoporous, Magnetic, Luminescent.

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Antioxidant activity of copper and zinc complexes with new water-soluble hydrazone ligand

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From the reaction of acetylhydrazide and bezhydrazide with the precursor 3-(3-formall-4-hydroxy-benzyl)1-methyl-1-hydrogen-imidazole-3-im chloride in methanol solvent two water-soluble Schiff base ligands H_2L1Cl, H_2L2Cl were synthesized in high yields and identified by UV-Vis, FT-IR, ^{1}HNMR and ^{13}CNMR techniques. The presence of OH and NH peaks in these ligands indicates that the ligands remain in phenolic and hydrozonic form. The metal complexes were prepared by the reaction of the ligands with the chloride salts of zinc(II) and copper(II) and characterized by UV-Vis, FT-IR, elemental analysis and cyclic voltametry methods. Antioxidant activity was tested at acidic, alkaline and neutral pHs by radical removal of DPPH (diphenylpicrylhydrazyl) and the results showed the ligands had better activity than their respective complexes [1-5].

Keywords: Antioxidant, Copper complex, Hydrazone ligand, Zinc complex, Schiff base.

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Synthesis and characterization of new aluminum and gallium complexes of water-soluble thiosemicarbazones

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Thiosemicarbazones are an influential family of Schiff bases that have been considered for their ability to form complexes having pharmacological, biological, and analytical properties. Three Schiff base thiosemicarbazone ligands with aqueous solubility, namely 3-(3-{[(aminocarbonothioyl)hydrazono]}-4-hydoxybenzyl)-1-methyl-1H-imidazol-3-iumchloride (H_2L1Cl), 3-[4-hydroxy-3-({[methylamino) carbonothioly] hydrazono} methyl) benzy]-1-methy-1H-imidazol-3-ium chloride (H_2L2Cl) and 3-(3-{[(anilinocarbonothioyl) hydrazono] methyl}-4-hydroxybenzyl)-1-methyl-1H-imidazol-3-ium chloride (H_2L3Cl) were synthesized respectively through reaction of thiosemicarbazide, 4-methyl-3-thiosemicarbazide and 4-phenyl-3-thiosemicarbazide with PL2 (name of PL2). The ligands were used for synthesis of the following Al(III) complexes with Aluminium chloride salt, named $[Al(H_2L1)_2Cl]$, $[Al(H_2L2)_2Cl]$ and $[Al(H_2L3)_2Cl]$. These compounds were characterized by elemental analysis, FT-IR, ^{1}H NMR, ^{13}C NMR, X-ray crystallography and UV-Vis spectroscopy. All the compounds have sufficient solubility and stability in water [1-5].

Keywords: Schiff base, Thiosemicarbazone, Al(III) complexes, Fluoresence.

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The electrocatalytic performance of Fe_2O_3/CuO nanocomposites for glucose detection

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The detection of glucose has important significance in the food industry and clinical medicine, especially in the diagnosis of diabetes. In recent years, electrochemical non-enzymatic glucose sensors have attracted intensive attention to detect the glucose level with great progress [1,2]. Up to now, different enzymatic glucose sensors are commonly used in glucose detection. However, considering some intrinsic disadvantages of these sensors, such as high fabrication cost and poor stability, non-enzymatic glucose sensors have attracted increasing research interest [3,4]. Herein, the activity of iron oxide/copper oxide heterostructure for glucose sensing was studied in KOH electrolyte by different electrochemical methods. Experiments revealed that the Fe_2O_3/CuO shows high sensitivity of 317.9 mA cm^{-2} mM$^{-1,}$ a wide linear range (0-50 mM), along with high selectivity, and applicability for glucose detection in real samples.

Keywords: Non-enzymatic glucose sensing, Metal oxide heterostructures, Electrochemical techniques.

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Investigation of the alcohol group protecting by nickel macrocyclic complexes from oxidation to aldehydes

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The oxidation of alcohols to aldehydes is a fundamental chemical transformation in synthetic chemistry [1, 2]. Most of the dioxygen activating catalysts are transition metal compounds [3]. On the other hand, the transition metal complexes are composed of a central metal atom and a surrounding organic ligand such as macrocyclic [4]. It is of continuing interest to design and synthesize novel macrocyclic host molecules because of their important roles in supramolecular chemistry [5]. In this work, the protection of the alcohol group (benzylic alcohol) from oxidation to aldehyde by two nickel macrocyclic complexes, $[Ni(L)]I_2$ and $[Ni(L)(NO3)_2]$ (Fig. 1), was investigated by Uv studies. These studies were carried out at elevated dioxygen pressure, different temperatures, the different molar ratios of complexes in alkaline aqueous solutions, and under reflux conditions. The results revealed that the titled complexes protect the alcohol group from converting to aldehydes. High conversions of benzylic alcohol to aldehyde were observed without of addition of macrocyclic nickel complexes.

Keywords: Catalytic activity, Macrocyclic, Oxidation, Alcohol, Aldehydes.

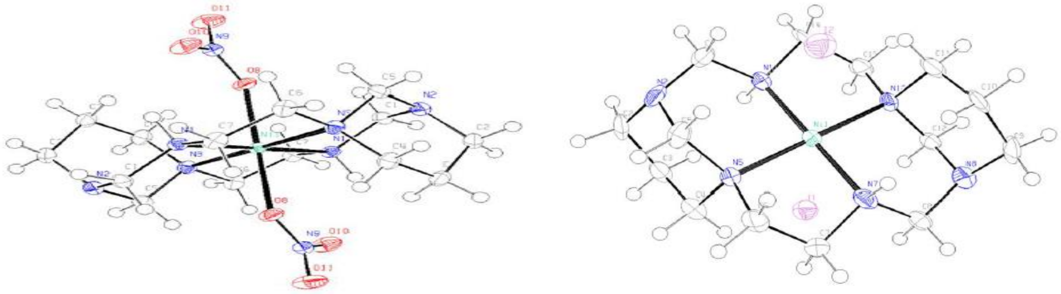

Fig1. Structure of the complexes used for catalytic effect studies.

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Removal of copper and Sulfate compounds from Sungun's acid mine drainage by sulfate-reducing bacteria in a DFFB anaerobic reactor

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Copper mine drainage contains large amounts of heavy metal and sulfate pollutants that can potentially pose serious risks to human and environmental health. Anaerobic bioreactors are considered to be the most suitable methods for the treatment of acidic effluents containing heavy metals due to some advantages such as the possible recycling of precious metals, the need for a small area, easy control, and better process prediction [1], [2]. In this experimental laboratory-scale study, the performance of sulfate-reducing bacteria (SRB) was investigated in a DFFB anaerobic reactor for SO_4 and Cu removal from the drainage of Sungun's acid mine drainage. To this end, 800 g of activated carbon granules with an average diameter of 0.63 mm, an apparent density of 0.58 g/cm^3, and an effluent volume of 2.5 L were introduced into the reactor in a non-fluid form with a height of 35 cm and 6-600 rpm. The rate of sulfate reduction and copper removal were studied at retention times of 24 hours or less. All parameters' samples were analyzed using the standard methods for experiments of water and wastewater. The analyzed results indicated that the DFFB reactor was an efficient and suitable method for the treatment of effluents containing large amounts of SO_4 and Cu. The concentrations of SO_4 and Cu in the samples decreased by 98.38 and 98.05%, respectively, after 24 h of retention time.

***Keywords**:* Acid Mine Drainage, Copper, Sulfate-Reducing Bacteria, Anaerobic Reactor.

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Crystal structures and properties of Topological Insulators $MnBi_2Te_4 \cdot (Bi_2Te_3)_n$ (n=0÷6)

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At the beginning of the XXI century, it was theoretically predicted about the possibility new material, which will have completely new properties. These materials are called topological insulators (TI), were first experimentally obtained in 2007. In recent years revealed that Bi_2Te_3 and some of its analogues are bulk topological insulators. The magnetic transition metals were used mainly for doping. Predicted in 2010 anti-ferromagnetic topological insulators (AFMTI), are of particular interest for creating spin electronics and quantum computers. An experimental confirmation of the presence of AFMTI was first published in 2019 [1], using the example of a Van der Waals type layered compound $MnBi_2Te_4$. They prove the results of both theoretical calculations and also experimental studies. In this case, theoretical calculations were performed by the methods of DTF and MC, and experimental studies consisted of structural, transport, magnetic measurements and angular emission spectroscopy. We studied the phase formation in the $MnTe\text{-}Bi_2Te_3$ system. It was found that in this system a series of homologous compounds are formed with the general formula $MnBi_2Te_4 \cdot (Bi_2Te_3)_n$, where n=0÷6. Their crystallographic characteristics for all of them have been determined, the crystalline structures for n=0÷3 are refined on the basis of single or powder XRD data, single-phase pieces are selected and some physical characteristics are measured. In the report will present the new results about general principles of crystalline structures and, crystal structures of mentioned homological crystalline phases of $MnBi_2Te_4 \cdot (Bi_2Te_3)_n$ terms of n=4÷6.

Keywords: Topological insulators, Structure, X-ray.

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Cadmium(II) complex with N_2O_2-donor salophen and azide ligands: Synthesis and spectroscopic properties

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Many efforts have been devoted to the study of transition metal azide complexes due to their structural diversities and attractive magnetic properties [1]. The bridging small pseudohalides, especially azide ions, are good condidates for magnetic exchange interaction between paramagnetic metal centers [2]. The azido bridges are bounded to the metal ions in various coordination modes, which the most common of them are end-to-end and end-on [3]. In this project, we report the syntheses, characterization and spectroscopic properties of Cd(II) complex with salophen-type and azide ligands. The ligand is prepared from the condensation reaction between 4-chloro-1,2-diaminobenzene and salicylaldehyde in ethanol. The complex is obtained from the reaction between 4-chlorosalophen, NaN_3 and $Cd(CH_3COO)_2.H_2O$ in methanol solvent. The FT-IR spectrum of the complex displays the characteristic bands of azide and imine groups. The absorption of –C=N– stretching vibration of imine groups in complex occurs as a strong band at 1616 cm^{-1}. This complex exhibits the sharp band at 2058 cm^{-1}, which is attributable to the coordination of azide ligand to the Cd(II) ion.

Keywords: Cd(II) complex, Azide, Salophen-type ligands

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Catalytic removal of chemical warfare simulant using UiO-66 and UiO-66(NH_2) MOFs

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In this study, two metal-organic frameworks (MOF) named UIO-66 and NH2-UIO-66 and a neurotransmitter named dimethyl 4-nitrophenylphosphate (DMNP) were synthesized. The synthesized chemicals were characterized by using Fourier transform Infrared (FT-IR), Ultraviolet (UV-Vis) Spectroscopy, Nuclear Magnetic Resonance (NMR), Powder X-ray Diffraction (PXRD). In addition, Nitrogen gas adsorption to estimate surface area (BET) was performed for more characterization. DMNP was selected and used as an alternative model of phosphorus neurotransmitters due to its similarity in properties and structure to these compounds. Removal of DMNP neurotransmitters was evaluated by using prepared MOFs [1]. UV-Vis spectroscopy was used to monitor the DMNP concentration during the removal process. The results showed that UiO-66 and NH2-UiO-66 have a very high ability to catalytically degrade DMNP by hydrolysis in the aqueous medium and neutral buffer. The removal percentage (R%) of DMNP from the organic medium was also studied and the results showed that the removal R% of 50 mL of DMNP (50 ppm) were about 76.5 and 66.8% for UiO-66 and NH2-UiO-66, respectively. Examination of the stability of the adsorbents after the adsorption process by the PXRD technique also showed that the adsorbents are recyclable.

Keywords: Metal-Organic Frameworks, Nerve agent, DMNP, Hydrolysis

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Synthesis and characterization of reduced graphene oxide/lanthanide ions nanocomposite for photo-degradation of methylene blue dye

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In a novel approach, the preparation of reduced graphene oxide/lanthanide ions (RGO/Ln^{3+}) as a novel nanocomposite is reported. The reduced graphene oxide was synthsized using sonochemical route [1,2]. The synthesized nanocomposite was characterized to study its various properties by infrared spectrometer (IR), scanning electron microscopy (SEM) and X-ray diffraction (XRD) techniques. The photocatalytic activity was evaluated for the degradation/oxidation of methylene blue (MB) dye under visible light irradiation and ambient temperature. The effective parameters on degradation process such as pH, the amount of photocatalyst and process time were optimized. RGO/Ln^{3+} nanocomposite resulted in an enhanced maximum degradation for MB dye molecules after short time of visible light irradiation.

Keywords: Graphene, Lanthanide ions, Nanocomposite, Degradation

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Leaching of sulfide concentrate of Sungun copper complex in sulfuric acid medium with addition of sodium chloride along with microwave irradiation

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In this study, the effect of microwaves along with chlorine ions on the leaching of sulfide concentrate of the Sungun copper complex has been investigated. To this end, a 10% by weight pulp solution before being utilized in the leaching process has been conditioned in a Bosch household appliances grade microwave oven with a frequency of 2450 MHz with different amounts of power. Microwave radiation causes more solvents to come into contact with the concentrate, increasing the mass transfer rate and reducing the time required for the process. In this research, the role and effect of microwaves in improving the acidic leaching of copper sulfide minerals have been investigated. The goal was to increase copper recovery and reduce the time required for the leaching process. The results indicate that the recovery of dissolved copper without sodium chloride and microwave irradiation was about 15.42%, with the addition of sodium chloride it has increased to 43.51%, and with microwave irradiation, it was increased by 15% which was equal to 58.63% [1-4].

Keywords: Leaching, Copper sulfide concentrate, Sodium chloride, Microwaves

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Leaching of sulfide concentrate of Sungun copper complex in sulfuric acid medium via oxygen application

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In this study, the leaching of sulfide concentrate of Sungun copper complex in atmospheric conditions by applying oxygen gas was investigated. The goal of this study was to investigate the effect of factors such as sodium chloride additive, temperature, and oxygen gas on the dissolution efficiency of copper from sulfide concentrate [1−4]. Since oxygen has a significant effect on the oxidation of sulfide minerals which is quite evident in the surface layers of the earth, throughout this research via the application of oxygen the transformation process of metallic sulfide to metallic sulfate was in progress and the final results indicated a pronounced effect of investigated factors especially sodium chloride and oxygen gas on extraction efficiency. In the experimental conditions of 1M sulfuric acid, a 20 g/l concentrate, the temperature of 80 °C, and a stirring speed of 800 rpm without the addition of sodium chloride and oxygen gas the dissolution rate of 16.7% was obtained. With the addition of sodium chloride, this amount increased to 45.2%. Also, by applying oxygen gas with a flow rate of 0.6 liters per minute in the most optimal condition a 15% increase in copper dissolution rate was achieved.

Keywords: Leaching, Copper sulfide concentrate, Sodium chloride, Oxygen gas

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Construction of carbon adsorbent to remove copper from Pakhir river drainage of Sungun copper mine

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Each river has the capacity to accept incoming pollutants and self-purify to a certain extent, so it is important to study the water quality of rivers and be aware of changes in self-purification capacity [1,2]. The effluent of Sungun copper mining activities in northwestern Iran, which flows in waterways and rivers, leads to an increase in the load of heavy metals in rivers [3]. Currently for this purpose, sampling is done in 9 stations of Sungun chai, Pakhir chai, Arghaneh Chai, Miyan Cafe and Ilgineh rivers in the area of Sungun copper mine and the parameters of pH, EC, TDS, TSS and heavy metal concentrations are analyzed. In this research, while making carbon adsorbent, the synthesis and structural study of pyrolysis carbon adsorbent in copper removal under different laboratory conditions has been investigated. Examination of the results of XRD, SEM and EDX analysis identified heat-absorbing carbon structure and almost complete copper removal was measured by AAS atomic adsorption method. In this study, by using KCT carbon adsorbent in aqueous media with acidic pH, we removed 99% of copper up to 100ppm and 67% of copper up to 300ppm and in real samples 56% of copper.

Keywords: Sungun, Heavy Metals, Carbon Absorbers, Pakhir River Drainage

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New Dual-Functional Metal Organic Frameworks as Platform for Hg^{2+} Ion Adsorption

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Designing adsorbents with accessible chelating sites and achieving high contaminant purification efficiency is still an important key to overcome environmental remediation challenge [1-3]. As one of the significant global concern, presence of heavy metal ions in environment has attracted increasing attention due to their toxicity, carcinogenicity and bioaccumulation in the food chain [4,5]. Herein, we targeted design a new dual functionalized metal organic framework (DF-MOF) by incorporating different percentage of N1,N3-di(pyridine-4-yl) malonamide ligang (S), into urea containing MOF (TMU-32); the produced material was labeled TMU-32S (with 33%, 65% and 100% incorporation percentages). Designing DF-MOF is our “design-for-purpose” approach for decoration of MOF walls by suitable functional groups result in high removal capacity of heavy metal ions. Among TMU-32S series with different concentration of S ligand, TMU-32S-65% was demonstrated an exceptional Hg^{2+} ion selectively. To the best of our knowledge, this is the first report of mixed urea-malonamide based MOF which provides a proper coordination site to coordinate strongly to Hg^{2+} ions, along with 1428 $mg.g^{-1}$ maximum adsorption capacity. Generally, we attributed the impressive implementation of TMU-32S-65% to synergistic effects of both hydrophilic chelating urea and malonamide functional group. Hence, the results reported in this work determined the exceptional potential of DF-MOFs for high accomplishment environmental remediation.

Keywords:Metal Organic Framework, Dual functionality, Mercury removal, Solvent Assisted Ligand Exchange

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Enhancing the efficiency of polyvinyl alcohol/ sodium alginate/ chitosan-based composites using algae biomass and Fe-MOF for wound healing and tissue engineering applications

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Wound healing mostly corresponds to skin healing. It starts immediately after an epidermal layer trauma and could last for years. In this project, we were able to generate wound dressings based on hydrogels for wound healing. Hydrogel dressings have been investigated for the treatment of skin wounds due to their capability to generate a moist environment for the wound, accelerate the healing process, and isolate the affected area from the external environment. As a result, the main objective of this work was to create a polymer wound dressing in the form of a hydrogel to aid in the process of healing the injured tissue. In this process, the Fe-Metal organic framework (Fe-MOF), which was synthesized by the hydrothermal method, was loaded on a mixture of polyvinyl alcohol (PVA)/sodium alginate (SA)/chitosan (CS) and Chlorella microalgae (nano-biocomposite as an appropriate hydrogel) which were then utilized as the upper and lower layers to successfully generate a bilayer composite dressing for wound healing. MOFs have been used for a variety of antibacterial applications in recent years due to their sustained release potential, porosity, and structural flexibility when combined with a wide range of chemicals and/or materials [1]. Three materials were adopted in this study for the purpose of improving the biocompatibility, biodegradability, and mechanical features of the gel, namely PVA, SA, and CS [2]. Chlorella Vulgaris is a green microalgae with several medical benefits. The bioactive components of microalgae hold antimicrobial, anticancer, and antioxidant properties as well as anti-inflammatory attributes. We have successfully incorporated (5%, 10%, 15%, and 20%) Chlorella into this structure to generate porous compounds, and the resulting hydrogel-based formulations have all of the essential features to manage moisture, enable gaseous exchange, prevent microbial lesions, and decrease toxicity [3].

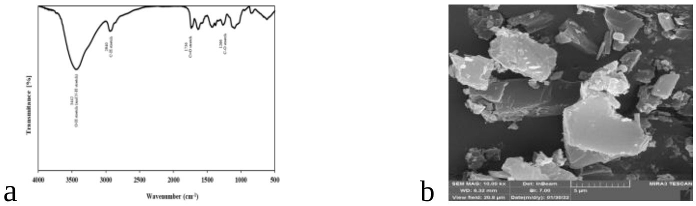

Fig. 1. (a) The FTIR spectrum of hydrogel sample depicting four absorption bonds displaying the presence of functional groups. (b) The SEM image of Fe-MOF.

Keywords: Chlorella Vulgaris, Hydrogel, Metal-Organic Frameworks, Tissue engineering, Wound healing

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Enhancing Hydroxyapatite characterization using some Microalgae as Porous Scaffold in Bone Tissue Engineering

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Bone is a complex and dynamic tissue that is somewhat capable of regeneration and reconstruction thus bone repair or reconstruction is a common and complex clinical problem in orthopedic surgery [1]. Bone is a highly organized composite material consisting of 50 to 70 percent minerals (mainly hydroxyapatite), 20 to 40 percent organic compounds, 5 to 10 percent water, and 3 percent lipids [2]. The goal of this study, is to develop new synthesized composite based on microalgae biomaterials, have led to the development of new engineering strategies to improve bone regeneration. Bone Tissue Engineering (BTE) is now taking an interdisciplinary perspective in search of new and better ways to address the challenges of biomedical engineering bone reconstruction [3]. In this work we synthesis a novel hydroxyapatite microalgae Ca-MOF composite for bone tissue engineering. Metal-organic frameworks (MOFs) are crystalline solids that have extensive lattices formed by coordinate bonds between mineral nodes [4]. Chlorella vulgaris is one of the green microalgae that has very useful contents for humans. The bioactive component of microalgae has antimicrobial, antitumor, antioxidant, antiviral, antifungal and anti-inflammatory activities. In addition, these bioactive components can produce collagen, a protein that supports cell regeneration, for example, in bone regeneration [5].We synthesized Hydroxyapatite and used green microalgae as binder and pore forming agent, also we loaded Ca-MOF on this substrate to increase the performance of the composite because of its porosity.

Keywords: Hydroxyapatite, Bone tissue engineering, Greenmicroalgae, Metal-Organic Frameworks

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Leaching of sulfide concentrate of Sungun copper complex in hydrochloric acid medium with addition of hydrogen peroxide and ethylene glycol

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In this study, the effect of hydrogen peroxide along with ethylene glycol on the leaching of sulfide concentrate of Sungun copper complex in a hydrochloric acid medium has been investigated. Hydrogen peroxide was utilized as a strong oxidizing agent and due to the instability of hydrogen peroxide at high temperatures, ethylene glycol was employed for stabilization and persistence of the suspension [1−4]. Experimental conditions consist of the utilization of 1M of hydrochloric acid, 1 M of hydrogen peroxide, 0.15 M of ethylene glycol, the temperature of 80 °C, and a stirring speed of 800 rpm. The goal of this study was to increase the recovery of copper from sulfide concentrate and the results indicate that the copper recovery without the addition of hydrogen peroxide and ethylene glycol, with the addition of hydrogen peroxide, and with the addition of ethylene glycol was 20.52, 57.63 and 77.58%, respectively.

Keywords: Leaching, Copper sulfide concentrate, Hydrogen peroxide, Ethylene glycol

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Structural and computational characterization of the homopolar dihydrogen interactions

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Herein it is illustrated how computational chemistry hand-in-hand with experimental outcomes can assist in describing non-covalent interactions, and more specifically, homopolar dihydrogen interactions [1-3]. Selected state-of-the-art computational approaches are conjunctly exercised in a tutorial-style manner to address the challenge for characterizing dihydrogen intermolecular contacts. In-depth tests were carried out to evaluate existence, nature and energetics of some O—H···H—C and C—H···H—C homopolar dihydrogen interactions. Satisfactory results, both in terms of accuracy and computational cost, were obtained. Readers with a general interest in computational non-covalent chemistry – from relative beginners to experts – will gain a lot from thinking through the different analyses and case study examples covered in this contribution.

Keywords: Non-covalent interactions, Density functional theory, Computational Inorganic chemistry, Structural chemistry, Dihydrogen interactions

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Surveying the elimination of Basic Red 18 colour by modified Zeolite

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The paint and textile industries produce large volumes of hazardous and toxic wastewater [1]. Adsorption processes are widely used in removing pollutants from wastewaters, particularly those that are not easily biodegradable such as dyes [2,3]. In this study, zeolite was modified with magnesium nitrate salt for better efficiency and faster removal of dye from alumina with a value of 0.01g. This study used modified zeolite was used as a low-cost adsorbent to remove dye from wastewater. The studies were carried out under various experimental conditions such as dye concentration, zeolite percentage, and absorbent contact time. The removal rate was monitore by Uv-Vis spectroscopy. The results showed that as the amount of the adsorbentincreased, the percentage of dye removal increased accordingly. The modified zeolite showed excellent elimination ability for the removal of Basic Red 18 so that 60 ppm of zeolite can eliminate the basic red 18 solutions (6 ppm) up to 87% in 90 min.

Keywords: Modified zeolite, Basic Red 18, UV-Vis, Adsorbent, Wastewater

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Green Synthesis of Zinc Oxide Nanoparticles by Hymenocrater Plastystegius and Investigation of Particle Morphology and Size

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The use of plant extracts in the synthesis of nanoparticles can be an eco-friendly [1], cost-effective and easy-to-synthesize method as well as an alternative to conventional methods such as physical and chemical ones; this has made the green synthesis of nanoparticles of interest to many researchers [2,3]. This study was to biosynthesize of ZnO nanoparticles by using extract of Hymencrater Plastystegius plant and its effect on morphology and size of NPs. The extract of Hymencrater Plastystegius is used as the reducing agent for Zn^{2+} in the biosynthesis of ZnO NPs in presence of 1 Mm $ZnNO_3$ solution. The physical and chemical properties of the Zinc oxide nanoparticles has been analyzed facility of X-ray diffraction (XRD), scanning electron microscopy (SEM) and Fourier transform infrared (FT-IR). X-ray diffraction (XRD) patterns have been investigated for the detection of phase and size and crystal structure as well as the proof of formation of zinc oxide nanoparticles, scanning electron microscopy (SEM) for morphology and Fourier Transform Infrared (FT-IR) analysis is for difference bonds checked. The results of various analyzes confirm the synthesis of ZnO nanoparticles .It seems that green Synthesis of nanoparticles using plant extracts can help to extracts can be of great help to the environment.

Keywords: Zinc Oxid, Easy-to-synthesize, Hymencrater Plastystegius, Eco-friendly, Green synthesis

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Leaching of copper arsenic mineral in hydrochloric acid medium with calcium chlorite additive

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Extraction of copper from sulfide sources by hydrometallurgical methods is one of the biggest challenges for mining researchers. Copper sulfide concentrates, especially chalcopyrite, are sometimes associated with arsenic minerals such as anarchite and tenantite, especially in deep mineral layers. Since sulfides and arsenic oxides are volatile compounds, an environmentally friendly method is needed to isolate them in order to prevent air pollution with toxic compounds. The aim of this study was to leach Sungun copper sulfide concentrate with the aim of extracting maximum copper from arsenic ores [1-5]. Leaching tests on Sungun copper flotation concentrate under operating conditions of 1 $_{\text{mol/l}}$ hydrochloric acid, 0.2 $_{\text{mol/l}}$ calcium chlorite and 0.15 $_{\text{mol/l}}$ ethylene glycol at 80$^{\circ\text{C}}$ and 800 $_{\text{rpm}}$ stirring conditions done. The results showed that the highest percentage of copper recovery was related to ethylene glycol additive and calcium chlorite additive in 15 minutes, which we saw an increase of 72.23% and 64.85%, respectively, compared to conditions without additive. These results indicate the high potential of calcium chlorite leaching in the extraction of copper from arsenic concentrates.

Keywords: Extraction; Leaching; Copper; Calcium Chlorite

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Synthesis of cadmium sulfide nanorods modified with Ag nanoparticles for photocatalytic degradation of Rhodamine B pollutant

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Photocatalytic decomposition of Rhodamine B by cadmium sulfide nanorods optimized with silver nanoparticles is a powerful method for wastewater treatment. In this study, silver nanoparticles are synthesized on the surface of CdS nanorods (NRs) which act as auxiliary catalysts. Successful reduction of silver ions through chemical reduction and close correlation between nanoparticles and NRs has been investigated using XRD, SEM, TEM, FTIR and UV-Vis spectra [1]. The obtained results showed that the composition of Ag nanoparticles and CdS NRs leads to the formation of new bonds with bridging sulfur in the form of Ag-S-Cd, which leads to a significant increase in the photocatalytic activity of CdS [2].

Keywords: Photocatalysis, Nanocomposite, CdS nanorods, Silver nanoparticles.

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Thermal decomposition of cyclopentadienyl compounds of Mn, Fe, Co immobilized on oxide surfaces

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Supported catalysts with metal particles smaller than 10 nm in size can be obtained by thermal decomposition of organometallic compounds immobilized on porous substrates. Development of the chemistry of organometallic compounds in recent years has made it possible to develop methods for the synthesis of various homo- and heterometallic clusters, which can be used to obtain catalysts containing ultrafine particles of transition metals on substrates of various organic and inorganic nature [1]. This paper presents the results of a study of the thermal decomposition of mono- and binuclear cyclopentadienyl compounds of 3d-metals (Mn, Fe, Co) deposited on oxide (aluminum oxide, silicon dioxide, aluminosilicates) substrates. The main goal of this work was to develop new approaches to the preparation of catalysts containing nanosized particles of 3d metals on oxide supports and to develop methods for controlling their catalytic properties in the hydrogenation of carbon dioxide to C_2,C_3 olefins. SEM JSM-6610LV, JEOL scanning electron microscope combined with an element analyzer (SEM/EDS) is used to control the surface morphology and distribution of active elements in the substrate structure. The phase analysis of the synthesized samples was studied using XRD 3500 TD diffractometer, China and Phaser D2, Germany, with CuK_α radiation. The textural characteristics (the specific surface area and total pore volume) of the samples was determined by low-temperature adsorption of nitrogen using Belsorp Mini II, BEL Japan Inc. instrumtnts device. The infrared spectra of the synthesized samples were recorded on an Alfa Fourier spectrometer, Bruker, Germany, and the EPR spectra - on an EMRmicro spectrometer, Bruker, Germany. Thermal analysis was carried out on a STA 449 C Jupiter setup (NETZSCH, Germany) in a nitrogen flow in the temperature range of 25–700°C at a temperature rise rate of 10°C/min, as well as in an isothermal mode at 120, 200, 400°C for 3 hours at each temperature. Test portions 10 mg, in the case of the original compound, and 25-30 mg, in the case of applied samples. The transformations occurring upon heating of the samples were judged from thermogravimetric (TG) and differential (DTG, DTA) curves.

Keywords: Thermal decomposition, cyclopentadienyl compounds of Mn, Fe, Co, oxides

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Efficient thin film photocatalyst of UiO-66/Ag_2O heterojunction within Cr(VI) reduction reaction

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The daily increasing demands for neat and healthy water resulted in development of new effective cleansing methods within household and industrial wastewaters. The pollutions like heavy metals, contaminant the drinking water so that, their photocatalytic remediation became more popular during the past decade [1,2]. In current study a new composite of Uio-66/Ag_2O having the different mass ratios was synthesized through the impregnation method [3] and then was characterized using FTIR, XRD, SEM, and EDS analyses. In following, the photocatalytic activity of compound was pursued for Cr(VI) reduction under the solar light simulator of LED lamp (200 W) [3]. The better photocatalytic results were observed for 30:70 mass ratio of Uio-66:Ag_2O contents that shown the significant capability of Cr(VI) reduction in comparison with the single form of Uio-66 and Ag_2O alone.

Keywords: Uio-66/Ag_2O composite; Photocatalytic reduction; Cr(VI).

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Effects of magnetic graphene oxide on the improvement of $ZnTiO_3$ nanocomposite for solar light-induced photodegradation of Azo dyes

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This work reports the synthesis of titanate peroskite with formula $ZnTiO_3$ via solvothermal method. The graphene-Zn titanate (GZnT) nanocomposites were synthesized by using the prepared $ZnTiO_3$ nanoparticles and graphene oxide as precursors. These materials were characterized by FT-IR spectroscopy, X-ray Diffraction (XRD), morphology was studied by transmission electron microscopy (TEM) and scanning electron microscopy (SEM), surface area determination by the BET method and analysis of particle size. Raman mapping of the GZnT nanocomposites revealed the homogeneity and distribution of ZT nanoparticles on the surface of graphene. The UV–visible absorption and photoluminescence spectra of the samples suggest that the GZnT nanocomposite can be used as efficient photocatalysts to remove organic dye from water under visible light irradiation. Since conventional water treatments are often ineffective in eliminating azo dyes, the heterogeneous photocatalytic oxidation advanced oxidation process (AOP) have been more efficient technologies in degradation of those contaminants [1,2]. The results showed that the photocatalytic activity of the GZT samples was obviously enhanced in contrast to bare $ZnTiO_3$ samples. The enhanced photocatalytic activity was mainly attributed to the conglomeration inhibition of $ZnTiO_3$ nanoparticles, the electron transfer between $ZnTiO_3$ and graphene, surface area and the extended absorption range. The possible electron transfer mechanism for graphene-ZT interface during the photocatalysis process is also proposed

Keywords: $ZnTiO_3$, Perovskite, Graphene oxide, Photocatalyst, Visible light

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Inorganic-organic hybrid based on the preysssler polyoxometalate, synthesis and application

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Polyoxometalates (POMs) are a class of metal oxides that exhibit a wide range of molecular clusters and can be easily employed in the generation of new materials [1]. These clusters occupy an extensive parameter space between the mononuclear metalates and the bulk oxide. It has been found that among POMs with different size and structures, $[NaP_5W_{30}O_{110}]^{14-}$, so-called Preyssler polyoxometalate, shows significantly distinct properties such as: (1) high thermal stability, (2) high hydrolytic stability (pH 0–12), (3) recyclability, (4) easy to handle safely, (5) low quantity of waste, (6) ease of separability, (7) low corrosiveness, (8) high oxidation potential and (9) being green [2]. In this paper, new inorganic−organic hybrid consisting of the Preyssler polyoxometalate, $[NaP_5W_{30}O_{110}]^{14-}$, PDA (p-phenylenediamine) and M = Mn^{2+} or Co^{2+} were successfully synthesized by an new straight forward method [3]. The hybrid nanocatalisis were fully characterized by field emission scanning electron microscopy (FE-SEM), Fourier transform infrared (FT-IR) spectroscopy, X-ray diffraction (XRD). Interestingly, the calcinated nanocatalysis samples showed excellent decomposition efficiency toward the organic pollutants such as the dyes of methylen Blue (MB) and rhodamine B (RhB). Moreover, the catalyst for RhB can be reused at least 4 cycles with only a slight dropping of catalytic efficiency, suggesting their promising applications in the treatment of wastewater [4,5].

Keywords: Polyoxometalates, Preyssler polyoxometalates, Inorganic−organic hybrid, Catalysis, Dyes

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Investigation of Catalytic Properties of Ruthenium Nanocomposites in Electroreduction of CO_2 to CO

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In an effort to address escalating environmental problems, using viable methods that rely on global efforts, atmospheric CO_2 accumulated (ACA), which is causing escalating ecological issues, has been converted into valuable chemical fuels [1]. Solar, wind, and tide energy are renewable sources that could potentially be used for electrochemical CO_2 reduction with high efficiency and selectivity to alleviate energy crises and environmental problems. Over the past few decades, numerous investigations have been conducted to find efficient catalysts for CO_2 reduction reactions (CO_2RRs), such as metals, metal alloys, and metal complexes [1,2]. However, due to the low abundance and high cost of these metal-containing catalysts, they are limited in their practical applications on a large scale. Instead, heteroatom-doped carbon-based catalysts' low cost, superior stability, and high catalytic ability have made them a promising alternative to metallic catalysts for CO_2RR [3]. As an example, Meyer and co-workers demonstrated that carbon nanotubes (CNTs) with N-doping as functionalized catalysts for CO_2RR in $KHCO_3$ aqueous solution achieved an 87% faradaic efficiency (FE) for formate [3]. On the other hand, mainly ruthenium-based systems have been reported to electrochemically or photochemically accelerate the reduction of CO_2 to CO [2]. Here, we report the synthesis and structural characterization of a new nanocomposite containing GO-NH_2 and a mononuclear complex of Ru(II), [Ru(tptz)(ACN)Cl_2] (where tptz=2,4,6-tris(2-pyridyl)-1,3,5-triazine and ACN=Acetonitrile). The electrocatalytic reduction of CO_2 to CO by the nanocomposite was investigated using cyclic voltammetry (CV) in $KHCO_3$ solution. Finally, the effect of prepared nanocomposite on the electrocatalytic performance of the initial complex was investigated.

Keywords: GO, Ruthenium, Electroreduction, CO_2 reduction, Carbon monoxide.

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Synthesis and characterization of immobilized phthalocyanine complex on cobalt oxide nanofibers using electrospinning for oxidation of alcohols

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Electrospinning is simple and versatile method to produce nanofiber and microfiber. Briefly, mechanism of nanofiber formation by electrospinning process as follow: (i) a strong electric field is applied between a polymer solution contained in a glass capillary and a conductive substrate; (ii) when the voltage reaches a critical value, electrostatic forces overcome the surface tension of the solution; (iii) charged droplets or jets are sprayed from the tip of the capillary, in a dry atmosphere; and (iv) the dried droplets or jets are finally collected on the substrate to form a thin film. The main electrospinning process parameters are polymer concentration, flow rate of the polymer solution, additives, humidity, viscosity, surface tension, applied voltage, and nozzle-to-ground collector distance[1-3]. Here, copper phthalocyanin was immobilized on cobalt oxide and the its nanofiber was synthesized using polyvinyl alcohol by electrospinning. It was characterized by SEM, TEM, FT-IR, and EDAX. This bio- nanofiber was applied as a heterogeneous catalyst for selective oxidation of primary and secondary alcohols. A long-term stability, using ideal oxidant, easy work-up, and solventless show the great potential in scalability with relatively low catalyst loading. These features as concepts in economical and sustainable modern oxidation systems along with good reusability of the bio-catalyst render a practical strategy to address the environmental and industrial applications.

Keywords: Electrospinning, Nanofiber, Oxidation alcohols

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Ni-Citric acid coordination polymer as a practical catalyst for multicomponent reactions

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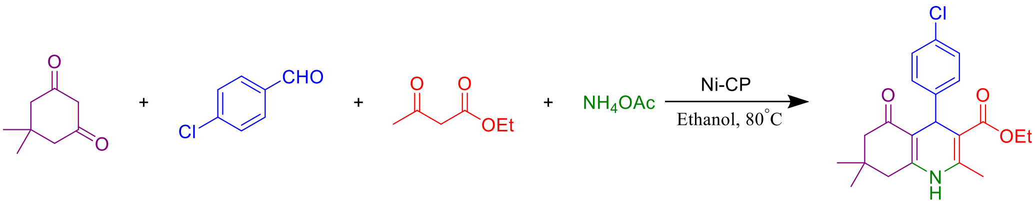
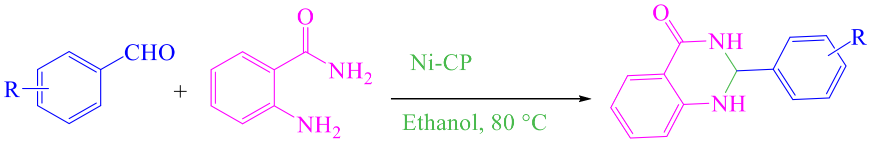
Coordinative polymers (CPs) are a subclass of Metal-organic frameworks (MOFs) with porous microstructures which have been widely synthesized in recent years and applied in various fields especially in catalysis science. In this work Coordinative polymers (CPs) of nickel and citric acid (CA) was prepared as a new catalyst (Ni-CPs) and applied in organic multicomponent reactions. The obtained catalyst was characterized by SEM, WDX, EDS, AAS, FT-IR, XRD and BET analysis. N_2 adsorption-desorption isotherms indicate good BET surface area for Ni-CPs; therefore can be employed as an efficient catalyst in multicomponent reactions for the synthesis of polyhydroquinoline and 2,3-dihydroquinazolin-4(1H)-one derivatives. Finally, this catalyst was recovered and reused several consecutive times (Scheme 1 and 2) [1-4]**.**



(Scheme 1)



(Scheme 2)

Keywords: Coordinative polymers, Polyhydroquinolines, Heterogeneous catalyst, 2, 3-dihydroquinazolin-4(1H)-ones

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Citric acid based Cu-MOF catalyzed the selective synthesis of biphenyls and sulfuxides

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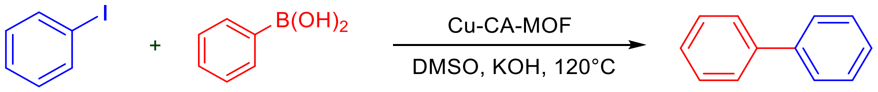
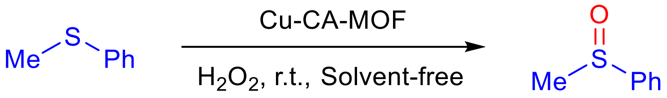
A highly stable heterogeneous and efficient catalyst was successfully prepared by hydrothermal reaction of Copper nitrate with citric acid. Citric acid with three carboxylic groups was used as an outstanding chelating agent was utilized for the preparation of Cu–metal–organic framework (Cu–MOF). The prepared MOF was characterized by FT-IR, SEM, AAS, EDS, XRD, BET and WDX analysis. N_2 adsorption–desorption isotherms indicated acceptable BET surface area for Cu–MOF. SEM images were shown that Cu–MOF has geometric polyhedral shapes. Also, catalytic activity of Cu–MOF successfully examined for the Suzuki–Miyaura cross-coupling reaction and chemoselective oxidation of sulfides to sulfoxides (Scheme 1 and 2) [1-5].



(Scheme 1)



(Scheme 2)

Keywords: Citric acid, Coupling reaction, Heterogeneous catalyst, Metal–organic framework, Suzuki–Miyaura reaction

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Synthesis of new copper oxide (II) nanostructure and its application as a sensor toward biomolecules

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CuO is a p-type semiconductor with a narrow band gap of 1.2 eV. It has been widely used and studied because of its numerous applications in field transistors, catalysis, semiconductors, gas sensors and biosensors [1,2]. Synthesis method of nanostructures has salient effect on their structrual features such as particles size and morphology along with their applications. In this work we have syntheiszed new copper oxide nanoparticle [3] and charachterized it by IR spectroscopy, XRD and SEM. Then it's used as a sensor for biomolecule detection. Copper nitrate slat was used with urea and a thioamine as surfactants with specific and precise ratio to make changes in particles shape and morphology and consequently their applications. Since a mixture of them prepared and stirred vigorously, using a teflon lined autoclave, the solution was aged up to 180 ^{0}C for 18 h. After reansing and dryring, the black precipitate eventually calcinated at 500 ^{0}C for 2 h. Fig.1 shows XRD pattern of sample and firmly confrimed preparation of CuO with monoclinic phase (JCPDS no. 01-080-1268). Obtained CuO has been employed as a sensing material to detect dopamine by electrochemical method. The results showed a good currecnt increase in the presence of dopamine. Also it has selectivity toward dopamine even in the presence of other interference species.

Keywords: Copper Oxide , Surfactant, Biosensor.

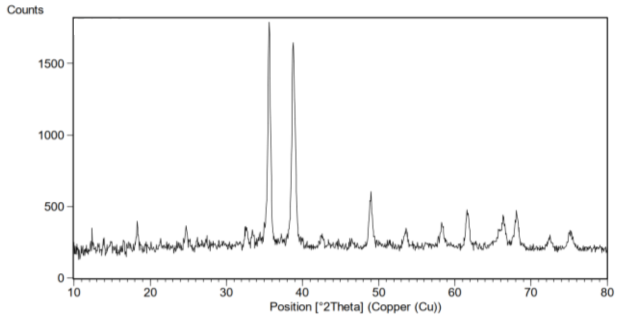

Fig.1 XRD Pattern of new CuO Nanoparticle

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Highly sensitive and selective dopamine biosensor using GCE modified by CuO-Ag decorated nanoparticles

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Dopamine is a neuromodulatory molecule that plays several important roles in cells. To detect it the bare sensor and all the nano-based sensors were used [1,2]. In this work we have used CuO Nanoparticles decorated by Ag as biosensor to modify the electrode surface. Synthesis of CuO-Ag decorated (5 % w/w) nanoparticles carried out using urea as a surfactant. The product was characterized by IR spectroscopy, XRD and SEM. Electrochemical studies were done by cyclic voltammetry and chronoamperometry methods using modified GCE electrode with CuO-Ag decorated/functionalized MWCNTs in order to examine its sensitivity and effectiveness toward biomolecules. Fig.1 shows Cyclic voltammogram of GCE modified in the absence and presence of dopamine. A significant current increase in the presence of dopamine (~ 600 μA) has been observed which is remarkable in comparison with many other dopamine sensors have been reported up to now. Also its selectivity in the presence of interferer species such as glucose were examined. The modified electrode had no electrochemical response toward glucose which makes it a reliable and selective dopamine biosensor.

Keywords: Biosensor, Dopamine, CuO, Ag co-doped

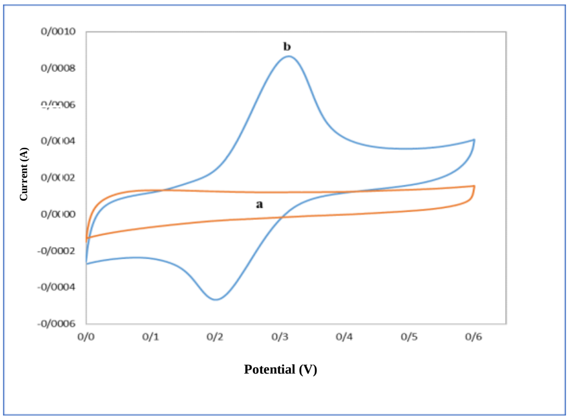

Fig. 1 - Cyclic voltammogram of GCE electrode modified with CuO-Ag decorated/functionalized MWCNT
a) in the phosphate buffer (pH=7)
b) in the 10mM dopamine solution (scan rate 50mV/s)

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Synthesis and Hirschfeld surface analysis of a tetranuclear Zn(II) complex with (E)-N'-(1-(4-hydroxy-6-methyl-2-oxo-2H-pyran-3-yl) ethylidene) picolinohydrazide

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Hydrazones are an important class of Schiff bases that are considered as one of the most extensively utilized ligands for the development of coordination chemistry of transition metals. This matter is related to their easy way of preparation, structural divergence, and solubility in commonly available solvents [1-3]. These are illustrious from the other members of the same class due to the existence of interlinked nitrogen atoms (-C(O)-NH-N=CH-) and can coordinate with the metal atoms in both neutral and deprotonated forms [4]. Picolinohydrazide, by having a pyridine ring connected to the hydrazone unit is one of the attractive compound for preparing diatopic Schiff base ligands. In this research, we report the synthesis, characterization and Hirschfield surface analysis of Zn(II) complexes with (*E*)-*N*'-(1-(4-hydroxy-6-methyl-2-oxo-2H-pyran-3-yl) ethylidene) picolinohydrazide. Tetranuclear zinc complex was synthezied in methanol solvent and its crystals were obtained by slow sovlent evaporating method. The obtained complex was characterized by spectroscopic methods and single crystal X-ray analysis which revealed it is a tetranuclear acetato-bridged Zn(II) complex and the picolinohydrazone ligand act as both bridging and chelating ligand. This copmpound is crystallized in monoclinic system and there are strong intermolecular interactions. The zinc ions are five coordinated and the acetato ligands act as briding group between metal cores. Intermolecular interactions in this compound were studied by Hirschfeld surface analysis. This analysis indicated there are strong C–H···O. O–H···O and O–H···N interactions in the crystal structur of the Zn(II) cluster.

Keywords: Hydrazones, Zn(II) complex, Picolinohydrazone, Single-crystal X-ray analysis

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Copper cobaltite nanoparticles as catalyst for direct alcohol fuel cell

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The decrease of fossil fuels such as crude oil, natural gas, and coal has urged researchers to explore sustainable energy resources and high-efficiency energy converters. Fuel cells are marked as efficient energy devices [1]. One commonly used fuel cell is the direct alcohol fuel cell in which the chemical energy stored in the organic molecules (e.g. alcohol fuels) is directly converted into electric energy through electrochemical reactions. Ethanol and methanol are among the most appealing alcohols for alcohol-based fuel cells owing to their low cost, ease of transfer and storage, and high energy density. The performance of a fuel cell depends on the activeness and lifetime of the catalyst [2]. The current study aims to investigate the electrocatalytic activity of copper and cobalt single and hybrid oxides during methanol oxidation. The nanostructures were synthesized using hydrothermal method, calcinated at different temperature points, and then used as nanocatalysts for methanol oxidation in alcohol fuel cells. The synthesized nanostructures were characterized and confirmed using X-ray diffraction analysis (XRD), transmission electron microscopy (TEM), and FESEM-EDX analysis. The performance of the synthesized nanostructures as catalysts was examined and compared during the electricity production procedure via methanol oxidation in fuel cells. The results confirmed that the $CuCo_2O_4$ nanocatalyst has excellent catalytic activity, high durability and stability compared to CuO and Co_3O_4 which indeed propose it to be as a promising electrocatalyst for future direct alcohol fuel cells.

Keywords: Copper cobaltite, Nanocatalyst, Methanol oxidation, Fuel cell

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Nickel ferrite nanoparticles as catalyst for methanol oxidation in direct alcohol fuel cell

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Direct alcohol fuel cells (DAFCs) have attracted considerable interest in their application to alternative power sources for portable electronic devices and electric vehicles [1]. The electrocatalytic reaction of alcohol oxidation in alkaline media is more facile, allowing to use low catalysts loadings and to select a wide range of catalysts [2]. In the present work, nickel oxide, iron oxide and nickel ferrite nanoparticles was synthesized by hydrothermal method. Synthesized nanostructures were characterized using Fourier transform infrared spectroscopy (FT-IR), X-ray diffraction (XRD), field emission scanning electron microscopy (FE-SEM), energy-dispersive X-ray spectroscopy (EDS), and high-resolution transmission electron microscopy (HRTEM). The performance of synthsized nanostructures was investigated in order to compare the activity and stability of these structures as anodic catalysts in the oxidation process of methanol in direct alcohol fuel cell. The results of methanol electrooxidation reaction were investigated and studied using electrochemical tests using a three-electrode system. The results confired that the $NiFe_2O_4$ nanocatalyst has excellent catalytic activity, high durability and stability compared to NiO and Fe_2O_3 which indeed propose it to be as a promising electrocatalyst for future direct alcohol fuel cells.

Keywords: Nickel ferrite, Nanocatalyst, Methanol oxidation, Fuel cell

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Plasmonic Metal-based Photocatalysis; an Efficient Method for Modifying Semiconductors

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Metal nanoparticles have shown great potential in heterogeneous photocatalysis. Noble metal nanoparticles such as Au, Pt, and Ag have drawn great attention in this area, due to their visible-light activity and selectivity in various chemical reactions [1-3]. But the challenge is that they are easily deactivated during the catalysis and their high cost. Therefore, composition of the metal nanoparticles with other metals and preparation of bimetallic nanoparticles based on surface plasmonic resonance effect becomes one of the most promising strategies to overcome the stability issue. In this paper, we provide a summary of the recent progress in the synthesis of Bi, Cu, and Ag nanoparticles as co-catalysts to improve the photocatalytic activity of metal oxides and metal sulfides. This paper begins with an introduction to the preparation method for synthesis of metal nanoparticles, and composition with semiconductors. The advantages of the designed materials are then discussed, such as improved photocatalytic efficiency for removal of organic pollutants, enhanced stability, and improved selectivity in photo-, and electrocatalysis.

Keywords: Photocatalysis, Surface Plasmon Resonance, Metal Nanoparticles, Bimetallic Nanoparticles, Organic Pollutants.

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Pd(II) and Zn(II) complexes of hydroxybenzhydrazide based Schiff base ligand. Synthesis, characterization, antioxidant activity and catalase inhibition

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The biological application of Schiff base compounds is expanding [1-3]. In this study, a new Schiff base ligand and its Pd(II) and Zn(II) complexes were synthesized from the reaction between 4-hydroxybenzhydrazide and diacetyl monoxime (Fig. 1). The prepared compounds were identified by elemental analysis and spectroscopic methods. Schiff base ligand showed stronger antioxidant properties after coordination (the trend of changes in antioxidant ability is as follows: Pd complex > Zn complex > ligand). Bovine liver catalase (BLC) was selected to investigate its binding interactions with Zn(II) and Pd(II) complexes. In the presence of the both complexes, the catalytic activity of BLC decreased slightly and reached about 87% (for Pd complex) and 83% (for Zn complex) at a concentration of 10^{-6} M. The prepared complexes interacts with BLC and are able to quench its fluorescence emission through a static mechanism. The thermodynamic parameters (in agreement with the docking results) indicated that interactions of both complexes with BLC were exothermic and main binding forces involved in the interaction process were hydrogen bonds and van der Waals interactions. The docking results revealed the locations of the binding sites for Zn(II) and Pd(II) complexes on BLC (locating at a cavity among the wrapping domain, N-Terminal arm and β-barrel).

Keywords: Schiff Base Complexes; Catalase; Inhibitor; Interaction Mechanism; Antioxidant

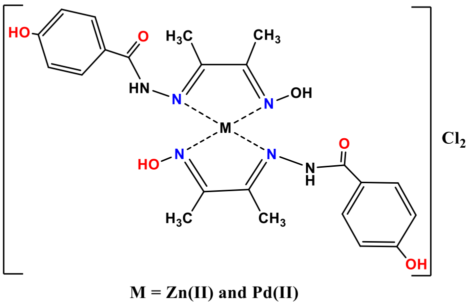

Fig. 1 Molecular structure of Schiff base complexes

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Fabrication of light-responsive CuO@COFs composite as photocatalyst for selective degradation of Fluoroquinolones

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A low-cost light-responsive CuO@COFs composite has been fabricated by a facile route. The designed photocatalyst has been investigated through various techniques, i.e. XRD, FTIR, SEM, and UV–vis diffuse reflectance. SEM images and FTIR spectra confirmed the growth of covalent organic frameworks (COFs) on the surface of CuO nanoneedles. The results from UV-Vis DRS showed that the COFs-modified CuO composite has a wider visible light response and smaller band gap compared to the pure phase CuO [1]. The visible light-driven photocatalytic degradation tests for various antibiotics showed that the designed composite has dramatically enhanced degradation efficiency in case of fluorquinolone type antibiotics during 90 min reaction time. The synergistic effects of light absorption of CuO crystals and the contact between COFs and CuO lead to high photocatalytic activity and selectivity of the designed nanocomposite [2].

Keywords: Copper Oxide, Photocatalysis, COFs, Nanocomposite, Dgradation.

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Mixed-ligand complexes with p-Toluic hydrazide derived Schiff base ligand and Glycine. Preparation, antioxidant study and interaction with catalase

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Efforts to produce antioxidants derived from metal complexes have greatly increased. Synthetic antioxidants have received more attention than natural antioxidants because they are cheaper and more effective.[1,2]. Bidentate Schiff bases (L) base on 2,3-butanedione monoxime and p-Toluic hydrazide and its complexes [M(L)(Gly)]Cl (M = Pd(II) and Zn(II) and Gly = Glycine) (Fig. 1) were synthesized. The prepared complexes thoroughly characterized by various techniques. The effects of the complexes on the catalytic function and structure of bovine liver catalase (BLC) were studied by spectroscopic and molecular docking methods. The results showed that Zn(II) and Pd(II) complexes inhibited catalase function by mixed-type inhibition. The prepared complexes quenches the intrinsic fluorescence of BLC via static quenching mechanism. The molecular docking simulation in the well coherent with kinetics results showed that there is one binding site for both complexes on BLC and these complexes did not directly bind to the catalase active site.

Keywords: Schiff Base; Catalase; p-Toluic hydrazide; Interaction Mechanism; Enzyme kinetics

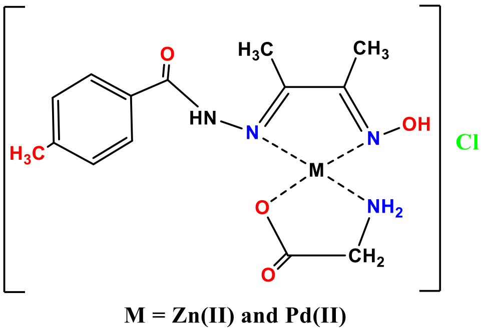

Fig. 1 Molecular structure of Mixed-ligand complexes

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UiO-67 and A-520 decorated with leaf extracts for targeted Doxorubicin delivery

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By exploring new knowledge of bionanotechnology, smart, accurate, and effective drug delivery systems are considered as one of the main goals. The development of drug delivery systems with the priority of green chemistry aspects is crucial to pursuing science and technology. Metal-Organic Frameworks (MOFs) are potential porous substrates for drug delivery systems and have been able to attract special attention due to their ability to load considerable percentages of drugs, provide smart diagnostic and therapeutic substrates, and rich host-guest chemical compositions, and slow diffusion[1,2]. However, the toxicity of coordinated-metals and their surface-based aggregations can greatly reduce their chances as a good candidate for clinical trials [3]. The use of leaf extracts as a coating in various stages of design and preparation of drug loaded nanocarriers can be considered a green and cost-effective solution. In this work, two MOFs, UiO-67 and A520 were used as the nanocarriers for the model drug, Doxorubicin (DOX), and coated with the mandarin extract. By preparing and comparing cytotoxicity data for MOF@Extract@DOX and MOF@Extract@DOX@Extract combinations, it was shown that green coatings at any stage can give a special function to the system including reduced toxicity, controlled drug release, and pH-sensitive release. The toxicity of the synthesized nanomaterials has been investigated by MTT on HEK-293, HeLa, MCF-7, and PC12 cell lines and showed more than 20% improvement in relative cell viability. The effectiveness of the synthesized nanocarriers have been investigated by treatment of the DAPI-stained cells with the drug loaded nanocarriers, and monitored by confocal laser scanning microscopy (CLSM) on the MCF-7 cell lines. All of the results showed sustained and slow-release of the drug from the porosity of the MOF, and also reduced toxicity and high biocompatibility towards different cell lines is another proof of using these kinds of porous nanomaterials as the next-generation chemical-modified carriers for biomedical applications.

Keywords: MOFs, Green Chemistry, Drug delivery, Interactions

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Investigation effect of synthesis variables of UiO-66 in Methylene blue adsorption

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Methylene blue is one of the cationic dyes that is widely used in industry and therefore can enter the environment as a pollutant [1]. Metal-Organic Frameworks (MOFs) are suitable candidates for absorbing pollutants and dyes due to their high surface-to-volume ratio [2]. UiO-66 is one of the popular MOFs with relative thermodynamic stability that has been reported by many applications in the industry [3]. Optimal synthesis conditions can increase the efficiency of structures in different applications. Here, the effect of different ratios of modulators and synthesis time and temperature was investigated [4]. It was shown that each of the variables could make a difference in the amount of methylene blue adsorption in the aqueous environment by affecting the structural properties. The relationship between adsorption graphs and properties created by different synthesis conditions, such as differences in crystallinity and particle size, indicates which of the porous material properties should be considered for each application. The slope of the adsorption diagram based on time is clearly related to the modulator to linker ratio. It was also shown that in a short time the system with high crystallinity acts like an amorphous system. Systematic studies of this kind can lead to a mechanistic view of the design and synthesis of MOFs.

Keywords: MOFs, UiO-66, Dye adsorbent, methylene blue

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Surveying the structure of modified Zeolite with Magnesium nitrate and Calcium Nitrate

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Zeolite is an active biomaterial with biocompatible, non-toxic, and high porosity properties [1,2]. In recent years, various groups have done a lot of research on applying and modifying of zeolite for different applications in different ways [3]. The aim of this study is to investigate the structure and morphology of modified zeolites with various metal salts, calcium and magnesium nitrate, to investigate the effect of these metal salts on morphology, crystalline structure, and size of zeolite pores. Samples were characterized by X-ray diffraction patterns (XRD), scanning electron microscope (SEM), and FT-IR spectra.

Keywords: Zeolite, Magnesium Nitrate, Calcium Nitrate, Biomaterial, Porosity properties

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Evaluation of alumina nanoparticles efficiency in removal of Reactive Red 141

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Dyes are usually present in trace quantities in the treated effluents of many industries. The discharge of large quantity of colored water from industries possesses serious environmental problems.Recently, the adsorpton of pollutants on the surface of adsorbent material has been intensively studied as a way to solve environmental problems [1,2]. In this study, alumina powder was used as an adsorbent for the removal of colore reactive red 141 from aqueous solution of wastewater. The studies were carried out under various experimental conditions such as: dye concentration, alumina percentage and absorbent contact time. The removal rate was monitoring by UV-vis spectroscopy. The results showed that as the amount of the adsorbent was increased, the percentage of dye removal increased accordingly. The alumina showed excellent elimination ability for the removal of Reactive Red 141 so that, 50 ppm of alumina can eliminate the reactive red 141 solution (6 ppm) up to 95% in 90 min. Alumina powder were characterized by X-ray diffraction patterns (XRD), scanning electron microscope (SEM) and FT-IR spectra.

Keywords: Alumina, Reactive Red 141, Elimination process, Industries, Pollutants

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Investigation of photocatalytic properties and band gap of cadmium and bismuth sulfides by experimental and computational (DFT) methods

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Herein, the novel visible light photocatalyst CdS/Bi_2S_3 were prepared by a facile solvothermal method. The structural, morphological, and optical studies have been carried out by using X-ray powder diffraction(XRD), FESEM, PL, UV-Vis techniques. Moreover, EDS and FTIR techniques have been used to obtain information about the elemental composition and functional groups associated with the synthesized nanoparticles. Theoretical calculations, based on density functional theory(DFT) and Experimental methods, have been performed to investigate Band Gap and Photocatalytic properties of chalcogenides (CdS, Bi_2S_3) [1,2]. The band gap value of Bi_2S_3 was about 1.3ev and for CdS was calculated approximately 2.4ev. The calculated Band Gaps were in good agreement with available experimental and theoretical results [1-3]. This study provides a new idea for the construction of novel and efficient heterogeneous photocatalysts, which benefits the practical application in environmental remediation.

Keywords: Cadmium sulfide, Bismuth sulfide, Photocatalytic properties, Density Functional Theory(DFT), Band Gap.

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Electrocatalytic Hydrogen Production with a Molecular Co(III) Complex

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Water splitting is one of the most effective ways to produce high-purity hydrogen and oxygen [1]. The most significant progress has been made in designing of the molecular catalysts for hydrogen production using earth-abundant transition metals as the catalyst. Cobalt complexes with polypyridyl ligands have received great interest because of their stability and electroactivity at both metal and ligand centers [2]. In this context, a Co(III) complex with the formula of $[CoL(X)(OH_2)]$, where L = N,N bis (pyridine-2-carboxamido) benzene dianion and X= N_3^-, has been synthesised and characterised by the CHN elemental analysis, IR, UV-Vis and X-ray powder diffraction techniques. The crystal structure determination of complex showed a dianionic ligand L providing N4 set is located in equatorial plane, and the two H_2O and N_3^- ligands occupy the two axial positions, leading to a distorted octahedral geometry around Co(III) center [3]. The electrocatalytic activity of this complex in water splitting reactions was investigated.. The results exhibit good electrocatalytic activity in hydrogen evolution reaction with a high TOF at neutral pH. Furthermore DFT computations provide further insights into the mechanisms, and explain the activities of the complex in H_2 production reaction. Our approach to synthesise effective and stable molecular catalyst with earth-abundant transition metal ions offers a simple way to design and fabricate molecular electrocatalysts for HER process.

Keywords: Water Splitting, Carboxamide, Co(III) Complexes.

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Synthesis and characterization of a new Pd(II) complex with piperidine ligand and it's interaction with CT-DNA

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Cancer is one of the greatest threats to human health, but fortunately with the development of anti-cancer drugs, cancer mortality rates have been somewhat controlled over the past thirty years. The first metal-based anticancer drug to be discovered was cisplatin, on which other anticancer drugs such as carboplatin and oxaliplatin were developed. Because cisplatin doses lead to side effects such as kidney and nerve disease, high blood pressure, nausea and vomiting, new approaches have been developed to address these side effects, one of the most important of which is the design of anticancer drugs. On other metals, especially palladium. Palladium complexes are very similar to platinum complexes in terms of coordination geometry and formation process. piperidine is a six-membered heterocyclic amine consisting of five methylene bridges and one amine bridge. Studies have shown that piperidine can exhibit biological properties including anti-cancer properties by acting on various cellular receptors [1-4]. In this study, a new Pd(II) complex with the formula cis-$[Pd(pip)_2Cl_2]$, in which pip is the piperidine ligand, was synthesized. This complex was characterized by FT-IR, UV-Vis and ^{1}H-NMR spectroscopies. The interaction of the synthesized complex with calf thymus DNA (CT-DNA) was studied by electronic absorption and competitive fluorescence titrations. In the electronic absorption spectroscopy, the apparent binding constant (K_{app}) values in the interaction of the studied Pd(II) complex with CT-DNA at 303 and 310 K were calculated to be 1.2×10^4 and 1.7×10^4 M^{-1}, respectively. Furthermore, the values of $L_{1/2}$ (the concentration of the Pd(II) complex at the midpoint transition of CT-DNA from nature to denature forms) were determined at these two temperatures to be 0.06 and 0.04 mM, respectively. In fluorescence spectroscopy, the binding constant (K_b) values in the interaction of the cis-$[Pd(pip)_2Cl_2]$ with CT-DNA were calculated to be 4.5×10^4, 1.7×10^5 and 6.1×10^5 M^{-1} at 298, 305 and 310 K, respectively. The number of binding sites (n) on DNA for this complex was found to be about 1. The results obtained from UV-Vis and fluorescence spectroscopic studies indicate strong interaction between the Pd(II) complex and CT-DNA groove binding. Using the results obtained from the fluorescence spectroscopy, the thermodynamic parameters $\Delta H°$, $\Delta S°$ and $\Delta G°$ in the interaction of the metal complex with DNA were also determined, which indicate spontaneous and hydrophobic interaction between the Pd(II) complex and DNA.

Keywords: Palladium(II) complex, Piperidine, DNA interaction, Thermodynamic parameters

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Copper and zinc complexes of curcumin-nicotinoyl chloride derivative: synthesis and characterization

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Curcumin is a natural product that can be used as drug for treatment of a wide variety of cancers such as breast, pancreas, lung and so on [1]. Also it can be used for non-medicinal applications. E.g. for detection of trace amounts of boron or use in the electrochemical modification of electrodes for oxidation reactions [2]. Unfortunately, curcumin is unstable and insoluble in water [3]. Two approaches to achieve more advantages is the use of metal curcumin complexes and structural modifications [4]. In this research, the structure of curcumin was modified by nicotinyl chloride hydrochloride. The produced derivative (Cur-Nic) was purified by chromatography column and characterized by several methods. Then this ligand was used to synthesis of copper (II) and zinc (II) complexes. To prevent the polymerization of the complexes, prior to the synthesis of these complexes, the copper and zinc coordination sites were locked (by H_2dipic as an observer ligand) except for one site to binding of Cur-Nic. Then the copper and zinc complexes, Cu(Dipic)$_2$Cur-Nic and Zn(Dipic)$_2$Cur-Nic were synthesized, purified, and characterized by IR, UV-Vis, NMR, and XRD methods. Solubility test showed that these complexes are not soluble in water and are not suitable for medicinal applications. However, these complexes can be used for non-medicinal applications.

Keywords: Curcumin, Water solubility, Non-medicinal applications

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Immobilization of bimetallic iron and nickel nanoparticles on nanosilica extracted from rice husk and their application as catalysts

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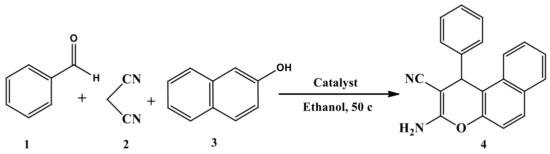
Use of agricultural wastes such as: rice husk, wheat bran, coconut husk, especially those containing silica, can be considered in the production of high value-added products as a potential adsorbent and cause extraordinary improvements in the synthesis of organic compounds [1]. The advantages of this type of waste include: environmentally friendly, renewable source, high availability and low cost, and can be considered as an option for the synthesis of catalysts [2]. First, nanosilica extracted from rice husk was prepared and then equipped with magnetic properties by fixing iron and nickel bimetallic nanoparticles on the silica surface. The synthesized compound was used as a recyclable magnetic catalyst in the three-component condensation reactions of 1-H-benzo [f] chromene. Easy separation of catalyst and products, efficiency and proper reaction time, mild conditions and reuse are some of the advantages of catalyst used. 1-H- Benzo [f] chromene and their derivatives are of particular importance due to their wide range of biological properties including antihypertensive, antispasmodic and anticancer activity [3]. In this work, 1-H-benzo [f] chromene derivatives 4 via a three-component condensation of aromatic aldehydes, malononitrile and b-naphthol were synthesized in the presence of Fe-Ni/RH-SiO_2 catalyst under optimal conditions with excellent efficiency. The resulting nanocomposite was studied by EDX, FESEM, TGA, FT-IR, VSM and XRD techniques.



Scheme 1. Synthesis of three-component reaction in the presence of catalyst

Keywords: Silica, Rice huck, Magnetic Nanoparticles, catalyst.

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Synthesis and characterization of TBA-PWFe @NiO@BNT nanocatalysts and investigation of its nanocomposite application in oxidative desulfurization

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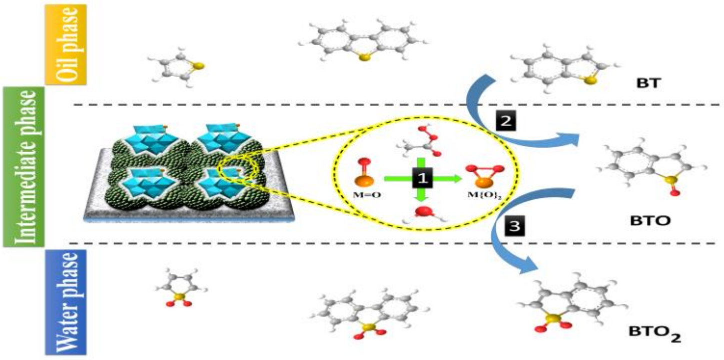
The sulfur oxides (SOx) emission from transportation fuel combustion is one of the serious environmental concerns [1]. That the oxidative desulfurization (ODS) process was proposed to reduce the sulphur-containing compounds in gas oil [2]. For this purpose, the TBA-PWFe@NiO@BNT nanocatalyst synthesized by the composition of quaternary ammonium salt of mono iron substituted phosphor tungstate, nickel oxide and bentonite clay via sol-gel method for the first time [3]. The catalytic activity of the catalyst was tested on ODS of real gas oil and model fuel using CH3COOH/H2O2 as oxidant at 60°C after 2 h, the removal efficiency of mercaptans and sulfur content of gas oil fuel could reach 97%; while the other properties of fuel remained unchanged. In the CODS system, the oxidation of sulfur-containing compounds is aided by the prior electrophilic attack of active oxygen of $M\{O\}_2$ on the electron pairs of sulfur atoms. Consequently, water-soluble sulfoxides (RSO) and sulfones (RSO_2) are produced, which can be easily removed by the polar extraction solvent such as acetonitrile to achieve deep desulfurization (Scheme 1). The prepared materials characterized by means of FT-IR, UV–vis, XRD, and SEM techniques.



Scheme 1: Schematic illustration of the proposed CODS mechanism of BT as a sulfur-containing compound

Keywords: Nanocomposite, Bentonite, Nickel oxide, Gas oil, Clean fuel, Desulphurization

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Preparation of WO_4/GO-IL magnetic nanoparticles as an efficient catalyst for the aerobic oxidation of alcohols

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Carbonyl compounds such as ketones and aldehydes are essential functional groups for chemical production in the laboratory and industry that are frequently prepared by oxidation of their corresponding alcohols or hydrocarbons [1]. In this investigation, an efficient novel heterogeneous catalytic system was designed and synthesized via immobilization of the tungstate ion on functionalized graphene oxide by magnetic ionic liquid. the configuration of WO4/GO-IL magnetic nanoparticles were characterized using Raman spectroscopy, X-ray diffraction, thermogravimetric analysis, electron microscopy transmission and scanning, and vibrating sample magnetometer. The generated catalyst's behavior was examined to aerobic oxidation reaction of primary and secondary benzylic alcohols. Utilizing air as an oxi- dant, operational simplicity, easy preparation, apt yielding, non-hazardous nature of the catalyst, and reusability are the essential advantages of this catalyst.

Keywords: Graphene, Tungstate, Magnetic Nanoparticle, Ionic liquid, Aerobic Oxidation

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Synthesis, Characterization and Antitumor Activity of New Cu(II) Mixed Ligand Coordination Polymers at Bulk-size and Nanopowders

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New cupper(II) mixed ligand coordination polymer at bulk and nanopowders $[Cu_3(\mu^3\text{-}BTCA)_2(Pyr)_3.3(H_2O)]_n$ [BDCA = Benzene 1,3,5-Tree Carboxylic Acid and Pyr = Pyridine], has been synthesized by the reaction of a mixture Cu(II) Acetate and BDCA in pyridine/water by simple Branched tube and sonochemical method. The nanopowders of CuO was prepared from the calcinations of the **NCP** at air atmosphere. The structure of the **CP** and **NCP** (**CP** = Coordination Polymers and **NCP** = Nano Coordination Polymers) were determined by X-ray crystallography, while nano-structural materials were characterized by X-ray powder diffraction (XRPD), Thermal Gravimetric Analysis (TGA) and Scanning Electron Microscopy (SEM) [1]. These binary complexes (**CP** and **NCP**) were tested in vitro as potential antitumor agents with Human Embryonic Kidney 293 cells. It was observed that the most stable NCP and CuO nanopowders exhibited a high antitumor activity respectively.

Keywords: Coordination Polymer; Nanopowders; Antitumor Activity; Cu(II)

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Biological Activity of Nano and Bulk Size Pb(II) Metal-Organic Frameworks, Branched-Tube and Sonochemical Assisted Synthesis

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New nanostructure lead(II) coordination polymer or MOFs $[Pb_5(\mu\text{-}L)_2]_n$ [L=4PCA=4-Pyridine Carboxylic Acid], has been synthesized by the reaction of a mixture lead(II) nitrate with 4PCA by Sonochemical method. Reaction conditions, such as temperature, time, concentration and initial reagents play important roles in the size, morphology and crystal growth of the final products. The PbO nanoparticles were prepared from the calcinations of the nanopowders of Nano-MOF at air atmosphere. The structure of the compound was determined by Single-Crystal X-ray crystallography, while nano-structural materials were characterized by X-ray powder diffraction (XRDP) and Scanning Electron Microscopy (SEM) [1]. Thermal stability of bulk and nano-sized particles of this Nano-Coordination-Polymer was studied and compared with each other. These CP, NCP and Lead(II) Oxide (LONPs) effects on the antibacterial activity *(against Staphylococcus epidermidis (Se) ATCC 14990, Bacillus subtilis (Bs) ATCC 6633, Bacillus cereus (Bc) ATCC 14579, Pseudomonas aeruginosa (Pa) ATCC 9027 and Escherichia coli (Ec) ATCC 25922 strains).*

Keywords: Nanopowder, Lead(II) Bromide, Lead(II) Oxide, Coordination Polymer.

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Synthesis of magnetically separable copper nanocatalyst and their application as an efficient catalyst for Sonogashira and Suzuki cross-coupling reactions

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A copper complex was immobilized on Schiff base modified magnetic $Fe_3O_4@SiO_2$ nanoparticles by covalent linkage. The obtained nanoparticles were identified with various characterization methods. The nanocatalyst shows good activity toward Sonogashira and Suzuki cross-coupling reaction in environmentally friendly solvent (H_2O/DMF) under mild conditions [1]. The catalyst shows not only high catalytic activity, but also offers many practical advantages such recyclability and air stability. Expectedly, the nanocatalyst can be applied in large-scale industrial synthesis. The SEM micrographs of the products Fe_3O_4 and nanocatalyst are given in Fig. 1(a) and Fig. 1(b) respectively. It was found that the nanoparticles were present as uniform particles with spherical morphology. SEM images reveal that Fe_3O_4 particles are aggregated particles having rough external surfaces (Fig. 1(a)) [2]. Silica coating makes the particles exhibit smooth and spongy surfaces (Fig. 1(b)) which indicatives the successful coating of silica over the magnetic nanoparticles. However, the nanocatalyst particles still fall in the nano-size range.

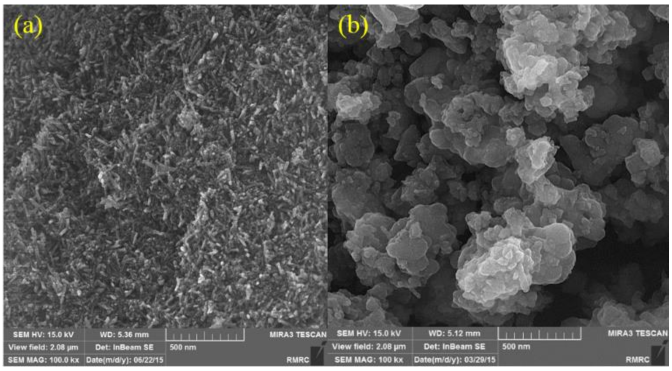

Fig. 1(a) SEM images of Fe_3O_4 and (b) nanocatalyst

***Keywords**:* nanocatalyst, magnetic $Fe_3O_4@SiO_2$ nanoparticles

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Magnetically separable nanocatalyst for selective oxidation of sulfides to sulfoxides

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A molybdenum complex, [$MoO_2Cl_2(DMSO)_2$], was immobilized on Schiff base magnetic $Fe_3O_4@SiO_2$ nanoparticles by covalent linkage. First, superparamagnetic Fe_3O_4 nanoparticles were prepared by the coprecipitation method [1]. Secondly, the surface of Fe_3O_4 was encapsulated with silica in order to increase the functionality and stability of nanoparticles. Then, the Fe_3O_4 nanoparticles were surface-modified with 3-aminopropyltriethoxysilane (APTS) which introduced -NH_2 on to the surface of support [2]. After functionalization by APTS, free amino groups on the surface can react with many different carbonyl compounds to form Schiff base ligand. For preparation of $Fe_3O_4@SiO_2$/Schiff base, $Fe_3O_4@SiO_2$-NH_2 nanoparticles were reacted with dialdehyde and then reacted with the $MoO_2Cl_2(DMSO)_2$ complex to synthesize Mo(VI) nanocatalyst. The resulting nanocatalyst are used as an efficient and recyclable catalyst for the selective oxidation of sulfides to corresponding sulfoxides using urea hydrogen peroxide as the oxidant. The characterization of catalyst was carried out by means of TGA, SEM, TEM, VSM, elemental analysis, FT-IR and Raman microprobe techniques.

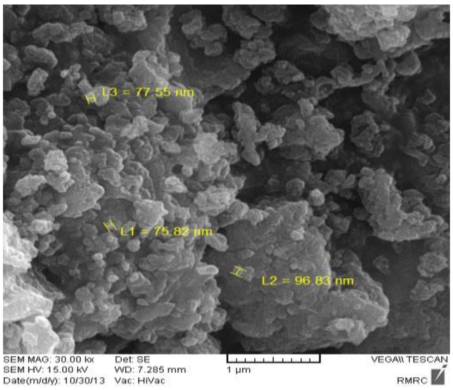

Fig. 1. SEM images of Mo(VI) nanocatalyst

Keywords: nanocatalyst, oxidation of sulfides

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4'-(4-chlorophenyl)-2,2':6',2"-terpyridine based Lead(II) complex: synthesis, crystal structure, and spectroscopic studies

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Since nanomaterials have a high percentage of atoms in unit area, a high ratio of particle volume to unit volume, and proximity of grain sizes with the size of atoms, they possess some specific properties, such as strength, high density, high chemical reactivity, and noticeable electrical and magnetic properties. Multidentate ligands containing heterocycle rings with nitrogen donors cover a wide area of coordination chemistry [1]. In addition to applicability and economic importance, studying coordination compounds plays a significant role in understanding chemical bonding, inorganic chemistry rules, and intermolecular forces [2]. 4'-(4-chlorophenyl)-2, 2':6', 2"-terpyridine (CPTP) ligand and other derivatives of terpyridine are among ligands that are widely applied in drug design, the chemistry of materials, and optical sensors [3]. In this study, we report the syntheses of the Pb(II) complex of 4'-(4-chlorophenyl)-2,2':6',2"-terpyridine with KSCN anion. $[Pb(CPTP)(SCN)_2]$ complex (CPTP=4'-(4-chlorophenyl)-2,2':6',2"-terpyridine) was synthesized using the side-branched tube method in bulk and hydrothermal treatment at the nanoscale, in presence of acid oleic surface-active material. Data obtained for the synthesis complex are in good agreement with its bulk properties and the formation of the synthesis complex is confirmed by scanning electron microscopy (SEM) and X-ray diffraction (XRD) techniques. the single-crystal X-ray analyses for complex $[Pb(CPTP)(SCN)_2]$ revealed that the coordination number in $[Pb(CPTP)(SCN)_2]$ complex is five and the complex structure is almost trigonal bipyramidal. this complex has been characterized by FT-IR spectroscopy, ^{1}H-NMR, and structurally analyzed by X-ray single-crystal diffraction.

Keywords: Lead(II) complex, Terpyridine, X-ray crystal structure.

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Selective and mild oxidation of sulfides and synthesis of various tetrazole derivatives catalyzed by Ni(II)-Schiff base complex immobilized into threedimensional mesoporous silica KIT-6

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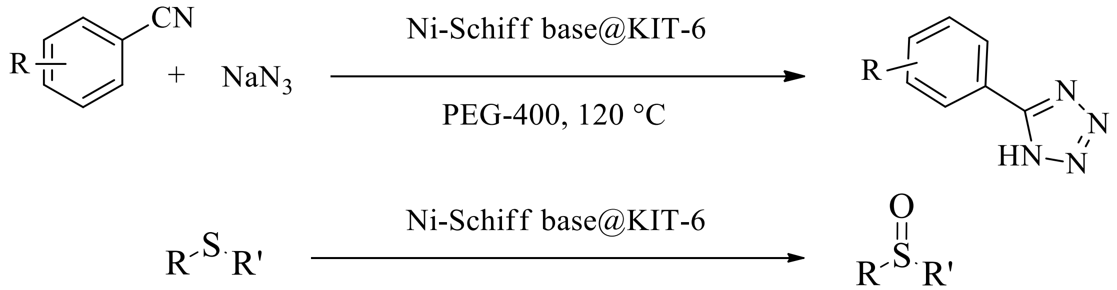
KIT-6 is a relatively new structure of mesoporous silica with thick expanded walls, thermal stable, open porosity and very accessible to guest species and metal complexes. Mesoporous KIT-6 exhibited wide range of application in various fields including catalysis, ion exchange, surface adsorption, and fabrication of applicable materials [1]. KIT-6 has symmetrical three-dimensional cubic structure with a network of intrusive channels, which make a lot of vacant space to accept guest species [2]. Therefore, due to the mentioned unique properties of mesoporous KIT-6, it can be used as a substrate for the synthesis of heterogeneous catalysts. In the present work, mesoporous KIT-6 were synthesized by pluronic surfactant P123 as a structure-guiding agent and conventional butanol as an auxiliary solvent in an acidic environment. The synthesized KIT-6 was then modified by 3-chloropropyltrimethoxysilane (CPTMS) and finally, a Schiff base complex of nickel was fixed on the modified mesoporous KIT-6 (Ni-Schiff base@KIT-6). The obtained catalyst was identified by IR, BET, XRD, EDS, SEM and TGA methods and was investigated in the selective oxidation of sulfide and synthesis of various tetrazole derivatives. All products were obtained with high purity which indicates the high catalytic activity of this catalyst.

Keywords: Mesoporous KIT-6, Heterogeneous Catalyst, Selective Oxidation of Sulfide, Tetrazole.



Scheme 1. Catalytic application of Ni-Schiff base@KIT-6 in the synthesis of tetrazoles and selective oxidation of sulfides

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Synthesis and characterization of a copper Schiff-base complex fixed on the mesoporous KIT-6 as a new catalyst for organic reactions

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Regular mesoporous compounds are a group of materials that have regular porosity in the range of 2-50 nanometer. Among them, silica mesoporous materials are the most considered by researchers and have wide applications, especially in the field of adsorbents and catalysts. Recently, block copolymers have been used to synthesize large mesoporous silica materials that exhibit Ia3d cubic symmetry [1-3]. KIT-6 is a three-dimensional symmetrical structure with a network of interconnected transverse channels. It has cavities with easy interchangeability, thick wall, high thermal stability, specific surface area and high cavity volume. Due to the three-dimensional structure of these materials between the cavities and the mentioned properties, it is expected that these compounds are better catalyst support than the other cavities compounds. In this project, Mesoporus KIT-6 is used as a mesoporous substrate fore perparation of heterogeneous catalysts. The synthesized mesoporus is first modified and then a copper- Schiffbase complex was stabilized on modified KIT-6. The prepared catalyst (Cu-Schiff base@KIT-6) was characterized by X-ray diffraction (XRD), scanning electron microscopy (SEM), X-ray energy distribution analysis (EDX) as well as Fourier transform infrared spectroscopy (FT-IR). The catalytic activity of Cu-Schiff base@KIT-6 was investigated in some organic reactions such as synthesis of tetrazoles. Because, tetrazoles were used in drugs and they are used as analgesics, herbicides, antimicrobial, anti-proliferative, anti-inflammatory, and anticancer agents [4-6].

Keywords: Mesoporous KIT-6, Heterogeneous Catalyst, Organic Reactions, Tetrazole

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Synthesis of KIT-6@SMTU@Ni as a novel, reusable and highly efficient nanocatalyst for the synthesis of 5-substituted 1H-tetrazoles and pyranopyrazole derivatives

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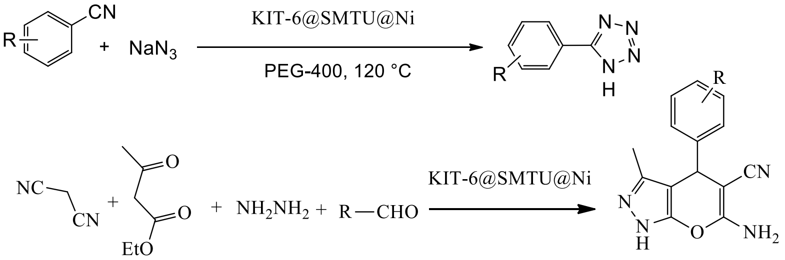
In the present study, KIT-6@SMTU@Ni was successfully synthesized using stabilization of a new Ni complex on mesoporous KIT-6 as a novel and green heterogeneous catalyst. The obtained KIT-6@SMTU@Ni catalyst was characterized by FT-IR, BET, SEM, XRD, AAS, EDS and TGA techniques. After full characterization, KIT-6@SMTU@Ni catalyst was successfully investigated in the synthesis of 5-substituted tetrazoles and pyranopyrazoles. Tetrazoles were synthesized from [3 + 2] cycloaddition of sodium azide (NaN_3) to the corresponding nitriles. Also pyranopyrazoles were prepared by the condensation reaction of benzaldehyde derivatives with malononitrile, hydrazine hydrate and ethyl acetoacetate. Because, tetrazole derivatives have been used as antiviral, anti-proliferative, anti-inflammatory, antibacterial, antifungal and anticancer agents [1-3]. Also, pyranopyrazoles composed of pyrazole and pyran rings, including significant biological activity such as anticancer, antimicrobial, anti-inflammatory, CHK-1 kinase inhibitor, and anti-viral [4-6]. Use of green medium, simple method, easy separation and workup, excellent reusability of the nanocatalyst, short reaction times, and high yields are outstanding advantages of these methodologies. Moreover, this catalyst can be easily recovered from the reaction mixture by simple filtration and reused for several consecutive cycles without noticeable change in its catalytic activity.

Keywords: Mesoporous KIT-6, heterogeneous catalyst, tetrazoles, pyranopyraoles.



Scheme 1. Catalytic application of KIT-6@SMTU@Ni in the synthesis of tetrazoles and pyranopyrazoles

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Homoselective synthesis of tetrazole derivatives using copper complex stabilized on mesoporous KIT-6 as a reusable and highly efficient nanocatalyst

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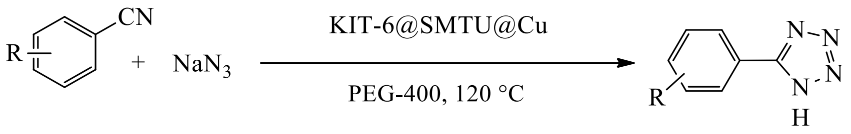
In this work, a novel heterogeneous catalyst of Cu(II) complex on modified mesoporous KIT-6 (KIT-6@DABP@Cu) was prepared via simple and inexpensive procedure using commercially available materials. The prepared catalyst was characterized by FT-IR, XRD, TGA, AAS, SEM, EDX and BET techniques. 5-Substituted tetrazoles were synthesized using nitriles and sodium azide in the presence of KIT-6@DABP@Cu catalyst in PEG as green solvent. Because, tetrazoles were used in drugs and they are used as analgesics, herbicides, antimicrobial, anti-proliferative, anti-inflammatory, and anticancer agents [1-3]. For example, Valsartan, Losartan, Candesartan and TAK-456 are several pharmacologically important of tetrazoles [4-6]. Ease of operation, high efficiency, eco-friendly procedure, easy separation and reusability of this catalyst are several advantages of this procedure. This catalyst can be recovered and reused for several consecutive runs without significant loss of its catalytic efficiency or copper leaching.

Keywords: Mesoporous KIT-6, copper, tetrazoles, heterogeneous catalyst.



Scheme 1. Catalytic application of KIT-6@SMTU@Ni in the synthesis of tetrazoles and pyranopyrazoles.

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A new Schiff base complex of neodymium stabilized on boehmite nanoparticles as an environmentally friendly nanocatalyst in the homoselective synthesis of tetrazoles

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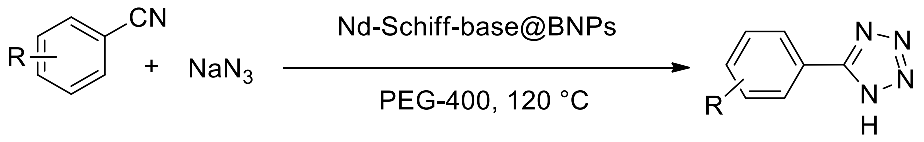
Boehmite nanoparticles are aluminum oxide hydroxide containing hydroxyl groups attached to their surface, which can synthesized by a simple procedure in water using commercially available materials [1-3]. In this study, boehmite nanoparticles (BNPs) were prepared using aqueous solution of NaOH and $Al(NO_3)_3.9H_2O$ at room temperature. After modification of BNPs surface by 3-choloropropyltrimtoxysilane (CPTMS) accorrding to repported procedure [4], synthesized Schiff-base ligand was anchored on the surface of modified BNPs. Finally, a complex of neodymium was stabilized on its surface (Nd-Schiff-base@BNPs) as a novel catalyst in the organic reactins. This catalyst was carachterized by TGA, BET, SEM, EDS, WDX, and XRD techniques. Then, the catalytic activity of Nd-Schiff-base@BNPs was investigated in the homoselective synthesis of tetrazole derivatives. Selectivity in organic chemistry is important from both green chemistry and industrial [5,6]. Therefore, homoselectivity of Nd-Schiff-base@BNPs was confirmed in the synthesis of 5-substituted tetrazoles *via* [3+2] cycloaddition of NaN_3 to the phthalonitrile and terephthalonitrile. Nd-Schiff-base@BNPs can be recovered and reused for several tims without significant loss of its catalytic activity. Besides, tetrazole products were obtained in exellent yields in the presence of Nd-Schiff-base@BNPs which revealed the practically and efficiency of this catalyst.

Keywords: boehmite nanoparticles; homoselective catalyst; neodymium; tetrazoles; Schiff-base



Scheme 1. Synthesis of tetrazole derivatives in the presence of Nd-Schiff-base@BNPs catalyst.

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Synthesis and characterization of a new single crystal of cadmium using N,N'-bis(2-aminoethyl)ethane-1,2-diamine as a ligand in coordination chemistry

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The centrosymmetric dinuclear cadmium title complex, $[Cd_2(C_6H_{18}N_4)_3](ClO_4)_4$, was obtained by the reaction of N,N'-bis(2-aminoethyl)ethane-1,2-diamine (trien) with $Cd(NO_3)_2.4H_2O$ and sodium perchlorate in methanol. The Cd^{II} cation is coordinated by four nitrogen atoms of a non-bridging trien ligand and by two nitrogen atoms of a bridging trien ligand in a slightly distorted octahedral coordination geometry, with a substantial departure from an ideal octahedral geometry [cisoid angles: 73.97 (8)–114.67 (9)°; transoid angles: 141.95 (1)–159.20 (6)°]. The bridging ligand shares another two N atoms with a neighboring symmetry-equivalent Cd^{II} cation. The structure displays C—H…O and N—H…O hydrogen bonding. The perchlorate anion is disordered over two sets of sites in a 0.854 (7): 0.146 (7) ratio. The distance between the two cadmium(II) centers of the dinuclear complex is 7.735 Å, which is longer than the corresponding distance in dinickel(II) complex (7.497 Å) of the same ligand (Cai et al. 2001b) due to larger radius of cadmium. Cadmium atoms in the dinuclear complex are related by a 2 fold symmetry operation. Bond distance of Cd-N(trien) are in the range of 2.62 (3)- 2.90 (3) Å. The structure exhibits disorder of one of the perchlorate anions in two positions with refined occupancy 0.854 (7) and 0.146 (7) for the major and minor componet,respectively. The disorder was described using the rigid body approach. In the title complex the C-H···O and N-H···O hydrogen bonds have been found between the amine nitrogen/carbon donors and perchlorate acceptors. All hydrogen atoms were discernible in difference Fourier maps and could be refined to reasonable geometry. According to common practice H atoms bonded to C were kept in ideal positions with C–H = 0.96 Å while positions of other H atoms were refined freely. In both cases $U_{iso}(H)$ was set to 1.2 $U_{eq}(C,N)$. Disorder of perchlorate anion was refined using rigid body refinement, with occupancy ratio 0.85:0.15 [1-3] .

Keywords: Coordination chemistry; Cadmium complex; crystal structure.

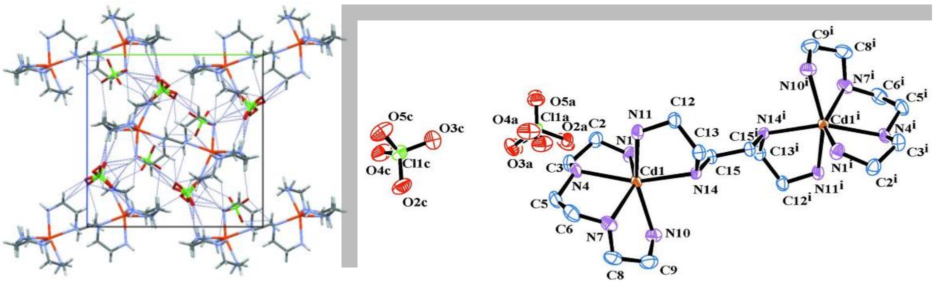

Figure 1. The molecular structure of the cadmium title complex.

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A complex of copper on magnetic MCM-41 nanoparticles: Preparation, characterization, and catalytic activity in the synthesis of tetrazole derivatives

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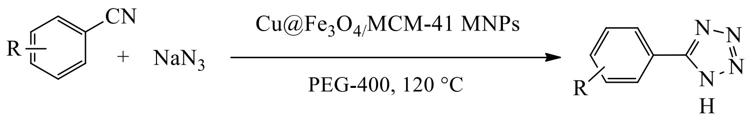
Magnetic nanoparticles (MNPs) and mesoporous materials are two important kinds of heterogeneous support in the synthesis of reusable catalysts [1,2]. MNPs have unique features such as easy functionalization, nontoxicity, and especially facile removing with assistance of an external magnet [3-5]. However, the major disadvantages of MNPs are low surface area and low stability. On the other hand, mesoporous materials have unique properties such as considerable stability, high specific surface area, and large and uniform pore size [6]. However, the major disadvantages of mesoporous materials are time consuming, difficulty, and expensive conventional work-up procedures. In order to combine advantages of both magnetic nanoparticles and mesoporous materials, magnetic MCM-41 nanoparticles (Fe_3O_4/MCM-41 MNPs) were synthesized in this work. Fe_3O_4/MCM-41 MNPs has a large surface area, and also can be recovered using an external magnet. Therefore, Fe_3O_4/MCM-41 MNPs can be considered as ideal support for the synthesis of reusable catalysts. In this regards, we repport a new complex of copper on Fe_3O_4/MCM-41 MNPs as efficient and reusable nanocatalyst (Cu@Fe_3O_4/MCM-41 MNPs) in the selective synthesis of tetrazole derivatives. Because, tetrazoles are an important class of heterocycle compounds with various applications in coordination chemistry, in medicinal chemistry, in catalysis science, in organometallic chemistry, in material chemistry, and in agriculture [7].

Keywords: mesoporous MCM-41, magnetic nanoparticles, copper, tetrazoles.



Scheme 1. Catalytic application of Cu@Fe_3O_4/MCM-41 MNPs in the synthesis of tetrazoles

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lead and cadmium uptake by Hibiscus tea residue as bio-adsorbent

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The most important environmental problems are heavy soil contamination of agricultural soils, and since agricultural products are directly linked to food hygiene, human health has faced serious challenges [1]. The metal biosorption is the removal of metal ions by inactive, nonliving biomass due to highly attractive forces present between them [2]. Heavy metals in agricultural soils such as lead and cadmium are not degradable in the ecosystem and pose a risk to human health due to their high toxin content [3]. The aim of this study was to investigate the capasity of Hibiscus tea residue as food waste bio-absorption in reducing the amount of heavy metals lead and cadmium in agricultural lands. The mint plant planted in five pots with the same conditions in the presence and absence of the adsorbent with a weight percentage of 0.5, 1, 3 and 5 has been investigated. The content of heavy metals in the samples of mint plant and pot soil in the presence and absence of Hibiscus tea residue in 30 days after the increase of this biological adsorbent to the soil, according to its different concentrations and the content of metals studied with the atomic absorption spectrophotometer was measured. The results showed that the amount of lead and cadmium in untreated samples was much higher than WHO standards, while the treatment of samples with biological adsorption had a significant absorption in heavy metals lead and cadmium ($P<0/05$). Based on the results obtained, it is recommended to use inexpensive and accessible bio-absorbers such as Hibiscus tea residue in removing heavy metals from contaminated soils where vegetables grow.

Keywords: heavy matal, Lead, Cadmium, Hibiscus tea residue

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Copper complex immobilized on SBA-15: as practical, reusable and selective nanocatalysts for the synthesis of tetrazoles

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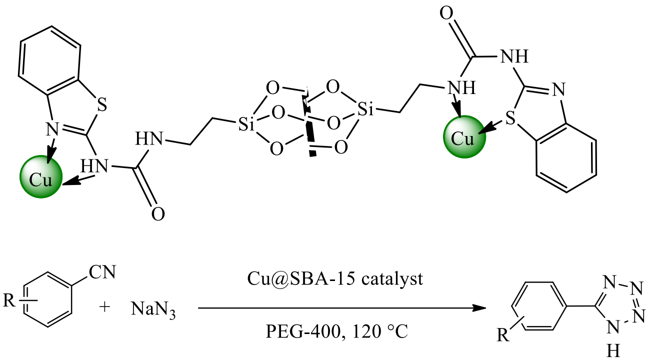
Tetrazoles have found use in various sciences, including photography and information recording systems [1,2]. Conventional procedure for synthesis of 5-substituted 1H–tetrazoles is [3 + 2] cycloaddition of azides to the corresponding nitriles. Based on this method, several methode have been reported [3, 4]. In this work, a green method is reported for homoselective synthesis of biologically active tetrazole derivatives in the presence of Cu@SBA-15 catalyst. The tetrazole derivatives was performed in green solvents in the presence of this catalyst. All products were obtained in high turnover frequency numbers and good yields in the presence of this catalyst, which revelved the high efficiency and catalytic activity of this catalyst. Cu@SBA-15 catalyst was characterized by BET, XRD, TGA, FT-IR, SEM, EDS, WDX, and AAS. This catalyst can be recovered and reused for several runs without significant change in its catalytic activity.

Keywords: SBA-15, reusable catalyst, copper, tetrazoles.



Scheme 1. Catalytic application of Cu@SBA-15 catalyst in the synthesis of tetrazoles

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Theoretical study on the dynamics of the reaction of CO($^1\Sigma^+$) with OH($^2\Pi$)

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We used stochastic one-dimensional chemical master equation (CME) simulation to gain insight into the dynamics of the reaction of CO($^1\Sigma^+$) with OH($^2\Pi$). The reaction takes place over a multiwell, multichannel potential energy surface that is based on the computations at the CCSD(T)/aug-cc-pVTZ//M11+GD3/6-311G** level of theory. The calculated multipath potential energy surface consists of three potential wells and two van der Waals complexes. In solving the master equation, the Lennard-Jones potential is used to model the collision between the collider gases. The fractional population of different intermediates and products in the early stages of the reaction is examined to determine the role of the energized intermediates and van der Waals complexes on the kinetics of the title reaction (Figure 1). The major products of the title reaction are CO_2 and H. The temperature dependence of the reaction over a wide range of temperature (200−2000 K) is studied. The calculated rate constants from the CME simulation [1] are compared with those obtained from the RRKM-SSA method [2] that is based on strong collision assumption. Our results indicate that the strong collision assumption increases the calculated rate constant for the formation of the main products (CO_2 + H) by a factor of 2 at 300 K and 1 atm pressure, compared to the results of CME simulation, although the results are in good agreement at higher temperatures.

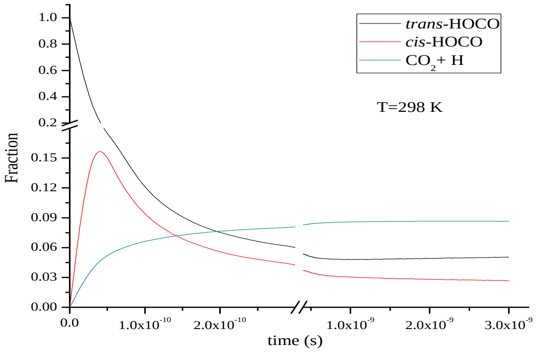

Fig. 1. The population fraction of the different species as a function of time.

Keywords: Atmospheric chemistry, Reaction kinetics, Chemical master Equation, Multichannel multiwell reaction

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A theoretical study on the dynamics of C(^3P_j) + H$_2$S($^1A_1$) Reaction on an interpolated potential energy surface

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The C + H$_2$S reaction is believed to play a key role in combustion and interstellar chemistry, particularly in cold and dense clouds. Quasi-classical trajectory calculations (QCT) are performed to to gain insight into the dynamics of the reaction between ground state carbon atoms, C(^3P_j), and hydrogen sulfide, H$_2$S(X^1A_1). The global potential energy surface has been constructed by interpolation technique following the method introduced by Collins [1] at high *ab initio* CCSD(T)/aug-cc-pVTZ level of theory. In the peresent study, the interpolated PES was grown from 40 initial set of data points up to 1500 set of data points. At periodical intervals through the itiration procedure to grow the initial PES, large scale clasical trajectory simulations are performed to estimate reaction cross section and other obsevable prpperties, based on the current data set. The PES is taken to be converged when the calculated cross sections do not change significantly with an increase in the number of data points. The reaction probabilities, total and individual classical reactive cross sections are calculated at collision energies from 2.6 kJ mol^{-1} to 78.8 kJ mol^{-1}. The total reactive cross section for the reaction is shown in Figure 1. These data are used to calculate the total rate constant for the title reaction by means of collision theory [2].

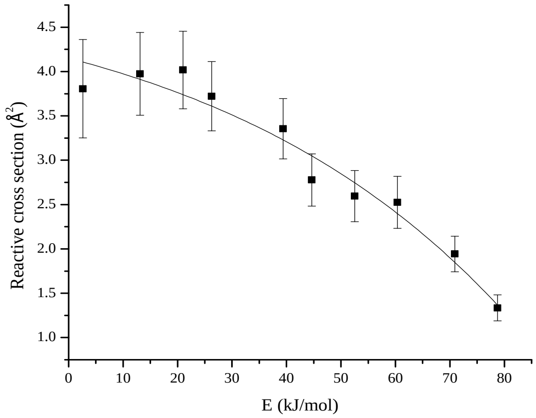

Fig. 1. Calculated reactive cross sections of the reaction as a function of initial collision energy. The error bars represent two standard deviations.

Keywords: Combustion chemistry, Collision theory, Potential energy surface, Reaction dynamics

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Investigation of Self-Association phenomena of Oxazine 720 in Aqueous Fructose solutions

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Oxazine dyes are a significant group of organic substances with special photophysical properties which make them suitable for many technological applications such as using in various optical and photonic devices as well as in fluorescent sensors, organic photoconductors/photodetectors, artificial light harvesters and organic transistors [1]. Nowadays the molecular association of these dyes in different solutions as a result of the attractive electrostatic forces is a well-known phenomenon [2]. The power of the aggregations depends on several factors like the dye concentration and structure, solvent environment, temperature, and pressure. The presence of the molecular associations in the dye solutions can noticeably affect their photophysical behavior; For example, the self-association in the dye molecules can cause a decline in emission quantum yield and life time of the first singlet excited state of the dye, and lower laser efficiency as a result [3].

The presence of additives in the dye solutions can change the properties of them due to the water-additive and dye-additive interactions. Molecular organic additives with various concentrations have many applications in science and technology, so it is very important to take their properties into consideration [4]. In this study, the aggregation behavior of oxazine 720 is investigated in the presence of fructose (which is a monosaccharide (carbohydrate)) as a neutral additive, using the UV-Vis absorption spectral data.

Keywords: Aggregation, Oxazine dyes, Fructose, UV-Vis absorption spectra.

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The DFT, AIM, NLO study of Sulfacetammide drug interaction with C24 nanocage

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Since after discovery of fullerene (C60) in 1985, various efforts were made on other fullerenes derivatives, including C20, C24, C30, C70, due to their unique physicochemical properties and potential applications as electronic, optic and magnetic materials [1–2]. Fullerene C24 represents one of the most active classes of nanostructures, and it has been used as an active material for important applications such as adsorbent or detector of toxic gas and drug delivery [3–4]. In the current work, we decide to investigate the interaction and adsorption of Sulfacetammide (SUL) drug on the surface C24 nanocage. For this aim, we consider different positions for adsorbing drug on the surface of nanocage and after optimizing all structures, the stable structures are selected. The selected structures are optimized at WB97XD/6-31G (d, P) level of DFT theory. From optimized structures the thermodynamic parameters, quantum parameters involve HOMO and LUMO orbital and gap energy, nonlinear optical (NLO) such as polarizability and hyperpolarizibility parameters, Uv-visible transition state and, atom in molecule (AIM) parameters are calculated and results are analyzed. The calculated results indicate that the adsorption of Sulfacetammide drug on the surface of C24 nanocage is favourable in view of thermodynamic approach. So the C24 nanocage can be used as delivery of SUL drug in the biological systems. On the other hand, the AIM results demonstrate that the adsorption of drug on the surface of nanocage is covalence bonding type. The NLO results reveal that the first polarizability and hyperpolarizibility values of SUL&C24 complex alter slightly from original state and the optical properties of system are almost unchanged. Moreover, the electrical properties of system change significantly from original state and this result confirm that the C24 nanocage is a good candidate to detect of SUL in biological system.

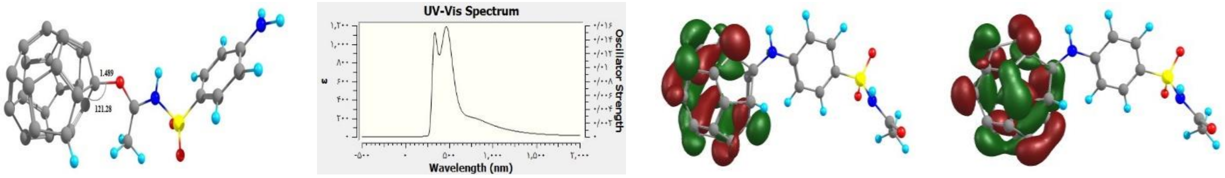

Fig. 1. The HOMO-LUMO, Uv-visible and opted structure of Sulfacetammide on the C24

Keywords: C24 nanocage, NLO, DFT, AIM, Sulfacetammide drug

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The interaction of 5 Flucytosine drug with $B_{12}N_{12}$ nanocage: A DFT, TD-DFT study

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5Flucytosine (5-FC) is an antifungal medication. It is specifically used, together with amphotericin B, for serious candida infections and cryptococcosis. It may be used by itself or with other antifungals for chromomycosis. 5FC is used by mouth and by injection into a vein [1–2]. Boron nitride ($B_{12}N_{12}$) nanocage materials with a bandgap energy of 6 eV and non-magnetism are also expected to show various electronic, optical and magnetic properties such as coulomb blockade, photoluminescence, and supermagnetism [3]. The $B_{12}N_{12}$ nanocage has been used as electronic devices, high heat-resistance semiconductors, nanocables, insulator lubricants and gas storage materials[4–5]. In this work, we decided to investigate the adsorption of 5-FC on the surface of $B_{12}N_{12}$ at different sites. The electrical, quantum parameters, thermodynanic and solvent effect parameters, UV-visible spectrum, natural bond orbital (NBO), atom in molecule (AIM) properties are calculated at cam-B3LYP/6-31G(d,p) level of theory and results are analyzied. The calculated results indicate that adsorption of 5-FC on the surface $B_{12}N_{12}$ is exothermic and spontaneous in thermodynamic approach. It is notable that in presence of ethanol solvent the adsorption of 5-FC is weak, and this property is sutible for making drug delivery in biological system. The results of electrostatic localaized field (ELF), HOMO-LUMO, PDOS and TD-DFT demonstrate that the electical properties, coductivity and reactivity of system alters significantly from original state(see Fig 1), and also the interaction drug with nanocage is electrostatic type. The calculated results confirm that $B_{12}N_{12}$ nanocage is sutiable candidate to making sensivitve sensors for 5-FC drug.

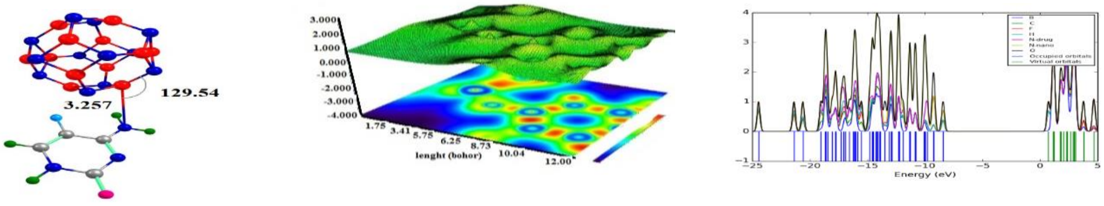

Fig. 1. The optimized, ELF and PDOS plots of 5FC adsorption on the $B_{12}N_{12}$ nanocage

Keywords: *$B_{12}N_{12}$, Solvent effect, Flucytosine, DFT, TD-DFT*

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Thermodynamic Properties of Ternary Thiophene + Ionic liquid + Hexane or Cyclohexane Solutions at 298.15 K

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The largest source of sulfur dioxide emissions comes from fuel combustion of sulfur-containing hydrocarbons to cause air pollution and acidic rain [1-2]. Therefore, the standards for reducing sulfur content in fuels has been set, which is expressed as the amount of gasoline and diesel that must be less than 10 ppm [3-4]. Thus, recently, aromatic sulfur compounds like thiophene are eliminated with non-HDS technologies such extractive desulfurization using ILs [5]. There is need to systematic study of the nature and their manner interactions of ionic liquids with systems consist of sulfur such as thiophene. The thermodynamic and thermophysical properties clarify the type and amount of solute-solute and solute-solvent interactions present in the systems studied and the proper ionic liquid to separation of thiophene from the fuels.

Therefore, effect of four ILs based on 1-buthyl-3-methylimidazolium cation with different anions, Cl^-, $[PF_6]^-$, $[BF_4]^-$, and Br^- on the thermodynamic properties of thiophene in hexane or cyclohexane solutions have been investigated. For this purpose densities, speeds of sound, and refractive indices of investigated solutions have been measured at T = 298.15 K and atmospheric pressure. These data have been used to calculate the standard partial molar volumes (V_φ^{o}), transfer partial molar volumes ($\Delta_{tr}V_\varphi^{\mathrm{o}}$), apparent molar isentropic compressibility (κ_φ), and molar refractions (R_D) for the solutions being studied. A comparison of the calculated thermodynamic properties for the investigated solutions indicates that the (V_φ^{o}) of thiophene for the solutions containing $[PF_6]^-$ and $[BF_4]^-$ anions are larger than those of the $[Cl]^-$ and $[Br]^-$ systems, respectively. These results are due to the larger sizes of the $[PF_6]^-$ and $[BF_4]^-$ anions compare to $[Cl]^-$ and $[Br]^-$ anions and subsequently attribute to the stronger IL-thiophene interactions. The isentropic compressibility and the apparent molar compressibility values increase when the anion size gets larger. Therefore, the interaction of $[PF_6]^-$ and $[BF_4]^-$ with thiophene are stronger than $[Cl]^-$ and $[Br]^-$ respectively, and the interaction between thiophene and cyclohexane, and thiophene and *n*-hexane are further weakened by $[PF_6]^-$ and $[BF_4]^-$ anions.

Keywords**:** Thiophene, Ionic liquid, Apparent molar volume, Refractive index, Solute-solvent interactions

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Molecular Interaction Studies of Volumetric Properties in Ternary Mixtures of Thiophene + Toluene / *n*-Hexane + Ionic liquid ([EMIM]EtSO$_4$ / [HMIM]Br / [BMIM]PF$_6$ / [MMIM]MeSO$_4$) at 298.15 K.

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The increasing use of the fuels containing sulfur in the industry and in the transport sector leads to the pollution of the environment [1]. A high content of sulfur compounds, i.e., thiophene, release sulfur oxides (SO$_x$) to the atmosphere [2]. This environmental issue caused that the EU and US legislation set the upper limit of sulfur content in diesel fuel to (10 and 15).10^6., respectively [3]. From an emission, economic, and efficiency point of view, the removal of thiophene is difficult because of catalyst surface interactions and stereo hindrance [4]. One of the most promising alternatives is the extractive desulfurization (EDS), where S-compounds remove through direct extraction by ionic liquids.

Thus, in this work, 1-Ethyl-3-methylimidazolium ethylsulfate ([EMIM]EtSO$_4$, 0.0999,0.4999 mol.kg^{-1}), 1-hexyl-3-methylimidazolium bromide ([HMIM]Br, 0.0998 mol.kg^{-1}), 1-butyl-3-methylimidazolium hexafluorophosphate ([BMIM]PF$_6$, 00999 mol.kg^{-1}), and 1,3-dimethylimidazolium methylsulfate ([MMIM]MeSO$_4$, 0.0999 mol.kg^{-1}) have been chosen to generate the density (d), speed of sound (u), and refractive index (n_D) data for the ternary mixtures of thiophene + toluene / *n*-hexane + IL at room temperature and atmospheric pressure. The values of apparent molar volume (V_φ), apparent molar isentropic compressibility (κ_φ), isentropic compressibility (κ_s), molar refraction (R_D), and so, the standard partial molar volume (V_φ°), the limiting apparent molar isentropic compressibility (κ_φ°) values of thiophene have been calculated at 298.15 K. The results expressed that the amplitude of the interactions between thiophene and the ionic liquids with the more concentration and the longer alkyl chain length as [EMIM]EtSO$_4$ (0.4999 mol.kg^{-1}) and [HMIM]Br are wider and the absorption capacity is favorer for molecules with higher density of the aromatic π electrons, namely, thiophene versus toluene and *n*-hexane. The positive ($\Delta_{tr}V_\varphi^{\circ}$) values obtained for thiophene in the solutions containing [HMIM]Br and [EMIM]EtSO$_4$ (0.4999 mol.kg^{-1}) suggested that the polar–ionic interactions and polar-polar group interactions are dominant. The interaction volumes of thiophene in the solutions containing [HMIM]Br and [EMIM]EtSO$_4$ (0.4999 mol.kg^{-1}) with the longer alkyl chain length and the more concentration of ionic liquid were greater than the others.

Keywords: Thiophene, Ionic liquid, Transfer adiabatic compressibility

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Hf_2CO_2: A High-Efficiency Photocatalyst for Water Splitting

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The conduction band minimum (CBM) must be higher (more negative) than the hydrogen reduction potential (H^+/H_2), and the valence band maximum (VBM) must be lower (more positive) than the water oxidation potential (H_2O/O_2) for an effective photocatalyst [1]. As a result, the smallest bandgap for a photocatalyst semiconductor is 1.23 eV. MXenes are a new 2D transition metal carbide/nitride family created by selective chemical etching of "A" from MAX phases. M is a transition metal, A is an element belonging to the IIIA or IVA family, and X is either C or N [2].

The Vienna ab initio simulation tool was used to perform the computations, which used Density Functional Theory (DFT) in conjunction with projector augmented wave (PAW) potentials (VASP) [3]. The Monkhorst–Pack scheme [4] automatically created k-points of 11*11*1 and 13*13*1 for structural optimization and static self-consistent computations. 520 eV was chosen as the cut-off energy. The VESTA code was used to investigate the atomic structures [5].We explored the structural and electronic properties of Hf_2CO_2 MXene in this study to explore the properties of MXenes as a photocatalyst for water splitting extensively. According to the findings, surface-functionalized M_2C-type MXenes, such as Hf_2CO_2, are semiconductors with a bandgap of 0.92eV. The bandgap for it with the HSE06 hybrid functional is 1.75eV at the same time. In addition to the bandgap size, the CBM and VBM must be greater (more negative) and lower (more positive) than the hydrogen reduction potential H^+/H_2 and the water oxidation potential H_2O/O_2, respectively, to assist the water-splitting reaction. Based on the computed imaginary component of the dielectric function, the optical absorption properties of 2D Hf_2CO_2 are also investigated. Calculating the phonon dispersion of 2D Hf_2CO_2 was used to investigate its lattice stability. As a result, the lack of imaginary frequency modes shows that the 2D Hf_2CO_2 structure is stable.

***Keywords*:** Photocatalyst, MXene, Density functional Theory (DFT), Water splitting, Dielectric function

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First-Principles Study of the Structural and Electronic Properties of Ti_2C and Ti_3C_2 MXenes by the Strain and External Field Effects

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The electronic, mechanical, and optical properties of two-dimensional (2D) materials have piqued interest. They're used in energy storage systems [1], nanoelectronic circuits, sensing, catalysis, and electronic devices [2], such as field-effect transistors [3]. Large surface areas and various characteristics distinguish 2D materials from their three-dimensional (3D) bulk counterparts. MXenes are a new class of 2D materials made by etching the sp element (A) layers from their corresponding MAX phases [4]. Transition metal nitrides, carbides, and carbonitrides make up these materials. External control, such as the composition of the external electric field, can alter its physical and chemical properties.

The SIESTA code was used to do all the calculations [5]. For the exchange-correlation functional, the Perdew-Burker-Ernzerhof (PBE) [6] generalized gradient approximation (GGA) was utilized. The VESTA code was used to investigate the atomic structures [7].

We examined the structural and electronic properties of two-dimensional Ti_2C and Ti_3C_2 MXenes using density functional theory, including compressive and tensile strain and external field effects. The magnitude of the strain is calculated to be $\varepsilon = \frac{(a-a_0)}{a_0} \times 100\%$, where a_0 and a are the calculated unstrained and strained lattice parameters**.** The metallicity of pure Ti_2C and Ti_3C_2 MXenes is indicated by the overlap of the valence and correlation bands. Mechanical strain influences bond length, the interaction between constituent atoms, and the electronic structure.

Keywords: MXene, Strain, External field, Electronic properties

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Application of Europium nanocomposite to fabrication of nanosensor for detection antidepressant drugs

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Antidepressant drugs such as Venlafaxine has been considered as one of the antidepressants belonging to the general family of the selective norepinephrine and serotonin reuptake inhibitors [1-2]. Fig.1 The present research successfully prepared the Eu3+-doped NiO modified carbon paste electrode (CPE), which has been utilized to selectively detect venlafaxine (VEN). Therefore, X-ray diffraction (XRD), scanning electron microscope (SEM) and energy-dispersive X-ray spectroscopy (EDX) have been applied for characterizing the Eu3+-doped NiO as a synthesized nanocomposite.. Moreover, differential pulse voltammetry (DPV) procedure has been exploited for successfully detecting VEN.

Thus, based on the optimized condition, a general linear association has been found in the experimental concentrations between 0.04 µM and 300.0 µM with 0.01 µM limit of detection (LOD) (S/N = 3). With regard to the outputs, our sensor had acceptable selectivity, significant stability, repeatability, and reproducibility. In addition, it has been substantially employed for determination of VEN in the drug and biological specimens.

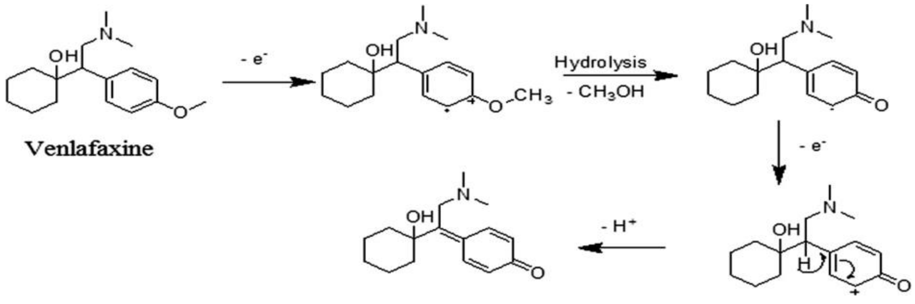

Fig. 1. Probable venlafaxine electro-oxidation mechanism at the Eu^{3+}-doped NiO/CPE.

***Keyword*:** Antidepressant drugs, Venlafaxine, Nanosensor

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Fabrication of biosensor by GO/Fe_3O_4@SiO_2 nanostructures and ionic liquid to measure gastrointestinal drugs

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The Gastrointestinal drugs as Sulfasalazine is an azo-salicylic acid derivatives with anti-inflammatory effect that was synthesized and used for treating rheumatoid arthritis from 1938 [1-3]. During treatment of autoimmune diseases the sulfasalazine prescribed as mainly drug in this process. Molecule of sulfasalazine has make by connection of pyridyl benzene sulfonamide and salycilic acid (SA) groups by azo bond.

In this study, A core-shell nanocomposite (GO/Fe_3O_4@SiO_2) in this case and ionic liquid have been used to improve the sensory properties of carbon paste electrode (CPE) entitle GO/Fe_3O_4@SiO_2/IL-CPE as new analytical approach. Fig.1. We validated the applications of GO/Fe_3O_4@SiO2/IL-CPE for the determination of sulfasalazine by using different electrochemical techniques. Under the optimized experimental condition, the linearity range and the detection limit (LOD) of GO/Fe_3O_4@SiO_2/IL-CPE were 1.0– 300.0 and 0.4 µM for sulfasalazine, respectively. The recording data showed that GO/Fe_3O_4@SiO_2/IL-CPE could be fabricated easily fabricated with outstanding stability. The sensor was applied to the detection of drug in real samples.

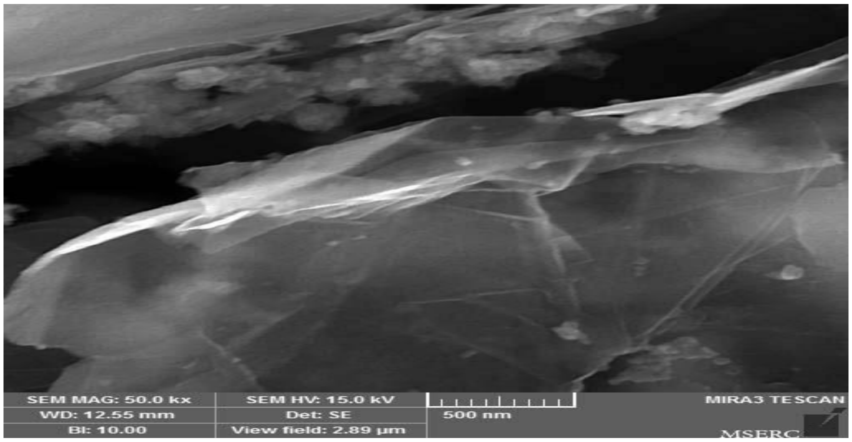

Fig. 1. SEM image of GO/Fe_3O_4@SiO_2

Keywords: Gastrointestinal drugs, Sulfasalazine, Biosensor

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Green synthesis of carbon dot from bio-source: A study of pH influence

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C-dots, new members of fluorescent carbon material with a diameter below 10 nm, are promising materials for bio-sensing, drug delivery and bio-imaging applications because of their excellent optical properties, high biocompatibility and low toxicity [1]. Various methods have been developed to prepare fluorescent C-dots, including physicochemical methods. The synthesis of nanoparticles using physicochemical methods can have toxic and dangerous effects on the environment and often requires expensive materials and tools. Therefore, it is crucial to use cost-effective, safer, simpler, more sustainable and environmentally friendly methods to prepare nanoparticles that comply with the principles of green chemistry. Herein, we report a straightforward route for synthesizing highly green-fluorescent C-dots by one-step hydrothermal treatment of bio-sourced at comparatively low temperature (120 °C) and in less time (150 min). The mechanism for the formation of C-dots involves polymerization, dehydration, and carbonization [2]. The resulting carbon dots exhibited concentration, excitation wavelength and pH-dependent luminescent behaviour in the visible range. The variation of PL intensity with pH (2–14) is studied, and as can be seen, the maximum PL intensity of aqueous dispersion of C-dots is intriguingly high within the interval of 6-8, whereas for higher or lower pH values, the PL intensity decreases. A strong PL intensity was observed in the physiological pH range. This is due to the electronic transitions of π–π^* and n-π^* that are changed by refilling or depleting their valance bands with the variation in pH. One possible explanation for this significant decrease of PL intensity as the acidity increases could be the protonation of nitrogen-containing functional groups; as a result, this protonation lowers the electron-donating efficiency. Despite that, a milder decrease of PL intensity from pH 8 to 14 could be accounted for the deprotonation of the carboxyl group on the surface of C-dot. In this pH range, the changes in the fluorescence intensity of the synthesized C-dots are minimal and subtle, which is due to the presence of many H and OH groups on the C-dots surface that neutralizes each other and prevents extinction. This study indicates that decreased PL of CD nanoparticles might hinder applications of the green CDs in non-physiological pH ranges.

Keywords: Carbon dots, Hydrothermal, pH, Photolumincense

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Solvatochoromic explains strong emission wavelengths of Carbon Dots

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Carbon Dots (C-dots) are a novel class of carbon-based nanoparticles discovered in 2004[1]. C-dots synthesis from bio-sourced has displayed excellent potential and ease of synthesis for applications in bio-imaging, printing inks, photocatalysis, biosensors, drug delivery and, light-emitting diodes (LED) owing to their remarkable properties [2]. The synthesized C-dots exhibit excellent solubility in a series of organic solvents and we have extensively investigated the C-dots + solvent interactions to understand the solvatochromic behavior of C-dots, which has hardly been studied. In this study, the photoluminescence (PL) emission spectra of C-dots indicate the blue-green color under UV light; various mechanisms have been proposed in relation to the color of C-dots releases. One of these mechanisms shows that surface heteroatoms such as nitrogen and oxygen from surface energy levels between HOMO and LUMO, leading to the propagation of long wavelengths from these surfaces [3]. In addition, we indicate exploring C-dots + solvent interactions to elucidate the nature of their tunable fluorescence. The photoluminescence quantum yield (QY) of the aqueous dispersion of C-dots was calculated to be 23.5%. Which increases as the lipophilic character of the solvent promote. The quantum yield of synthesized C-dots was studied in the range of protic and aprotic solvents. If surface states are complicated in the emission mechanism, the interactions of C-dots with the surrounding solvent should be vital in causal their optical properties. The result shows the fluorescence of C-dots is a combination of an excited state of the -COOH group and an excitation wavelength-dependent fluorescence from the polar groups such as the -OH moiety in the C-dots. Additionally, solvatochromic provided a semi-quantitative method to analyze the C-dot behaviors in connection with its surface localized electronic transitions in terms of non-specific and specific solute-solvent mutual interactions. The results of C-dots + solvents and photoluminescence influence will be useful for future application of drug delivery, cell imaging, biosensors and, another medical study.

Keywords: solvatochromic, Carbon dots, photoluminescence

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Study of catalytic reaction of thiol and amine to sulfonamide on silicon carbide nanotubes: A DFT approach

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According to the increasing prevalence of bacterial infections, it needs to produce drugs to combat these bacteria. Sulfonamide as a medicinal compounds are more noticeable [1]. The catalytic reaction of thiol and amine is a known useful method for production of sulfonamide [2-3]. First, the possible adsorption of thiol and amine structures on the surface of silicon carbide nanotubes was investigated. In some case there was adsorption between thiol and/or amine and the silicon carbide nanotube. For more study the surface activity of aluminum doped silicon carbide nanotube were investigated, too. The results were shown, for this surface the possible adsorption configurations has been increased. After adsorption process, the reaction of thiol and amine is studied to production sulfonamide on the surface of the mentioned nanotubes. For this purpose several possible reaction pathways were designed and studied individually. All calculations were performed with using GAMESS program suite [4] at m06 theoretical level and 6-311g(d) basis sets. The transition state configurations were calculated with using the QST3 keyword at the same level of theory. Thermodynamic parameters, potential energy surfaces and density of states diagrams for thiol and amine before and after adsorption were studied. Also, some important bond lengths and angles in the adsorption process were investigated. The results were shown only one of the designed pathways was feasible and this reaction pathway is thermodynamically desirable at some step and so, the improved silicon carbide nanotubes can act as an applicable catalyst for this reaction.

Keywords: Thiol, Amine, Sulfonamide, Silicon carbide nanotubes, DFT

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Isopiestic Investigations of the Interactions of Water-Soluble Polymers With 1-butyl-3-methylimidazolium hydrogen sulfate in Aqueous Solutions

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Aqueous biphasic systems (ABS) are usually formed by mixing two structurally different polymers or one polymer and one salt in an aqueous solution above a certain critical concentration. Liquid−liquid extraction utilizing ABS has found this platform to be a powerful technique for purification, extraction, and enrichment both in industry and academia [1,2]. Ionic liquids (ILs) are a new type of ionic solvent that exists as a liquid below 373.15 K. Because ILs possess some green characteristics, such as negligible volatility, a large liquid range, strong solubility power, and a number of possible variations in cation and anion features that allow the fine-tuning of their properties [3]. Furthermore, in recent years it was found that a new class of IL-based ABS can be formed when a hydrophilic IL and a certain salt or a certain water-soluble polymer are combined in an aqueous solution [4]. In this work, To obtain a detailed understanding of the molecular-level interactions in the salting effect of water-soluble polymers on the addition of ionic liquid is 1-butyl-3-methylimidazolium hydrogen sulfat ([C4mim][HSO4]), the isopiestic equilibrium molalities of aqueous solutions of PPG400, PPG725, PEG400, and PEG10 000 in the presence of the IL at 298.15 K as well as liquid−liquid equilibrium phase diagrams for the ternary aqueous [C4mim][HSO4] + PPG400 and [C4mim][HSO4] + PPG725 systems that form ABS were determined. It was found that there is a relationship between the salting-effect of ionic liquid and the deviations of the constant water-activity lines from the linear-isopiestic relation. For polymer−IL water systems that are not capable of inducing phase separation (the salting-in effect) because of the favorable polymer−IL interactions, the water molecules are allowed to relax to the bulk state; therefore, the water activity of these ternary systems is larger than those that we expect for a semiideal solution of the same concentration. The result is that these systems show positive deviations from the linearisopiestic relation and the salting-in effects are expected. However, in the case of the ternary aqueous polymer−IL solutions that form ABS (salting-out effect), the interaction between solute one and water becomes more favorable in the presence of solute two; therefore, the water activities of these ternary solutions in the one-phase region are smaller than those we expect for a semi-ideal solution of the same concentration. These systems show a negative deviation from the linearisopiestic relation; therefore, the salting-out of the polymer by salt occurs.

Keyword: Ioniq liquid, Aqueous biphasic systems (ABS), salting in and salting out

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Catalytic role of graphitic nitrogen atoms in the CO oxidation reaction over N-containing graphene: a first-principles mechanistic evaluation

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The release of air pollutants like carbon monoxide (CO) into the atmosphere is one of the most serious challenges for mankind in the current century. Although CO is produced in part by ambient photochemical oxidation of methane and other volatile organic molecules, incomplete combustion of fossil fuels and biomass are the primary sources of CO emission [1-2]. The negative impacts of acute CO poisoning on human health and the environment have been well documented. The oxidation of CO by O_2 is an efficient strategy that converts toxic CO into less harmful CO_2 at room temperature [3]. However, under normal conditions, this process usually requires large activation energy. Also, extensive scientific efforts have been made to design efficient catalysts for the CO + O_2 reaction [4-5]. Nitrogen-doped graphene has sparked a lot of interest due to its exceptional catalytic activity in a variety of chemical processes. We examine the catalytic ability of a series of nitrogen-containing graphene surfaces for CO oxidation using first-principles computations. The activation of the O_2 molecule in these systems is affected by the number and distribution of nitrogen impurities. According to the results, O_2 may be readily decomposed to O* species adsorbed on the nearest carbon atoms in the most active nitrogen-doped structures. The oxidation of a second CO is the rate-limiting step of the process due to the strong binding of the remaining O* moiety on the surface. Based on our findings, N-doped graphene can provide excellent metal-free catalytic performance for CO oxidation.

***Keywords**:* CO oxidation, Density functional, Adsorption, Elimination, The environment

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Study of thermal and adverse reactions of lithium ion batteries

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The performance, aging and safety of lithium ion batteries are all affected by their performance and / or storage temperature. In this research, the main thermal issues that require thermal management of lithium ion batteries are presented. These include reduced capacity / capacity, heat escape, electrical imbalance between multiple cells in the battery, and variable temperature performance. Pairing between electrochemical reactions and transfer phenomena is considered, which in turn affects temperature. Capacity / Power Reduction - The reduction in performance of lithium-ion batteries can be determined by the loss of available energy, ie capacity or power. The active substance inside the battery is converted to inactive phases, which reduces the capacity at any rate of discharge [1]. The basic mechanisms of battery aging in this study from 298 to 328 K are investigated and according to related topics [2], the reasons for battery aging and reduction of battery storage energy due to temperature conditions are given in this study.

Keywords: Temperatures, Capacity, Li-ion batteries, Side reaction

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DFT Study of Ionic Liquids as electrolytes in Li-Battery

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The ion mobility and charge transfer are two main challenges for scientists to design batteries with optimal charging time and lifetime. The bis(trifluoromethylsulfonyl)imide anions are applicable in batteies[1].The DFT study was performed on triethylsulfonium triethylsulfonium bis(trifluoromethylsulfonyl)imide ([S_{222}][TFSI]). The ionic liquids with and without Li cation are selected to examine the effect of cations on mobility, charge transfer, and other properties of this electrolyte. The optimized structure of [S_{222}][TFSI] and [Li][S_{222}][$TFSI]_2$ are shown in Figure 1. The structures and orbitals of ionic liquids were analyzed to determine the interaction between ions. Also, the effect of Li cation on structure, charge, and IR spectra was studied.

Results show that in the presence of Li cation, the anions go far from [S_{222}] to interact better with Li cation. Also, the Li cation is in the middle distance between two anions. Furthermore, IR spectra of these ionic liquids were affected by this observation. The frequency of C-H stretching mods in [S_{222}] at Li-ionic liquid takes the blue shift, which indicates that [S_{222}] tends to move away from anions and make weaker interactions with other cations. The wavelength of cations is also changed. Due to the strong attraction between anions and Li cation, S-O or S-F [TFSI] 's stretching and bending modes accrued in higher frequency numbers. Analyzing molecular orbitals shows that HOMO and LUMO orbitals are located on [TFSI] and [S_{222}], respectively.

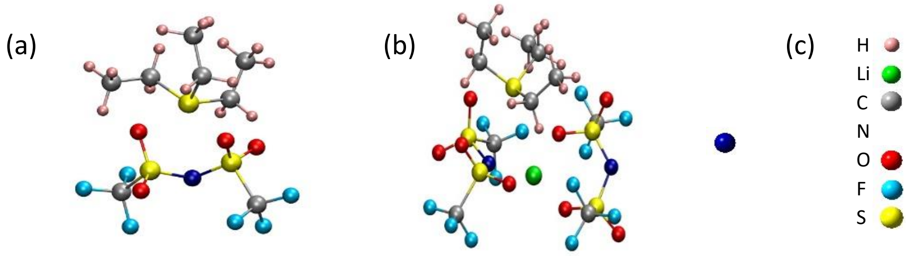

Fig. 1. Optimized structer of (a) [S_{222}][TFSI], (b) [Li][S_{222}][$TFSI]_2$ and atom types (c) are shown in figure.

Keywords: Li-battery, Ionic liquid, Lithium salts electrolyte.

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CO_2 capturing by Cr-graphdiyne surface: a DFT-D2 computational study

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Because of the remarkable growth in industrial activity and the consumption of fossil fuels in world, CO_2 emissions are increasing in the air and causing many concerns about climate change and global warming. Hence scientists are facing with related challenges to CO_2 trapping to protect the environment and reduce pollution. For this purpose a variety of nanostructures have been studied for CO_2 adsorption and trapping [1-2].In this study, we used the new carbon structure named graphdiyne (GDY) which synthesized in 2010. GDY has different hybridized C atoms (sp^2, sp) and different adsorption sites, unlike graphene. All computations were executed using DMol3 module available in Materials Studio software· All structures were optimized via the generalized gradient approximation (GGA) with Perdew, Burke, and Ernzerhof (PBE) of the exchange-correlation functional. For all of them, DFT method contains Grimme's D2 correction include dispersion and van der Waals forces and DNP basis set was applied. Calculations showed that the adsorption energy of CO_2 on pristine GDY is -0.206 eV and with the decoration of Cr on the GDY surface, this energy increases to -0.581 eV due to charge transferring and strong interactions. Therefore, GDY decorated with Cr can be applied to CO_2 capture and storage.

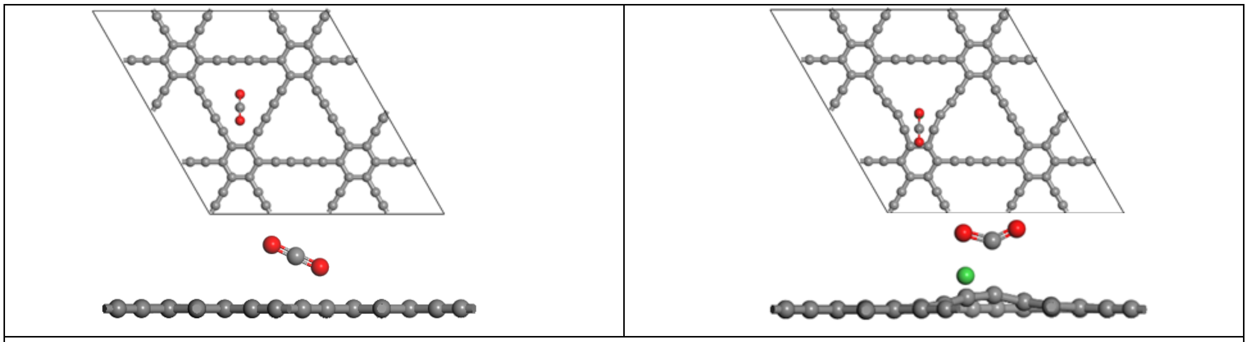

Fig. 1. The top and side view of the most stable structures of CO_2 adsorption on the pristine GDY(left) and Cr-GDY (right)

Keywords: Graphdiyne, CO_2 capture, DFT-D2

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Protonation states of titrable residues in Escherichia Coli Glyoxalase I

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Properties of most enzymes strongly depend on electrostatic interactions, both within the active site and between the groups of the active site and the surrounding protein. Such interactions crucially depend on the protonation state of the various residues, i.e., whether they are charged or not [1]. Protonation or deprotonation of titratable groups can cause changes in binding affinities, enzymatic activities, and structural properties. Very often, protonation or deprotonation are the key events in enzymatic reactions [2]. In this work, we have studied the protonation states of several groups in Escherichia Coli Glyoxalase I (GlxI). There are five residues in which the protonation-state assignment was not fully conclusive, two histidines (His-5, and -74), two glutamates (Glu-56, and -122), and one aspartate (Asp-115). We have performed molecular dynamics (MD) simulations to determine the most stable protonation states of these (besides the standard procedure of studying the surroundings, the solvent accessibility, and the H-bond network around the residue). MD simulations have been run on a 1.50 Å crystal structure of GlxI (Protein Data Bank entry 1F9Z) [3]. The entire enzyme was included in the calculations. The protein is a dimer, and the two subunits were treated the same way. The enzyme was solvated in a periodic truncated octahedral box of TIP3P water molecules, extending at least 10 Å from the solute using the *leap* program in the Amber suite. The final system contained ~30 000 atoms. After the solvation, we minimized the structure followed by a 500 ns production simulation, during which coordinates were sampled every 10 ps. The root-mean-square deviation (RMSD) from the starting crystal structure as has been done before for His residues in three proteins [4], titratable residues in the active site of myrosinase [5], and homocitrate and nearby residues in nitrogenase. It is possible to determine which protonation state is more realistic based on the RMSD from the crystal structure. It is believed that if an incorrect protonation state is used, the atoms in that residue or nearby residues will move to reduce steric or electrostatic clashes or to form new favorable interactions. Therefore, the RMSD will be higher in the case of incorrect protonation states (assuming the reference structure is representative of the studied state). The results show that His-5 and -74 are protonated on the ND1 atom, not on the NE2 atom, Glu-56 and -122 and Asp-115 are deprotonated.

Keywords: Glyoxalase I, Molecular dynamics simulations, Protonation state, Enzyme

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Experimental study on the calorimetric data of Cyclohexanol + Alkylamine (C4 and C6) at 303.15 K

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Excess molar enthalpies, H_m^E, of two binary mixtures of cyclohexanol (CYC) with butylamine (BUT), hexylamine (HEX) were measured using a Paar 1455 solution calorimeter at T = 303.15 K and ambient pressure. Experimental data was used to calculating the excess partial molar enthalpies, $H_{m,i}^E$. Negative or positive values of H_m^E indicate that the interactions between components in such a way that the system can absorb heat (endothermic) or repel heat (exothermic) [1-2]. The value of H_m^E for these systems over the whole of composition range were negative. The magnitude of the H_m^E values increases with increasing alkyl chain length because of the formation of hydrogen bonding and dipole – dipole interactions. The magnitude of H_m^E values for all binary systems are follow: CYC + BUT: $-3169.3 < H_m^E < -997.9$ j.mol^{-1} and CYC + HEX: $-2437.9 < H_m^E < -956.5$ j.mol^{-1}. Viewing these values is due to various factors such as hydrogen interactions breakdown, number of interactions between unlike molecules, intra-molecular polar interactions, the type of geometric connections and chain length between the components. These values reflect that the mutual-association between the unlike-molecules are greater than self-association between the like-molecules. In order to theoretical study these binary mixtures, the experimental excess molar enthalpy data have been fitted by Redlich – Kister equation and correlated with three thermodynamics models (Wilson, NRTL and UNIQUAC) [3-4]**.** All three models well confirmed the experimental results which the NRTL model had the best prediction.

Keywords: Excess molar enthalpies, Aniline, Butylamine, Hexylamine

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Isopiestic study on ternary polymer-polymer nonaqueous solutions

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Nonaqueous solutions of polymers, especially polyethylene glycols and polypropylene glycols, are broadly used in various processes in lubricants, carriers, coupling agents, pharmaceuticals, and purification of bioactive compounds [1-2]. Vapor-liquid equilibrium (VLE) investigation in ternary solutions composed of two polymeric solutes and a nonaqueous solvent provides valuable information regarding predominant factors that control the phase behavior of these systems. An overview of the literature shows that although VLE data have been obtained for binary nonaqueous solutions of polymers [3-4], as far as we know, there is no study about ternary nonaqueous polymer-polymer solutions. In this work, the isopiestic technique has been used to study the VLE behavior of ternary systems composed of polymer 1 (polyethylene glycol) + polymer 2 (polyvinylpyrrolidone) + organic solvent (ethanol or 1-butanol). The effects of polymer structure and concentration on the slope of constant solvent activity lines and the magnitude of deviations from the semi-ideal behavior (Zdanovskii−Stokes−Robinson rule) [5] have been explained and related to the soluting-in or soluting-out effects occurring in the investigated systems.

Keywords: Polymers, Isopiestic equilibrium, Soluting effects, Semi-ideal behavior

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Synthesis, Characterization and Improving Photocatalytic Properties of Cobalt Titanate Perovskite and Its Nanocomposites in Degradation of Persistent Organics dye

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Titanium based perovskite oxides suchlike $ATiO_3$ are a type of considerable photocatalyst for the perfect photocatalytic degradation of poisonous pollutants [1]. On the other hand, among visible light photocatalysts, nitrogen-rich carbon nitride materials are excellent options for photocatalytic activity [2]. Therefore, we decided to synthesize of $CoTiO_3$ and C_3N_5 and their nanocomposite. Cobalt titanate ($CoTiO_3$) nanostructures were synthesized in the form of nanorods by hydrothermal method and calcined in 600 °C. C_3N_5 nanosheets also were synthesized by simple thermal treatment, then, $CoTiO_3/C_3N_5$ nanocomposites were prepared by reflux method. The phase structure and crystalline properties of the synthesized samples was investigated using X-ray diffraction (XRD) technique. The morphology and optical properties of the synthesized materials were investigated by Field-Emission Scanning Electron Microscopy (FESEM), High-Resolution Transmission Electron Microscopy (HRTEM) and UV–Visible Diffused Reflectance Spectroscopy (UV-DRS). Also, the surface properties of materials were determined by adsorption-desorption isotherms of N_2 gas. Photocatalytic measurements of $CoTiO_3$ and $CoTiO_3/C_3N_5$ photocatalyst were evaluated towards the degradation of methylene blue (MB) as a model coloring organic pollutant, and tetracycline hydrochloride (TC) as a model antibiotic, under simulated visible light illumination. The results showed that $CoTiO_3/C_3N_5$ (1:3 wt%) was the best photocatalyst, with the complete MB (10mg L^{-1}) and TC (100ppm) degradation efficiency within 60 min of radiation compared with pristine $CoTiO_3$ nanorods and C_3N_5 nanosheets.

Keywords: Photocatalyst, $CoTiO_3$, Nanocomposite, Dye.

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Clouding behaviour of aqueous 1-butanol solutions in the presence of organic and inorganic ammonium salts

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The liquid-liquid and vapor-liquid phase behavior of mixed solvent systems meaningfully changes in the presence of a non-volatile solute [1]. This issue appears as the soluting-out or soluting-in phenomena and is profitably used in distillation and solvent extraction. The butanol-water mixed solvent systems have significant importance as a reaction media or extractant in a wide variety of chemical processes and the manufacturing of cosmetics, pharmaceuticals, and essential oils [2-3]. In this respect, there is a well-sustained interest in studying the soluting effects of various additives on mixed solvents composed of 1-butanol and water. In continuation of the previous works [4-5] , herein, we have studied the soluting effects of several organic and inorganic ammonium salts on the liquid-liquid phase diagram (cloud points diagram) of aqueous 1-butanol solutions. The impacts of cation alkyl chain length, anion type, and concentration of ammonium salts on the clouding phase behavior have been discussed. The main driving force of phase separation in the investigated systems has been determined by correlating the obtained results with the relevant thermodynamic functions.

Keywords: Cloud point, Butanol, Ammonium salts, Thermodynamic functions, Soluting effects

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Soluting effect study in aqueous solutions composed of sugars and tetraalkylammonium salts

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Sugars are renewable, biodegradable, non-toxic, and non-charged hydrophilic materials owning soluting-out aptitude in aqueous media due to their high affinity for water [1-2]. During the past decade, there have been significant efforts to study sugar-based aqueous two-phase systems (ATPSs) as alternative extraction platforms [1-5]. However, despite its importance for optimum designing of green separation processes, the mechanism of ATPS formation in a ternary aqueous system composed of a sugar and a second solute is still unclear. Aiming to study the main driving forces that control the phase behavior of these systems, this work focuses on the vapor-liquid equilibrium investigation for ternary systems of {water + sugar + tetraalkylammonium salt} via the isopiestic method. The magnitude and the type of deviation of constant water activity curves from the linear isopiestic relation (semi-ideal behavior) have been taken as a benchmark to study the soluting effect occurring in the investigated systems. The impacts of cation alkyl chain length and anion type of ammonium salts, and also the structure and stereochemistry of sugars on the deviation from the semi-ideal behavior have been scrutinized and explained based on soluting-in and soluting-out phenomena.

Keywords: Carbohydrates, Tetraalkylammonium salts, Soluting-in, Soluting-out, Isopiestic

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Investigation on Molecular Structure and Electronic Properties of Zinc (II) Complex with 2-acetylpyridinenicotinichydrazone ligand

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The metal-organic supramolecular systems continue to attract the attention of researchers because of their potential applications as functional materials in various fields [1-2]. Acyl-hydrazone having different heteroatoms in its structure used as ligands in coordination chemistry as polydentate ligands for the synthesis of metal complexes [3]. In this work, a new zinc(II) complex, [CuI2(HL)], with 2-acetylpyridine nicotinichydrazone ligand (HL) was modeled theoretically and the structural and physical properties of the complex has been investigated by using the Density Functional Theory (DFT) based on B3LYP density functional with basis set combinations. In calculations, LANL2DZ and a mixed basis set of LANL2DZ (for Zn and I) and 6-311G (for other atoms) were used in the gas-phase geometry optimization. The vibrational frequency, polarizability (α), dipole moment (μ) and the first-order hyperpolarizability (β), E_{HOMO} (the highest occupied molecular orbital energy), E_{LUMO} (the lowest unoccupied molecular orbital energy), energy gap (ΔE), of complex was calculated by using the same method. Also, the ^{1}H as well as ^{13}C NMR chemical shifts values of studied compound in the ground state for DFT/B3LYP/GENECP/LANL2DZ-6-311G have determined using Gauge independent atomic orbital (GIAO) technique. In addition to, UV-Visible absorption property of the complex was also investigated the same method. Equilibrium state (ground state) dipole moment value of the studied complex was calculated as 12.61 and 12.74 Debye by B3LYP/GENECP/LANL2DZ-6-311G and B3LYP/LANL2DZ method, respectively. The calculated structural parameters of the complex were compared with the previous experimental data of analogue compounds in the literature and a good agreement was found between the structural parameters. The approximate geometry of the molecule in three dimensions was drawn in the GaussView 5.0 molecular imaging program, and all theoretical calculations were used with the Gaussian 09W package program.

Keywords: LANL2DZ-6-311G, Dipole moment, Polarizability, Hyperpolarizability, ^{1}H and ^{13}C NMR.

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NMR characterization, conformational energy and nonlinear optical property calculations of 1,3-bis(2,4-dimethoxyphenyl) imidazolidine-2-thione molecule

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Thioureas and their cyclic derivatives are known to exhibit a broad spectrum of biological activities such as antibacterial and antifungal properties and regulating activities for plant protection in agriculture [1-3]. They also have a wide variety of uses in the mining industry. Therefore, the interest in these compounds continues to increase [4-5].Conformational analysis of the 1,3-bis(2,4-dimethoxyphenyl) imidazolidine-2-thione molecule was performed by calculating the molecule's potential energy surface (PES) as a function of the θ[C4-C3-N1-C2] and φ[C13-C12-N2-C11] dihedral angles. In potential energy surface calculation, density functional DFT/B3LYP methods and the 6-31G basis set were used and and θ[C4-C3-N1-C2] and φ[C13-C12-N2-C11] torsion angles were scanned from -180° to 180° at intervnals of 15°. By performing geometry optimization calculations of the lowest energy conformations on the PES, the ground state geometry of the molecule was determined. Using the optimized structure, the geometry of the molecule, the highest occupied molecular orbital (HOMO), the lowest unoccupied molecular orbitals (LUMO), harmonic vibration waves, linear optical properties (polarizability) and nonlinear optical properties (NLO) (hyperpolarizability) values has been examined at both *ab initio* Hartree Fock (HF) and DFT/B3LYP methods using the 6-311++G(d,p) basis set. The energy gap ($\Delta E = E_{LUMO}-E_{HOMO}$) of the molecule were determined using E_{HOMO} and E_{LUMO} energy values of the molecule. The total energy distribution (TED) of the studied molecule was calculated in VEDA4f program. Also, the ^{1}H as well as ^{13}C NMR chemical shifts values of studied compound in the ground state have determined by both methods employing different basis sets such as the 6-31G, 6-31+G, 6-31+G(d), 6-31++G(d,p), 6-311++G(d,p) and 6-31+G(2d,p) using Gauge independent atomic orbital (GIAO) technique. The structural parameters of the 1,3-bis(2,4-dimethoxyphenyl) imidazolidine-2-thione molecule calculated in both methods were compared with the previous experimental data on the molecule in literature [3]. The approximate geometry of the molecule in three dimensions was drawn in the GaussView 5.0 molecular imaging program, and all theoretical calculations were used with the Gaussian 09W package program.

Keywords**:** Conformational energy, NMR characterization, Dipole moment, Polarizability, Hyperpolarizability.n

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Vapor-liquid equilibrium in aqueous systems composed of amino acids and quaternary ammonium salts

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Amino acids are the building blocks of proteins, which are a type of the most important biological macromolecules. The thermodynamic investigation of aqueous amino acid solutions in the presence of second solutes, especially electrolytes, provides valuable information about the complex behavior of proteins in biological systems. Further, distinct pairs of amino acids and a second solute in aqueous media can undergo the soluting-out phenomenon as aqueous biphasic systems (ABS) formation[1-2] or precipitation[2]. Such systems have a significant place in designing green extraction and separation strategies[1-3]. Quaternary ammonium salts own a tunable hydrophobic/ hydrophilic character because of the possibility of changing the ammonium alkyl chain length. Therefore, this kind of salts can be a good choice for a comprehensive study of soluting effects of electrolytes on aqueous amino acid solutions[4-5].

This work addresses soluting-out and soluting-in effects occurring in ternary aqueous solutions composed of amino acid and quaternary ammonium salts. For this purpose, the vapor-liquid equilibrium properties of several ternary systems of {water + amino acid + quaternary ammonium salt} have been measured by the use of the isopiestic method at 298.15 K. The effects of amino acids type, alkyl chains length of ammonium, and anion type on vapor pressure, osmotic coefficients and the slope of constant water activity lines have been determined. The concave or convex shape of constant water activity curves has been taken as a benchmark to study the type and magnitude of deviation from the semi-ideal behavior and therefore the soluting effects occurring in the investigated systems.

Keywords: Vapor-liquid equilibrium, Constant water activity line, Amino acids, Quaternary ammoniums, Soluting effects

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PEGylated PAMAM Dendrimers as Eptifibatide Nanocarriers: An Atomistic View from Molecular Dynamics Simulations

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Acetylation and PEGylation can decrease cytotoxicity, improve biocompatibility, and reduce the rate of elimination of PAMAM dendrimers from systemic circulation [1]. However, atomic level information on the microstructure, drug loading capacity, and release pattern of drug molecules from PEGylated dendrimers is very limited [2]. We have performed molecular dynamics (MD) simulations to explore the association of eptifibatide (EPT) drug with native acetyl-terminated G4-PAMAM dendrimer and its partially (25, 50, and 75%) PEGylated analogues. The impact of PEG length was investigated using PEG chains with molecular weight of 500 and 1000 Da. The results showed that PEGylation does not affect the overall microstructure of dendrimers. The maximum loading capacity was achieved by G4-16PEG1000 system (1:7) through the encapsulation of 4 EPT in its internal cavities and conjugation of 3 EPT on its surface. Potential of mean force calculations revealed that G4-48PEG500 possesses the highest value of free energy barrier and holds EPT molecules tightly. In view of loading capacity, preferential binding sites of drug molecules, and release patterns, G4-16PEG1000 can be considered as the most promising carrier for EPT. In general, partially PEGylated dendrimers can increase the plasma half-life of the EPT molecule and reduce its clearance rate by up to 2 times.

Keywords: PAMAM dendrimer, PEGylation, Targeted drug delivery, Eptifibatide, Molecular dynamics (MD) simulations.

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Hydrolysis of *S*-D-lactoylglutathione By Glyoxalase II, a Theoretical Study

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The glyoxalase system catalyzes the conversion of toxic methylglyoxal to D-lactate. Glyoxalase II (GlxII) catalyzes the second step of this conversion, namely the hydrolysis of *S*-D-lactoylglutathione (SLG), which is the product of the Glyoxalase I (GlxI) reaction. In this study, we investigated the reaction mechanism of GlxII by the quantum mechanics/molecular mechanics (QM/MM) method. A model of the active site of GlxII was constructed based on the crystal structure of the human GlxII (1QH5 PDB ID) [1]. Its active site contains two zinc ions, an aspartic acid (Asp-58), several histidine ligands (His-54, His-56, His-59, His-110, and His-173) and a bridging Asp-134 group, a hydroxide (μ-OH), and SLG as the substrate (Figure 1). The results showed that the first step of the mechanism is the nucleophilic attack of the bridging oxygen (Oμ) on the carbonyl carbon (Cs) of the substrate (the atom names are defined in Figure 1) that concurrently with this attack, the S-Cs bond dissociation occurs. Then the mechanism proceeds with two successive proton transfers, first the transfer of H2w from a water molecule to the S atom. After that, the transfer of the Hμ to the O1 atom of the substrate produces a lactate ion. Our results indicated that the initial nucleophilic attack is the rate-limiting step which contradicts previous calculations on other dinuclear zinc enzymes [2-3].

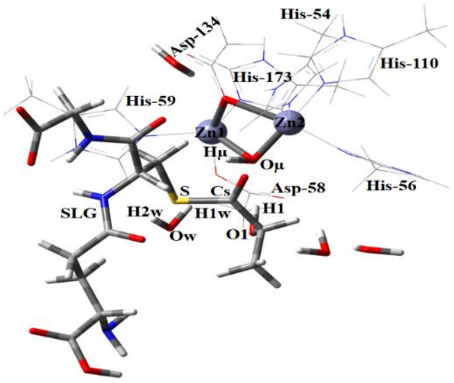

Fig.1. The active site model of GlxII. The substrate, bridging atoms, and water molecules are shown by tubes, amino acids in the wireframe, and Zn atoms by ball.

Keywords: Glyoxalase II, QM/MM, Mechanism

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Effects of metal ions substitution on Glyoxalase I activity

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Glyoxalase I (GlxI) is one of the enzymes that shows a high metal dependency in its catalytic activity. For the catalytic activity, GlxI requires divalent metal ions (Zn(II), Ni(II), Co(II), or other metal ions, depending on the organism). It has been suggested that the metal specificity is related to the amino-acid sequence and the length of the enzyme. For example, Zn(II)-active GlxIs comprise additional short regions that are missing in the Zn(II)-inactive ones [1]. Despite all studies of the reaction mechanism of GlxI [2-4], the metal preference of this enzyme has not gained much attention. In this study, we have used the QM/MM method to study the metal preference of GlxI from humans (*Hu*GlxI) and corn (*Zm*GlxI), prototypes of Zn(II)-active and Zn(II)-inactive GlxIs, respectively. This enzyme can act upon a mixture of methylglyoxal (MG), glutathione (H-SG), and hemithioacetal (HTA). Depending on the number of substrates, there could be two mechanisms for the reaction of GlxI (single- and two-substrate mechanisms). We studied energy profiles for the two- and single-substrate mechanisms of *Hu*GlxI and *Zm*GlxI with the Zn(II), Ni(II), and Co(II) ions. Our results show that the Zn ion gives the lowest barrier for the two- and single-substrate reaction mechanism of *Hu*GlxI. This agrees with the experimental observation that *Hu*GlxI is most active with Zn. However, the barriers diverge from the experimental results for *Zm*GlxI (cf. Figure 1).

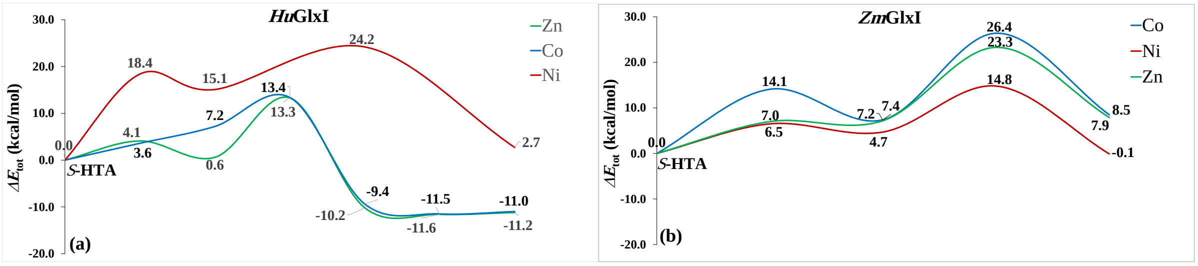

Fig. 1. The ΔE_{tot} energy profiles for the single-substrate reaction of *S*-HTA with the three metal ions in (a) *Hu*GlxI and (b) *Zm*GlxI.

Keywords: Glyoxalase I, Metal preference, QM/MM, Mechanism

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The effect of mono vacancy defect on the interactions of F_2, Cl_2 , O_2 , N_2 , CO , NO and Boraphene

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Among various allotropes of boron, B36 is the smallest boron cluster with crystalline atomic monolayer of boron forming of 36 bonded boron atoms. This material has been suggested to be one of the unique adsorbents for CO, N_2, H_2O, O_2, HF, H_2, and NO gas molecules[1-3]. On the other hand, it is well known that structural modifications including atom doping, decorating, and even vacancy imposing are effective tools to increase the interaction between 2D host materials and guest gas molecules[4].

Therefore, according to the findings of previous researchs in this study using density functional theory, the effects of three types of mono-vacancy defects on electronic structure of B36 were investigated to find the outcome of these changes on the amount of adsorption energy of F_2 , Cl_2 , O_2 , N_2 , CO and NO in relation to B36.

The results reveal that the changes of the energy gap of defects are very significant. So that the energy reduction for defects of the first, second and third rows of B36 was -57.46%, -57.10% and -57.68% respectively. The electronic structure features of these defects are very different from one another. Namely, each of them specifically affects the entire structure of the absorbent.

DOS diagrams and UV spectra of mono-vacancy defects are compared to pristine Boraphen and discussed. In addition, adsorption spectra were compared before and after the adsorption of B36 and three types of mono-vacancy defects.

Besides, external electric field was introduced to increase adsorption energy for cases with low adsorption energy.

Keywords: Boraphene, Mono-vacancy, Energy gap, UV spectra

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Calculation of the Intermolecular Potential Energy Surface and Transport Properties for He… HBr Van Der Waals Complex Using CC, MMA and MD Simulations

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In this work, the intermolecular potential energy surface (IPES) for He-HBr van der Waals (vdW) [1] complex has been calculated using the ab-initio calculations method in the CCSD (T)/Aug-cc-pv5z-BF level of theory considering the BSSE correction [2]. The influence of different basis sets and addition of the virtual mid bond functions (BF) was also investigated. There are two minimum in the obtained potential for linear He-HBr and He-BrH linear structures. The obtained IPES than was used to calculate the interaction second virial coefficients along with the cross viscosity (η_{12}) and diffusion coefficients (D_{12}) over a wide range of temperatures. The full-quantum mechanical close coupling (CC), classical Mason-Monchick approximation (MMA), and classical molecular dynamic simulations (MD) were done to calculate the η_{12} and D_{12}. It was found that the Vashishta force filed (FF), in which 3-body and 2-body interactions were considered simultaneously is better in calculation of η_{12} and D_{12} than the Lenard-Jones (12,6) potential model, where only 2-body interactions were incorporated in derivation of the FF.

Keywords: He, HBr, IPES, vdW, MD, MMA.

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Investigation of Solvatochromism Properties of Mg-Al-Acid Orange-7 LDH Nanohybrid

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The solvent characteristics play a significant role in both the chemical and physical processes by regulating the photo chemical/photo physical behavior of the molecules[1]. The position of the absorption/emission bands of the molecules are either shifted, or the intensities of these bands are shrunk due to the interaction of molecules with the solvents of different polarties [2]. In this research work, Mg-Al-Acid Orange-7 LDH, was synthesized by chemical co-precipitation method [3]. XRD patterns indicate that a kind of large anion has been intercalated into the interlayer space of the LDH. Also, increasing the interlayer distance from 14.43 A^0 to 22.43 A^0 reflects the bilayer structure of acid orange 7 in the LDH Gallery. Infrared spectrum of AO7-LDH shows that the product has the characteristic absorption bands of both azo and hydrazone forms of AO7 anion, as well as the Mg-O and Al-O vibrations of LDH layers, well convincing the intercalation of AO7 anions successful. The $E_T(30)$ values for the LDH were evaluated in the persence of different solvents. By employing KAT framework, the polarity parameters were assessed(α, β, π^*). With increasing polarity of the environment, it was observed that the resulting peaks shifted to shorter wavelengths and higher energies(hypsochromic).

Keywords: Solvatochromism, Layered Double Hydroxide, KAT equation, Polarity

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Calculation of non-equilibrium thermodynamic properties of He…BeH_2 Van der Waals complex based on the quantum and classical kinetic theory and classical molecular dynamic simulation methods.

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The He-BeH_2 is a van der Waals complex synthesized when BeH_2 placed under He atmosphere at 1500°C [1]. Intermolecular potential energy surface (IPES) has been calculated for this complex, at CCSD(T)/aug-cc-pv5z level of theory as a function of distance and angle between He and the BeH2 molecule. The obtained potential data then was fitted with a great precision to a mathematical potential model by Legendre expansion of the potentials. Also, in order to achieve thermodynamic parameters through molecular dynamics (MD) simulation method, the developed classical LJ (12,6) and the Vashishta potential models were fitted to the ab-initio potentials. The devopled potentials models then were used to calculte the second virial coefficients along with the cross viscosity (η_{12}) and diffusion coefficients (D_{12}) over the the temperature range of T = 100-2000 K. It was found that, the results of Vashishta force filed is better than the LJ(12,6). Also, η_{12} and D_{12} form quantum close coupling and classical Mason-Monchick (MM) [2] showed that, classical MM approximation is only valid in the temperatures far from the quantum effects, i.e., ~ room temperature and beyond.

Keywords: He-BeH_2, Non-equilibrium thermodynamics, Viscosity, Diffusion coefficient

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Electrochemical reduction of NO on fullerene doping by boron atom: a computational study

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Nitric monoxide (NO) is a main environmental pollutant generated by the burning of fossil fuels in different industrial processes and internal combustion engines [1]. NO species in the atmosphere can interact with water molecules, resulting in acid rain, which has a detrimental impact on plants, forests, soil, buildings, and human health. Additionally, NO contributes to photochemical smog and ozone depletion [2]. The electrochemical reduction of nitrogen monoxide (NO) is one of the most promising approaches for converting this harmful gas into useful chemicals.

In recent years, single-atom catalysts (SACs) have emerged as a distinct branch of heterogeneous catalysts due to their high metal performance and long-term durability [3]. Carbon nanostructures like fullerenes, nanotubes, and graphene have gained a lot of interest in the recent decade due to their unique chemical and physical characteristics [4]. Buckminsterfullerene (C_{60}) is an important member of the carbon fullerenes, composed of twenty six-membered and twelve five membered carbon atom rings with sp^2 hybridization. Using density functional theory calculations, the work examines the potential of a single B atom doped C_{60} fullerene ($C_{59}B$) for catalytic reduction of NO molecules. NO may be strongly activated over the B atom of $C_{59}B$, and that the subsequent reduction process can result in the formation of NH_3 and N_2O molecules at low and high coverages, respectively. Based on the Gibbs free energy diagram, it is inferred that the $C_{59}B$ has excellent catalytic activity for NO reduction at ambient conditions with no potential-limiting. At normal temperature, the efficient interaction between the $^*NOH$ and NO species might lead to the spontaneous formation of the N_2O molecule.

Keywords: Electrochemical, Fullerene, Electrocatalyst, Reduction

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Electrochemical reduction of NO over Si-N_4 embedded graphene: Theoretical investigation

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Nitric oxide (NO) is an important air pollutant, primarily emitted from the burning of fossil fuels in vehicles and industrial activities. When produced, oxidation of NO leads to formation of NO_2 molecules in the atmosphere and then by interacting with water molecules, converted into acid rain, which is hazardous for the environment and human health. In addition, NO is regarded as a major cause of the photochemical smog and ozone layer depletion [1]. Therefore, it is needed to develop effective ways for removing or reducing toxic NO molecules from the atmosphere. Electrochemical reduction of NO is an efficient method for removal of harmful NO molecules from atmosphere and their converting into useful components. Graphene with its exceptional mechanical, electronic, thermal and optical properties has many potential applications in energy storage, sensors and solar cells. Recently, doping heteroatoms in graphene have attracted much attention in many different chemical reactions [2-3].There are a variety of N atoms containing graphene surface, including pyridine N, graphitic N and pyrrole N [4]. Particularly, incorporating four pyridinic N atoms around pre-existing di-vacancy in graphene (N_4Gr) is one of the high potentials for metal atom substitution to improve its catalytic activity towards many applications.

In this article, we study for the first time the catalytic cycles of NO reduction over a Si atom coordinated N_4 centers in graphene (Si-N_4Gr) by application of density functional theory (DFT) calculations. Based on our findings, NO can be highly activated over Si-N_4Gr electrocatalyst and the subsequent reduction of this molecule can produce N_2 molecule at high coverages or NH_3 at low coverages. The Si-N_4Gr electrocatalyst exhibits outstanding catalytic activity for reduction of NO molecule with a limiting potential of 0.56 eV under ambient conditions.

Keywords: Electrocatalyst, Reduction, Graphene, Electrochemical

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Study of the effect of polymer molecular mass on the phase equilibria of the aqueous two-phase systems composed of polyethylene glycol 1000, 1500, 2000, 4000, and 6000 + tri-lithium citrate + water

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In this study the temperature effect on the Liquid–liquid Equilibrium (LLE) for PEG 1000, 1500, 2000, 4000, and 6000 + tri-lithium citrate + water at T = 298.15 K was investigated, and the binodal curves and tie-lines were measured experimentaly. It was found that, with increasing molecular mass, the two-phase region expanded and the slating-out ability of the system were increased. The experimental binodal data were fitted with the Merchuk equation. The fit of the experimental tie-line data performed using the Seteschenow equation and the salting-out parameters (K_{ca}) were calculted [1]. The calculations shows that, K_{ca} increased with increasing molecular mass of the polymer, which shows that, the K_{ca} parameter can be used as a quantitave index for scaling the slating-out ability of ATPSs. Also, the experimental tie-line data were syccesfully modeled using Osmotic-Virial, Othmer-Tobias, and e- Wilson, e-NRTL models [2]. The poposed ATPSs than was used to partition the salbutamol drug. It was found that, partitioning coeffeicient of the sulbutamol drug was decreased by increasing the molecular mas of the polymer.

Keywords: LLE, PEG, Tri-lithium citrate, Salbutamol

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DFT Studied on The Possibility of Chitosan Nanoparticles as Potentials Drug-Delivery Carriers of Favipiravir: A COVID-19 Drug

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In this work, the possible complexation of Favipiravir, a COVID-19 drug, with pure chitosan, and the nitro, carboxylic acid and amino functionalized chitosan nanoparticles was investigated using quantum density functional theory [1] methods at B3LYP-D3/6-311g(d,p) level of theory. In this respect, different FP/nanoparticle complexes were constructed and optimized in gaseous state and in aqueous media using integral equation formalism of the polarizable continuum model (IEPCM). The interaction energies (E_{in}) between the FP and nanoparticles were calculated using a supramolecular approach, and the noncovalent interaction (NCI), quantum theory of atoms in molecules (QTAIM) [2] and natural bond orbital (NBO) analysis were done to explore the nature of the interactions between FP and chitosan nanoparticles. The values of the E_{in} reveal the physisorption of FP on the considered nanoparticles. Furthermore, we found that, the functionalization of chitosan has no considerable effect on the obtained E_{in}. The NCI, QTAIM and NBO analyzes also confirm that, the physisorption of FP on nanoparticles is through the van der Waals interactions and hydrogen bonding. Overall results show that, the chitosan has the potentials of being a nontoxic carrier for targeted nano-based drug delivery of favipiravir drug.

Keywords: COVID-19, Chitosan, Favipiravir, DFT, nanoparticle

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Theoretical and computational investigation on the Choline chloride based deep eutectic solvents

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Deep eutectic solvents (DES) have received substantial applications and development in the field of green chemistry during last decades [1]. Using quantum mechanical density functional theory (DFT), the possisblity of the DESs generation of Choline Chloride (ChCl) as hydrogen band acceptor and six carboxylic acids including Glycolic acid (Gly), Glutaric acid (Glu), Oxalic acid (Oxa), Lactic acid (Lac), Itaconic acid (Ita) and Levulinic acid (Lev) as hydrogen band donnors were investigated [2-3]. Geometry optimization, and vibrational analysis were performed by applying three DFT functionals, i.e., B3LYP-D3(BJ), M06-2X, and ωb97X-D3. Then, QTAIM, natural bond orbital (NBO), non-covalent interaction (NCI) analysis, and bond orders calculated from WBI method were implemented to explore the nature of the interactions between choline chloride and various carboxylic acids. It was found that, the ion-covalent interactions due to the chloride ion of the choline chloride is the main interaction that generates the DES of the studied acids with choline chloride.

Keywords: Deep eutectic solvents (DES), Choline chloride, Density functional theory (DFT)

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Experimental and Quantum Density Functional Studies on the IR, UV-Vis and NMR Spectra of 5-Amino Pyrazole Derivatives

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Pyrazole is a 5-membered heterocyclic compound extensively used as a medical in treatment of patient, inflammation, fever and other types of disease. In recent years, new derivates of Pyrazole have also been synthesized and extensively used in treatment of different and vesting area of disease [1]. In this work, 5-amino pyrazole derivatives were synthesized and characterized experimentally and theoretically. The IR, NMR, and UV-Vis spectra of the compounds were measured experimentally in different solvents, and calculated using time independent and time dependent quantum density functional methods at B3LYP/6-311++g(d,p) level of theory. The effect of the polarity of the solvent on the observed bathochromic effect of the UV-Vis spectra was discussed based on the linear solvation energy relationships, the Kohn-Sham molecular orbitals, the charge transfer, and the hole-electron analysis methods. The scaled quantum mechanical (SQM) method was applied on the calculated IR spectra, and the deviation of ~ 6 cm^{-1} was obtained between the calculated and experimental IR spectra, so, the observed vibrations were assigned ultimately with the minimal possible error. The absolute average deviation (AAD) between the calculated and experimental NMR spectra for ^{1}H-NMR and ^{13}C-NMR were found to be $AAD\%_{H\text{-}NMR} = 6\%$ and $AAD\%_{C\text{-}NMR} = 4\%$, respectively.

Keywords: 5-amino pyrazole, NMR, DFT, UV-visible

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Theoretical and computational studies on deep eutectic solvents of choline chloride

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In the last decades, deep eutectic solvents (DES) have found significant application and development in the field of green chemistry [1]. The mian feature of the presnet study is to demostrate the feasibility of the DESs composed of Choline Chloride (ChCl) as hydrogen band acceptor and malonic acid, succinic acid, and adipic acid carboxylic acids as hydrogen band donnors was studied using quantum mechanical density functional theory (DFT) [2-3]. Geometry optimization and vibrational analysis were done using three various DFT functionals, i.e., B3LYP-D3(BJ), M06-2X, and ωb97X-D3 functionals. The quatum theory of atoms in molecules, natural bond orbital, non-covalent interaction, and the Wiberg bond index (WBI) were subsequently utilized to study the nature of the interactions between ChCl and the carboxylic acids. Generally, from the obtained results, it can be deduced that, the Chloride-induced ion-covalent interactions mainly infulenced the generatation of the DES of the investigated acids with ChCl.

Keywords: Deep eutectic solvents (DES), Choline chloride, Density functional theory (DFT), QTAIM, NBO,

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Calculation of the Intermolecular Potential Energy Surface and Transport Properties for He… CO2 Van Der Waals Complex Using CC, MMA and MD Simulations

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In this work, at the level of the CCSDT/aug-cc-pvQz-BF theory, the intermolecular potentials of the He...CO_2 van der Waals (vdW) complexes at different configurations, with the consideration of the BSSE correction were calculated[1]. The effect of different basis sets and the inclusion of the dummy mid bond functions were also studied. There are two minima in the obtained potential for T-shape He…CO_2 and linear He-OCO configurations. Using Legendre polynomials, the obtained potential was fitted to a fairly exact mathematical model. The generated potential was also utilized to compute the cross viscosity (η_{12}) and cross diffusion (D_{12}) coefficients using the classical Mason-Monchik[2] approximation (MMA), classical molecular dynamics simulations (MD)[3] and full quantum mechanical close coupling (CC) approach. The classical molecular dynamics (MD) simulations were further done using the Leonard-Jones force fields (i.e., with the consideration of just 2-particl interactions) and Vashishta potential models (i.e., with the consideration 2-particl and 3-particl interactions). The observed results support the importance of 3-particl interactions in MD simulations for such a small (vdW) complex.

Keywords: He, CO_2, IPES, MD, MMA

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Detection of thiopropamine by inorganic BC_3 nanotube and nanosheet: DFT studies

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The findings showed that large amounts of chemical sewage is released into the environment by pharmaceutical factories. The other sources of contamination are as folows: expired and unused drugs, and excreted pharmaceutical metabolites formed during drug metabolism in humans and animals. Unfortunately many researches confirmed that the conventional water treatment processes are not effective for reasonable purification of drinking waters. Additionally, due to the long half-life of some drugs especially antibiotics, the risks of drug resistance, mutagenic effects on microorganisms and other cells, and their environmental accumulation are high and may lead to hazardous consequences. So the study of detection methods and removal of drug contaminants from the environment seems necessary [1].

In this study, we investigated potential application of BC_3 nanosheet and nanotube in thiopropamine drug detection. Structural optimization, frontier molecular orbitals and electron density analysis for all structures were performed using dispersion corrected B3LYP-D density functional with 6-31G* basis set which all of them have been implemented in GAMESS program [2]. The B3LYP functional was chosen because it has been previously indicated that it is a good functional for investigation of nanomaterials, and reproduces experimental data[3-4]. The electronic properties of sheet and tube are not affected by Thiopropamine drug which makes them inappropriate for detection process. To overcome this problem, they are doped with Si atom. The reactivity and sensitivity of the Si-doped systems significantly increase and these structures may be promising sensors for Thiopropamine detection. The electrical conductivity of the Si-doped nanotube much more increases at the presence of Thiopropamine compared to the Si-doped sheet.

Keywords: Detection, BC_3 nanosheet and nanotube, Thiopropamine, A DFT study

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Kinetics Study of Hydrogen Generation over Co/g-C_3N_4 Nano Catalyst

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Extraction of hydrogen gas from its compounds is necessary because hydrogen gas can be found rarely in its pure form. Fossil fuels, biomass and water electrolysis are the most resources for hydrogen generation. Sodium borohydride as a non-fossil inorganic energy sources has been suggested as a source for hydrogen gas under mild conditions [1-2]. Among the certain catalysts, $NaBH_4$ can be hydrolyzed and hydrogen gas released. The hydrolysis of $NaBH_4$ is expressed as follows (1).

$$NaBH_4 + 2H_2O \rightarrow NaBO_2 + 4H_2 \uparrow \qquad (1)$$

It is found that, $NaBH_4$ solution hydrolyzed only when certain suitable catalysts are added. As known, it is necessary to stabilize metal nanoclusters in an aqueous solution because of aggregation and agglomeration phenomenon. In this work, in order to reduce particles aggregation and then enhance the catalytic activity of nano powder, graphitic carbon nitride (g-C_3N_4) is used as a stabilizing matrix in preparation processes. A thermolysis method is conducted to prepare g-C_3N_4 from melamine as non-expensive precursor. g-C_3N_4-stabilized Cobalt nano catalyst was synthesized with chemical reduction method. XRD, Fe-SEM, EDS, TEM, TGA/DTA techniques are used for characterization of powders. The catalytic activity of catalyst is tested for hydrogen generation through hydrolysis of alkaline sodium borohydride solution. Kinetic studies on the hydrolysis reaction of $NaBH_4$ are investigated through three factors: (i) initial concentration of $NaBH_4$, (ii) catalyst dosage and (iii) temperature. Arrhenius equation was used to calculate Ea of hydrogen generation reaction at different temperatures. The activation energy (Ea= 55 KJ/mol) was achievement indicated that the compound of Co/g-C_3N_4 has the lowest agglomeration and the highest rate of hydrogen generation. Catalytic hydrolysis of $NaBH_4$ is first order with respect to the catalyst dosage and also first order to $NaBH_4$ concentration in the case of Co/g-C_3N_4.

Keywords: Graphitic carbon nitride, Co nanoparticles, $NaBH_4$, Hydrogen generation, Kinetics

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Study of Effect Phenyl Rings On Electrical Field Power Of The Molecular Switch Containing Fullerene C20 To Be ON State

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In this work, using DFT calculations, the effect of additional phenyl rings on the ON / OFF electric field of a molecular switch made of fullerene C20 as the central skeleton was investigated. By studying the effect of electric fields with strengths ranging from 0 to 80 × 10-4 a.u. on structural changes, it was found that the switch with phenyl groups will be ON in the lower electric field than structures without phenyl groups. Since fullerene is used as the electronic source of the conjugate system in the switch structure [1-2], fullerene resonance with additional phenyl rings causes this phenomenon. When the external electric field changed the energy of the orbitals changes also too. Since the switch is ON whenever the difference in energy levels of the HOMO and LUMO orbitals is zero, it can detect structural energy changes by changing the range of the external field strength [3]. The study of the partial atomic charges of the Au and S atoms with the dihedral angles and the length of the bonds, confirms the reduction of the necessary field to be the switch ON.

Keywords: Molecular switch, Electric field, HLG, NBO.

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Application of Modified screen-printed Electrode as Electrochemical Detector for anti cough drugs

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Anti cough such as Noscapine is a phthalideisoquinoline non-narcotic alkaloid. It is derived from the poppy family through potential antineoplastic, antitussive and mild analgesic activities. This factor mostly is used for its antitussive (cough-suppressing) effects. Its major pharmaceutical action, antitussive activity, is reported to be equal to that of codeine. According to the research, noscapine can cause apoptosis in different kinds of cells and it has a powerful antitumor effects on human breast, solid murine lymphoid tumors, and bladder tumors implanted in nude mice. Noscapine presents in opium in concentrations of 2–8% and is the second most alkaloid in it.A wide range of Noscapine concentration is reported in illicit heroin samples: from none up to 46% of the sample weight [1-4].

In the present study, a La3+doped Co3O4 nanoflowers modified graphite screen-printed electrode (La3+doped Co3O4 nanoflower/SPE) were prepared and used for voltammetric determination of noscapine. Presence nanoflowers lead to a substantial improvement in current in compare to an unmodified electrode. The diagnostic methods used for the purposes of the study include chronoamperometry, differential pulse voltammetry (DPV) and cyclic voltammetry (CV) approaches. The modified SPE was used to determine noscapine in the range of 0.3 to 600.0 μM (LOD= 0.1 μM).

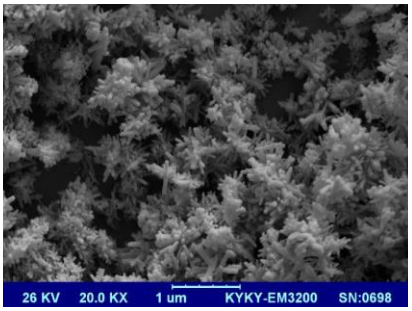

Fig. 1. SEM image of La3+/Co3O4nanoflowers

Keyword**:** Anti cough, Noscapine, Modified electrode, La3+/Co3O4 nanoflower, Voltammetry

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Application of MOWS$_2$ Nanocomposite to fabrication of biosensor for detection food additives

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For many years, sulfite (SO_3^{2-}), has had a global widespread usage as a kind of food additives as sulfite, bisulfite, sulfur dioxide, and metabisulfite. It has been widely applied as an anti-oxidant, food additives, and bacterial growth. Moreover, it modulates enzymatic and non-enzymatic browning responses while protecting and storing food [1-2].

The present study reports synthesis of MOWS$_2$ nanocomposite followed by its characterization using energy dispersive X-ray spectroscopy (EDS), X-Ray diffraction (XRD) and field emission scanning electron microscopy (FESEM). Chronoamperometry (CHA), differential pulse voltammetry (DPV), and cyclic voltammetry (CV) have been used to examine electro-chemical behaviors of sulfite on MOWS2 nanocomposite modified SPE. Electro-chemical specification indicated very good electro-catalytic activities and surface area impact of MOWS$_2$ nanocomposite. Oxidation signals of sulfite on MOWS$_2$/SPE has been considerably increased in comparison to the bare SPE. Within optimum conditions, quantification of sulfite might range between 0.08 to 700.0 μM with a small determination limit of 0.02 μM based on S/N=3.The impact of scan rates has been explored. Finally, the MOWS$_2$/SPE has been employed for detection of sulfite in real specimens. In general, an easy experimental method for manufacturing MOWS$_2$ nanocomposite has been suggested that takes advantage of selectivity, reproducibility, and sensitivity toward electro-active specimens, as well as biological matrices.

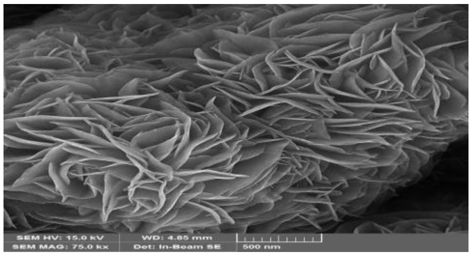

Fig. 1. FESEM Image of MOWS$_2$ composite.

***Keyword*:** Anti-oxidant, Food additives, Biosensor, Nanocomposite

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A non-visual bubble-pressure experimental method for measuring solubility of light hydrocarbons in aqueous solutions

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Aqueous alkanolamine solutions are currently used in industrial natural gas treating and sweetening plants. These solutions must have a high capacity of acid gases (H_2S and CO_2) absorption, low vapor pressure and viscosity, high thermal and chemical stability, and at the same time negligible absorption tendency toward hydrocarbons for efficient gas recovery [1-2]. The solubility of hydrocarbons in gas sweetening solutions is generally physical. The extent of this solubility at a specified temperature and pressure is determined primarily by Henry's law. This work presents features of a new experimental setup that has been recently developed in our laboratory for measuring the solubility of light hydrocarbons, from methane to propane, in aqueous solutions of multi-component mixtures in a wide temperature range of (263 – 373) K and pressures up to about 12000 kPa. The experimental method is based on the synthetic non-visual bubble pressure procedure coupled with an asymptotic Padé approximant technique, devised in this work. The experimental data obtained for methane + water and methane + water + MDEA (*N*-methyldiethanolamine) are in quite good agreement with the reliable experimental values reported in the literature [3-5].

Keywords: Gas solubility, Vapor-liquid equilibria, Gas sweetening, Alkane, Bubble pressure

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Thermodynamic study of electrolytic system "Potassium chloride + water + lysine" based on Pitzer ion interaction model

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Having an accurate knowledge of the thermodynamic properties of electrolytes, especially electrolytes with biochemical compounds such as proteins, sugars and amino acids, is of great importance. The study of the electrolytic system "potassium chloride + lysine + water" is important because potassium chloride is an important compound in metabolic systems and having its thermodynamic properties along with lysine is important. Amino acids are the basic building blocks of proteins and important compounds in organisms, and a deeper understanding of the effect of electrodes on amino acid solutions is needed. These features can be very useful as a basis for efficient design and simulation of separation processes such as extraction, precipitation or drying. Potassium in the living organism helps balance osmotic pressure and maintain moisture inside and outside the cell, as well as the normal functioning of nerves and heart and other physiological functions. In this research, the above electrolytic system was investigated from a thermodynamic point of view based on the ion-Peter interaction model. For this purpose, the mean activity coefficient was measured by potentiometric method using galvanized cell without liquid bonding. Also, potassium ion selective electrodes based on PVC membrane and Ag / AgCl electrode were used [1]. Measurements were performed at 298 K in solutions containing 0, 2, 4, 8 and 10% by weight of lysine in a water-lysine solvent mixture.. In this study, by determining the potentiometry of the average activity coefficients of potassium chloride electrolyte in water and comparing it with the average activity coefficients calculated by the Pitzer ion interaction model, the efficiency of the method and the electrode pair were evaluated. Pitzer parametres were determined. Finally, using the obtained adjustable coefficients, the thermodynamic properties of the solution such as the osmotic coefficient were calculated based on the Pitzer ion interaction model. The results show that the Pitzer ion interaction model is successful for describing the electrolytic system under study [2].

Keywords: Thrmodynamic study, Pitzer equation, Lysine

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Electrochemical Behaviour of NMC/C Cathode in Li-ion Batteries

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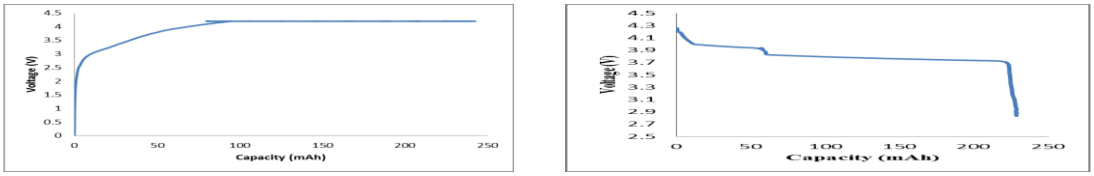
Batteries are consuetude of: an anode, a cathode, and electrolyte [1]. Among various types of batteries, since Li-ion batteries have higher energy densities than that of their counterparts, they have gained much more attention. Current studies take advantage of Ni-Mn-Co (NMC) as a cathode in order to increase reversible capacity, enhance safety, reduce toxicity, and reduce the cost of it. Since the cathode is the limiting part of Li-ion batteries, major advances at the material level are needed to achieve a desired increase in their energy density and power capability [2]. We aim to dope NMC to enhance its stability, increase power and energy density, and cycling. We underlined Li-ion batteries as a promising alternative for small scale and large scale application, and NMC was proposed to enhance such batteries capacity. They suffer from several issues, among which lower conductivity of both electron and ion is the most important one, thereby resulting in lower power efficiency at elevated current densities, which constitutes the main obstacle to the application of the NMC. Using conductive carbon is a promising advance to conquer the insulating nature of NMC. The surface coating tactics stipulate a pliant and active means of improving the electrochemical behavior of lithium-ion batteries (LiBs) since it can help cathodes/anodes from contact humidity and better the thermal fixedness and cyclability of LiBs [3]. Electrochemical charge tests were done at 25°C. Charge curves of NMC cathode materials in the voltage range of 0.2−4.2 V at 25°C are shown in Figure 1(a). The initial cycle was measured at the rate of 0.2C to activate the cathode and to form a stable solid electrolyte interface film. The general charge profile of NMC is observed as relatively flat regions around 3.8 v. And its capacity is 220 mAh. Similarly, the discharge process was performed in the voltage range of 4.2−2.8 V at 25°C, and the capacity is 228 mAh.



a b

Fig. 1. (a) Charge, (b) Discharge

Keywords: Li-ion batteries, NMC, Carbon, Capacity

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Application of Dortmund-UNIFAC thermodynamic model to investigate changes in cola activity coefficient in black beverage model systems

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Beverages are one of the most widely consumed foods in the world, among which black beverages have a significant acceptance worldwide. The most common type of packaging to protect this type of beverage is aluminum cans. The main function of the package is to protect the food from adverse changes such as changes in the taste of the food. Among these changes is the reduction in the taste of the food due to its absorption by the aluminum can varnish, which affects the marketing rate. Over time, at a rate that depends on the temperature, this taste decreases in the food environment [1]. Due to the reduction of this taste, the coefficient of activity of the taste also changes, which by knowing its trend, we can understand the process of reducing the taste at different temperatures and times. The taste is typical in black cola drinks. The purpose of this study is to use an appropriate thermodynamic model to predict changes in the index flavor activity coefficient at different times and also the effect of molecular component changes due to the effect of temperature on the cola activity coefficient as an index flavor. In this research, the effect of three parameters of molar component, time and CO_2 gas on the cola activity coefficient in black beverage model systems was modeled using Dortmond-Unifac thermodynamic model and after determining the model parameters. Gas chromatography was used to determine the concentration of cola in the samples.The results showed that increasing the molar component will reduce the activity coefficient. Also, during storage for 30 days, the amount of cola activity coefficient will be minimal and will increase before and after. The introduction of CO_2 into the beverage system further reduced the cola activity coefficient [2].

$$\ln \gamma_i^C = \ln \frac{\Phi'_i}{x_i} + 1 - \frac{\Phi'_i}{x_i} - 5q_i\left(1 - \frac{\Phi_i}{\theta_i} + \ln \frac{\Phi_i}{\theta_i}\right)$$

Keywords: Activity coefficient, Black beverage, Dortmund-UNIFAC model

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Electronic and nonlinear optical features of a new bowl-shaped subunit of C_{70} decorated with alkali metals (Li, Na and K)

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The design and synthesis of novel materials with excellent nonlinear optical (NLO) properties has attracted great interest in experimental and theoretical fields over the past several decades due to their potential application in optical, electro-optical devices, optical switching and other laser devices [1-2]. Among many strategies for enhancing the NLO response of materials, introducing the diffuse excess electron, such as alkali metals, proposed an efficient approach to improve the NLO properties of different systems [3-4].

Density functional theory (DFT) and time-dependent (TD-DFT) computations have been carried out to study the nonlinear optical response of a new bowl-shaped of C_{70} fullerene [5] ($C_{22}H_{12}$) with alkali metals (Li, Na and K). These interactions result in six, five and four stable conformations for $Li@C_{22}H_{12}$, $Na@C_{22}H_{12}$ and $K@C_{22}H_{12}$ structures, respectively. The electronic and optical properties of decorated structures strongly depend on the type and position of alkali metals. The Na interaction surprisingly causes the remarkable first hyperpolarizability (β_0) enhancement. As a result, the β_0 value of $Na@C_{22}H_{12}$-S1 is 2500 times of pristine $C_{22}H_{12}$ structure. Additionally, the HOMO-LUMO gaps of decorated structures are significantly narrowed due to interaction. These results might introduce new views for the development of designing novel electro-optical nanomaterials.

Keywords: Bowl-shaped $C_{22}H_{12}$, Alkali metal, Hyperpolarizability, DFT calculation, NLO

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Unusual behavior of the sumanene substitute (3BN-3NB) structure relative to similar structures and pristine sumanene

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Sumanene is one of the bowl-shaped fragments of fullerene C_{60} that has six spoke positions[1]. Replacement of polarized unit of BN in C-C bonds produce new heterocyclic with different chemical and electronic properties[2-4].The 3BN-3NB sumanene is formed by replacing the 6BN groups with two different orientations in one by one in the spoke positions of sumanene. At first glance, this molecule seems to have average properties of 3BN and 3NB molecules, or perhaps these two groups will neutralize each other, and this molecule will have properties similar to the pristine sumanene.

In this study, the geometry and electro-optical properties of 3BN-3NB sumanene investigated employing density functional theory (DFT). Afterward results of these calculations are compared with data reported in our previous article in 2021[5]. Despite the first idea, 3BN-3NB sumanene shows no resemblance to pristine sumanene or even other similar molecules in BN and NB orientations. 3BN-3NB sumanene has the greatest HOMO-LUMO gap (4.93 eV) in BN-embedded sumanene structures. The lowest optical properties in consider structures have been obtained for this molecule so that its first static hyperpolarizability (β_0) is 1.12 au. In the dipole moment (1.85 D) it behaves similarly to BN-orientation molecules. The 3BN-3NB sumanene by depth of 1.22 Å is deeper than pristine sumanene (1.06 Å) and BN-structures. By analyzing the structure of this molecule, can examine more closely the factors affecting the nonlinear optical properties.

Keywords: Sumanene nanobowl, BN orientation pattern, Optical properties, DFT

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Study of the effects of fullerene and five anticoagulants drug with computational chemistry

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By combining the science of nanomaterials and medicine, scientists were interested in a new topic centered on drug delivery. One of the most important goals of drug delivery systems is to reduce the side effects of consumption and increase the drug's effect on the tissue. Designing drug delivery systems in laboratories and experimentally, in turn, has many difficulties. With the advancement of computational chemistry and the more efficient use of cloud computing in computing, both financial costs and time can be saved [1-2].

The drugs considered in this study were five essential drugs in the control of blood coagulation, rivaroxaban, warfarin, edoxaban, dabigatran, and Apixaban, which interacted with fullerene of C60 and formed a complex.

In this study, Gaussian09 software was used to calculate the energy composition, Gaussview5 was used to arrange the drugs and complexes, and Spartan was used to calculate the energy of the LUMO and HOMO. Chemoffice compounds to obtain the most likely structure of fullerene. The equation used in this study was the DFT of the basic function B3LYP-6-311G * presented in SPARTAN software and on HIKCHEM online servers running Windows according to the software output data of all five drugs Rivaroxaban, Warfarin, and Edoxaban [3-5]. They are Dabigatran. And Apixaban has the lowest total energy, and due to the negative absorption energy of the reaction between drugs and fullerene, it can be performed in the laboratory and experimentally.

Keywords: Computational chemistry, Fullerene, Drug delivery, DFT, Anticoagulants

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Catalytic Activity of Zeolites Modified by Cr and Mo Nanopowders in the Conversion of Methanol to Hydrocarbons

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The study of methanol conversion may help to solve one of the global issues finding alternative raw materials to obtain petrochemical products [1-2]. Methanol-to-light and aromatic hydrocarbons (MTH) over zeolites and zeolite based catalysts are considered as suitable choice for these processes due to their unique structure and catalytic properties.

Over the H-form zeolite at 350-400ºC temperature methanol conversion rate was as the same 100% as it was on the modified samples. The main products of methanol conversion are olefins C_2-C_4 (30-40%), aliphatic hydrocarbons C_{5+} (15-25%) and aromatic hydrocarbons C_6-C_{10} (25-40%).

We have studied the effect of metal nanopowders (Cr, Mo) modified zeolites on the selectivity of p-xylene at the temperature (400ºC). It is shown that the modification of HZSM-5 nanopowders by Cr and Mo led to an augmentation in the selectivity of formation of p-xylene. The enhancement of molybdenum nanopowder content from 2.0 wt% to 6,0wt% in HZSM-5 consequentially increases the selectivity of p-xylene from 45.3% to 62.5%.

Modifying Mo/HZSM-5 with 6.0wt% Cr changes the activity and para-selectivity of catalyst, as result of the acid sites redistribution and change in properties of molecular-sieve zeolite. Thus, the possibility of usage the pentasil type of zeolite modified by the Cr and Mo nanopowders for selective synthesis of aromatic hydrocarbons from methanol is shown. It was found that the addition of Mo and Cr nanopowders to HZSM-5 leads to a decrease in the concentration of strong proton sites and an increase in the concentration of medium strength acid sites.

Thus, the modification of zeolite with chromium and molybdenum leads to redistribution of its acid sites by strength and the formation of new active sites. Due to this point the ratio of weak acid sites to strength sites changes, which affects its catalytic properties in conversion of methanol. A certain combination of weak and strong acid sites is necessary to obtain an effective catalyst for the conversion of methanol to aromatic hydrocarbons, which is achieved by controlling the amount of modifiers in the catalytic system.

Keywords: Methanol, ZSM-5, aromatic hydrocarbons, nanopowders, molybdenum, chromium

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Use of artificial neural network to predict the thermodynamic properties of organic solvents in ionic liquids at infinite dilution

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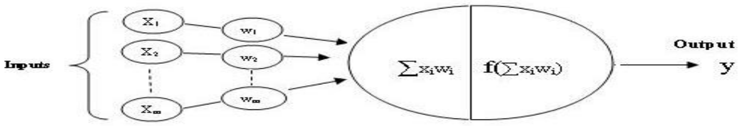
In recent years, the use of ionic liquids as green solvents in various chemical and biochemical processes has increased significantly. Thermodynamic properties such as activity coefficient in infinite dilution is one of the essential parameters in solvent design and selection. On the other hand, artificial neural networks have been widely used in various fields of chemistry, including physical chemistry, to successfully predict and model the various properties of chemical systems. In this study, using artificial neural network, activity coefficients in infinite dilution (∞γ) of organic solvents in ionic liquids were predicted. The systems used in this design include imidazolium-based mixtures of two components of alkanes in ionic liquid. The neural network program code was written in MATLAB language by the project manager. After testing different networks, finally the feed forward network with topology 1-10-8 and sigmoid and linear activation functions were selected for the hidden and output layers, respectively. The reverse diffusion method with Levenberg-Marquardt algorithm is used to train the lattice. And according to the purpose of natural logarithm research, the coefficients of activity in infinite dilution of solutes are considered as output. In order to calculate the dipole moment of ionic liquids and the softness of organic compounds, first the structure of all compounds was plotted in HyperChem software. Then, using GAMESS software, the three-dimensional structure of the compounds was optimized by B3LYP / G-31 (d, p) method, and finally the dipole moment of ionic liquids and the softness of organic compounds were calculated.Comparison of the network results with experimental values of ∞γ showed that the artificial neural network can be used as a powerful computational tool to predict the thermodynamic properties of systems containing ionic liquids. RMSE and R2 are the data predicted by the network designed for the training series of 0.104 and 0.997 and for the test series of 0.126 and 0.993[1].



Keywords: Organic soluble, Activity coefficients, Ionic liquids, Artificial neural network.

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Study of the temperature effect on the aqueous two-phase systems composed of polyethylene glycol 6000 + tri-lithium citrate + water at and the partition of salbutamol drug *T* =288.15, 298.15, 308.15 and 318.15 K

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Liquid-liquid equilibria (LLE) for the PEG 6000 + tri-lithium citrate + water teraary system was measured at the temperatures 288.15, 298.15, 308.15, and 318.15 K . The effect of temperature on the binodal curves and the tie-lines of the investigated aqueous two-phase system were measured experimentally. It is found that, an increase in the temperature caused significant expansion of the two-phase area. Merchuk equation was used to represent the experimental binodal curves [1]. Also, tie-line compositions were correlated with Seteschenow, Othmer-Tobias, Osmotic-Virial, m-NRTL, and e-Wilson models, and the parameters are reported. The result of the correlation using the e-Wilson model was also compared with the m-NRTL model [2] and it was shown that the e-Wilson model works better and more accurately. In addition, the partitioning of the salbutamol drug in the investigated aqueous two-phase system was studied. It was found that, the partitioning coefficient of the salbutamol drug was decreased by increasing the temperature of the system.

Keywords: LLE, PEG, Tri-lithium citrate

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Study of photocatalytic activity of $ZnO/Bi_{24}O_{31}Br_{10}$(40%) nanocomposite for rapid degradation of Methylene blue in wastewater

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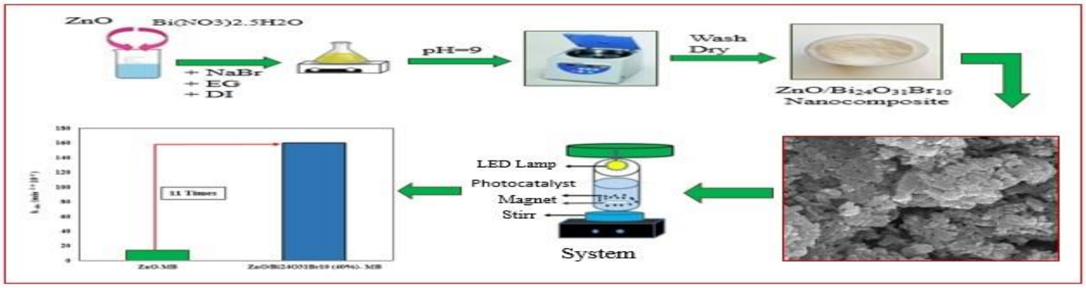
Over the last decade, Industrial wastewaters contain hazardous contaminants that pollute the environment thus demanding the recruitment of impressive remediation methods such as photocatalysis [1]. Advanced oxidative processes (AOPs) have gathered a lot of attention as a promising route to decontamination of water [2].

In this work, a novel $ZnO/Bi_{24}O_{31}Br_{10}$(40%) was synthesized a facile method. The as prepared $ZnO/Bi_{24}O_{31}Br_{10}$(40%) was characterized by FESEM. Fortunately, unlike other heavy metals which are highly toxic, bismuth is non-toxic and non-carcinogenic [3]. Fig. 1 illustrates the respective FESEM images of $ZnO/Bi_{24}O_{31}Br_{10}$(40%).

It can be observed that the $ZnO/Bi_{24}O_{31}Br_{10}$(40%) samples prepared all show a multi-plate structure without obvious stacking. The $ZnO/Bi_{24}O_{31}Br_{10}$(40%) photocatalyst displayed the highest ability for photodegradation of methylene blue, which was almost 11 times as high as the bare ZnO. It was beneficial for developing new nano struture and improving the catalytic performance.



Keywords: Methylene blue, $ZnO/Bi_{24}O_{31}Br_{10}$(40%), Photocatalytic activity, Wastewater

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First-principles calculation the magnetic properties of Mn-doped ZnSe

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Diluted Magnetic Semiconductors are very useful materials for spintronics and optoelectronics devices [1]. The studied wurtzite ZnSe compound is also extremely photosensitive in the entire range of spectrum, with bulk direct band gap of 2.7 eV at room temperature [2].

The magnetic moments for Mn and its neighboring host atoms have also been calculated in detail using DFT-LSDA+U method. It is known that undoped ZnSe is non-magnetic material but on doping Mn, the main contribution to magnetization of supercell comes from impurity atom and small contribution of host atoms. The investigations performed for 16-, 32-, 64-, 128- and 256-atom $Zn_{1-x}Mn_xSe$ systems show that Zn substitutions by Mn^{2+} ion lead to a paramagnetic spin ordering. The mainly contribution to the magnetization comes in essence from *d*-states of Mn impurity atom. Results of the energy difference between the DLM and the FM state for $Zn_{1-x}Mn_xSe$ nearly present a stable DLM state. The value of the total magnetic moment of investigated supercells was found 5.0 μ_B.

The band gap energy of ZnSe supercells are observed to be decreasing after Zn replaced by Mn atom. The presence of Zn vacancy in Mn doped ZnSe system affect the magnetization, where increases the magnetic moment of the supercell and behaves half-metallic state and total magnetic moment for $Mn_xZn_{1-x}Se$ with one Zn vacancy-defected system is about ~6 μ_B.

The calculations results of exchange splitting constants approve that paramagnetism exists in Mn-doped ZnSe and this material is useful for magneto-optical devices.

Keywords: ZnSe, magnetization, half-metallic, spin-glass

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Dielectric Investigation of binary systems of alcohol-solvent using different dielectric models

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In this study, models for predicting the dielectric behavior of binary systems with the aim of explaining them were improved. In this regard, the required information was extracted from reliable sources. Excel software the required relationships was used as an add-on to specify the interaction factor as well as to match the experimental information with the theory models [1]. We classified forty systems into four main groups: alcohol-alcohol, alcohol-ketone, alcohol-ester, and alcohol-hydrocarbon. Our purpose of this classification was to be able to examine the changes a (improvement factor) in a particular model during the change of the binary system type. Then the results obtained in Excel environment in seventeen models (Oster, Lichteneker-Rother, Bruggeman, Looyenga, Krazewski, Bottcher-Bordewijk, upper Hashin-Strickman, Peon-Iglesias, Iglesias-Peon, rayleight-Maxwell, Weiner, Gross- Graph, sen, ideal state, Onsager-Bottcher, Iglesias, Brown) were plotted [2].

First, we compared the data deviation from the experimental results before and after improvement, as well as the improvement factor and the rate of improvement in groups and subgroups. Finally, the obtained information emphasized that the improvement made on the systems by the models will increase the improvement of all systems [3]. But along with this initial goal, we also came to the conclusion that the alcohol-alcohol group responded better to the models than the other three groups [4]. Then, the effect of chain length and number of branches connected to the alcohol-carrying atom on the improvement factor of alcoholic systems was investigated and the results show that alcohols that have more branches around the carbon-bearing carbon of the alcoholic agent or have a larger chain next time, as a result, the improvement factor has the most change compared to the initial model.

Keywords: Alcohol, Improvement, Solvent, Binary, Dielectric model

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Adsorption of SO_2 gas on two different SWCNTs: A DFT study

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To develop novel nano materials for online detection of insulated faults in SF_6 insulated equipment [1], two single wall carbon nanotubes (SWCNTs) with 32 and 64 atoms are proposed and their sensing capabilities for the measurement of typical decomposition products of SF_6 insulated gas (SO_2) are investigated based on density functional theory (DFT), in this work. Furthermore, adsorption energies, densities of states, band structures, partial densities of states (PDOS) and their conductivities were analyzed to interpret the mechanism of gas adsorption on the surfaces of SWCNTs. All calculations were performed using the Quantum Espresso package, which is based on the density functional theory (DFT) methods [2]. Our calculations were performed on two super cells with 32 and 64 atoms in a hexagonal lattice. All structures were relaxed before and after SO_2 adsorption. The structural results show that after optimization, the gas molecule was located at a distance bout 2.9945 Å and 4.3028 Å for (SWCNTs) with 32 and 64 atoms, respectively. The relaxed structures were applied for future calculations. The results of electronics reveal that the band gap of (8, 0) SWCNT with 64 and 32 atoms are close to each other. However, SO_2 adsorption reduces the band gap of 64 atoms SWCNT more evidently. Therefore, by adsorbing SO_2 to SWCNT the conductivity increases which can be used for detecting SO_2 gas. Doping CNT can improve the adsorption, considerably.

Keywords: Single walled carbon nanotube (SWCNT), Density functional theory (DFT), Adsorption.

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Adsorption kinetics of surface-modified nanoparticles onto a solid surface

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Polymer-coated nanoparticles which are responsive to their micro-environment in a controlled manner are colloidal nanoparticles that are coated with at least two physico-chemically distinct moieties. Recent advances in the synthesis and characterization of nanoparticles have made it possible to produce responsive surface-modified nanoparticles with hydrophilic and hydrophobic surface groups. These nanoparticles act like colloidal surfactants [1-2]. In various applications, understanding the effect of nanoparticle surface chemistry on the kinetics of nanoparticles' adsorption onto solid surfaces is of great importance for nanoparticle engineering. The aim of this study was to experimentally study the adsorption of the surface-modified nanoparticles, bonded with hydrophobic and/or hydrophilic agents, onto a silica surface. While no measurable adsorption was observed for solely hydrophobic or hydrophilic nanoparticles, a significant amount of adsorption was observed for nanoparticles coated with both hydrophilic and hydrophobic agents. Various kinetic models were used to model the adsorption kinetics of the responsive nanoparticles. The results show that adsorption-reaction models predict the kinetics better than the adsorption-diffusion models.

Keywords: Adsorption, Kinetics, Nanoparticle, Silica surface

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First principal study of structural and electronic properties of nitrogen and boron doped superprismane

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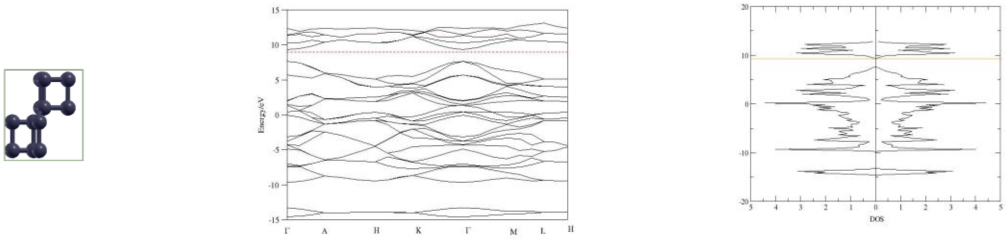
Carbon present numerous allotropes (fullerenes, carbon nanotubes(CNTs), graphene, graphite, diamond and amorphous carbon) thanks to its ability to form sp-,sp2- and sp3-hybridized bonds. cold compression of graphite, single-walled and multiwalled CNTs [1] results in super hard allotropes of carbon, which were found to be naturally different from hexagonal (or cubic) diamond. Joining of two three-membered rings to one another by three single bonds leads to a prismane [2]. The superprismane is composed of prismane units, which are inherently made up of carbon triangular networks. In this study, we have investigated the structural and electronic properties of superprismane and the effect of N or B doping on these properties using first-principles density functional theory (DFT).The results show that this doping does not change the structure of superprismane, considerably. Band structure and DOS results show that superprismane is a semiconductor with 1.65 eV band gap. After doping superprismane with N and B atoms the band gap removes and the semiconductor superprismane tunrs into a conductor. Therefore, doping superprismane with B and N atoms change its electronic properties, considerably which can be used in electronic devices.



a **b** **c**

Fig. 1. a) relaxed structure b) bandstructure c) DOS of superprismane

Keywords: DFT, Superprismane, Band Structure, Dopping

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Density Functional Study of Structural Stabilities, Electric and Magnetic Properties of Formamide Adsorption on pure Nanotube

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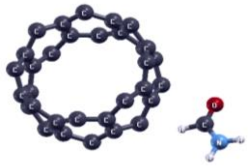
Recently, carbon nanotubes (CNT) have proved their suitability as adsorbents and catalyst aids [1]. It has been shown that pristine carbon nanotubes can adsorb some special molecules. However, CNTs have high surface area and porosity that help them to adsorb small catalyst particles which can improve the nanotube's sensing performance. Formamide ($HCONH_2$,FM) is the simplest amide, which can is considered as an appropriate model molecule to search the nature of amide-surface interactions [2]. Moreover FM is considered as model molecule for the investigation of a basic building unit in proteins and the simplest model of nucleic base linkage due to its simple yet rich structure, which includes an amide bond [3]. In this work, formamide ($HCONH_2$,FM) molecule adsorption on pristine (8,0) single-walled carbon nanotube (SWCNT) was studied by the dispersion corrected density functional theory method, in the spin polarized mode, along with the Quantum-ESPRESSO computational package.The formamide molecule was adsorbed from the oxygen and nitrogen side vertically on pristine nanotube. Both structures were relaxed, and the structural and electronic properties were investigated before and after FM adsorption. Obtained results show that adsorption energies of (FM) O-SWCNT and (FM) N-SWCNT are -0.0479eV and -0.0162eV, respectively .Therefore, oxygen side of FM can be adsorbed more strongly more strongly to SWCNT. However low adsorption energies show the physical adsorption. Moreover, band structure and DOS results show that FM adsorption increases the bandgap of pristine SWCNT from 0.4 eV to 0.6-eV. Spin polarized calculations show that SWCNT has no magnetic properties which doesn't change after adsorption.



Optimized structures

Keywords: Density functional theory, SWCNT, $HCONH_2$, Electronic properties

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Influence of a salt on the liquid- liquid equilibrium data of (water + propanoic acid + ester) ternary system

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Propanoic acid is an organic acid produced by chemical synthetic or fermentation processes. Due to the importance of this acid, its purification and recycling from dilute solutions are essential. Since these acids give rise to azeotropic mixtures in the extraction process, it is impossible to separate them by distillation. One of the best methods for their separation from aqueous solutions is the liquid-liquid extraction method. Liquid-liquid equilibrium data are essential in every extraction process. The presence of salt can affect the extraction capacity. Considering the importance of the effect of salt on extraction, in this study, phase equilibrium data were determined by the cloud point titration method for the water + propanoic acid + isopentyl acetate ternary system in the presence of Na_2SO_4 salt under the atmospheric pressure and 298.15 K [1-3]. On the basis of this liquid-liquid equilibrium (LLE) data, the distribution coefficient of propanoic acid between the aqueous and organic phases was specificated. The results show that the distribution coefficient of propanoic acid is high due to the low miscibility of isopentyl acetate and water. The presence of Na_2SO_4 salt in the aqueous phase leads to an increase in the distribution coefficient of propanoic acid. The amount of selectivity for the salt-free system is in the 9.1-32.2 ranges and in the presence of Na_2SO_4 salt is in the 126.1-279.9 ranges [4]. The results show that in the presence of Na_2SO_4 salt, better extraction is performed. The Eisen-Joffe equation as a common model for the quaternary systems containing salt was used to examine the consistency of the experimental data and also NRTL model was applied to correlate them. Usually, NRTL and UNIQUAC thermodynamic models are used for the correlations of LLE data but in some cases, the results of the NRTL model are better [5]. In the presence of Na_2SO_4 salt, the root mean square deviations of compositions for the NRTL model, was 0.0132.

Keywords: liquid- liquid equilibrium, propanoic acid, isopentyl acetate, Na_2SO_4, NRTL model

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Design of Novel Molecular Switch Using the C24 Fullerene and Electrode of Ag

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In this research, the possibility of using the fullerene C24 and silver electrode to design a molecular switch has been investigated. Different electric fields were applied to the molecular switch and its effects on structural and electrical properties were studied [1]. It was shown that the structure of the molecular switch changed due to the application of electric fields with different strengths. The energies of HOMO and LUMO orbitals are also affected by field strength and energy changes. In a particular electric field, their difference reach to about zero, which is equivalent to the electric field required to change the molecular switch to the on state. In different electric fields, the dihedral angles Au-S-C-C were analyzed and showed that they change with the applied electric fields [2-3]. A noteworthy point is that a sharp change was observed in a specific field related to the switch to ON. The overall of the results of frequency analysis, molecular orbital and structural analysis of molecular switches in different electric fields confirm each other.

Keywords: Nono switch, Fullerene C24, HLG, DFT.

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A density functional theory study on the defect stabilized Fe atom on porous BN sheet as a potential electrocatalysts for oxygen reduction reaction

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The slow kinetics of the cathodic oxygen reduction reduction (ORR) remain a significant issue in the development of polymer electrolyte membrane fuel cells (FCs) [1]. Currently, precious Pt-based materials are the most efficient cathodic catalysts for the ORR process [2]. However, the high cost, scarcity, and catalytic instability place significant constraints on their widespread commercial implementation [3].In this study, Fe-doped porous BN (*p*-BN) nanosheet is proposed as an efficient and noble-metal free electrocatalyst for the ORR process in FCs using first-principles calculations. Electronic structure spin-polarized calculations were carried out by the DMol^3 [4], employing the dispersion-corrected PBE functional.

The calculated formation energies show that the Fe atom is more stable on the *p*-BN with a boron vacancy than one with a nitrogen vacancy. The ORR process on this electrocatalyst begins with the cleavage of the O-O bond of chemisorbed O_2, followed by the hydrogenation of the separated O atoms to produce two water molecules. The rate-determining step in the ORR process is the formation of the second H_2O molecule with an energy barrier of 1.12 eV. As a result, ORR prefers a direct four-electron route on the Fe-doped *p*-BN catalyst. Our findings can help in the design and manufacturing of novel electrocatalysts for ORR in FCs.

Keywords: Porous boron nitride, ORR, Electrocatalyst, DFT, Fuel cell

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Investigation of curcumin solubility in the presence of deep eutectic solvents as novel green solvents

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Curcumin is a biologically active substance and a natural antioxidant, but it is almost insoluble in water and has low bioavailability. A possible solution to this barrier could be to use solvents that are low toxicity and biodegradable. Choline chloride-based DES can be used as a co-solvent to increase the solubility of curcumin [1-2]. The objectives of this study are to introduce and prepare DESs, to measure the solubility of curcumin in water and DES as well as in water - DES mixtures with different weight percentages. In this perspective, the solubility of Curcumin is measured in the mixtures of water with some DESs based on choline chloride (ChCl) and in pure solvents at T = 298.15 K to 313.15 K. The measured solubility data were correlated by the activity coefficients models e-NRTL and UNIQUAC. Finally, the thermodynamic functions entropy, enthalpy, and Gibbs free energy were estimated for dissolution using van't Hoff equation [3-5].

Keywords: Curcumin; Solubility; Deep eutectic solvent; Thermodynamic functions.

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Effect of choline-based deep eutectic solvents on the thermodynamic properties of phenytoin drug

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Thermodynamic studies provide complete information about the interactions in the mixture and the choice of proper solvent for the different fields of pharmaceutical sciences. Especially, the study of antiepileptic drugs in solutions (ethanol + co-solvent) has been a subject of interest owing to their effect in the systems using interaction with a number of important biological membranes [1-5]. This work focuses on the measurement of density and speed of sound of the Phenytoin (PTH) in ethanol + deep eutectic solvents (choline chloride/ethylene glycol, and choline chloride/glycerol) solutions as the innovative class of green solvents at temperature range (288.15 to 318.15) K.

Some thermophysical parameters including apparent molar volumes V_{ϕ}, apparent molar isobaric expansion E_{φ}^{0}, and Hepler's constant, apparent molar isentropic compressibility κ_{φ} are obtained and calculated using the density and speed of sound data. For fitting the experimental V_{ϕ} and κ_{φ} the Redlich-Meyer equation is used to define a number of quantities containing standard partial molar volume and partial molar isentropic compressibility. The thermodynamic analysis of the studied system also plays a crucial role in the pharmaceutical industry.

Keywords: Density, Speed of sound, Phenytoin, Deep eutectic solvent (DES), Hansen solubility parameter, Redlich-Meyer equation.

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Ultrasonic-assisted extraction of curcuminoids from turmeric by using some green solvents

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Curcuminoids (CURs), bioactive and antioxidant polyphenols, are major components of turmeric. Commercially available component in CURs are curcumin (C) as the main constituent and the other two demethoxycurcumin (DMC) and bisdemethoxycurcumin (BDMC) as minor components [1-5]. Extraction and analysis of these components from turmeric may pose specific challenges and yield different results. The organic solvents applied in traditional solvent extraction systems are not eco-friendly owing to their properties such as flammability, toxicity and volatility. For this reason, in this research work, ten deep eutectic solvents (DESs) and three ionic liquids (ILs) were selected to investigate the extraction of CURs from turmeric. Further, DES and ILs-based extraction was performed under ultrasound. Under extraction conditions, the CURs in the turmeric powder was measured by the use of high performance liquid chromatography (HPLC). The maximum CURs amount of 164.51 mg/g was attained using effective ultrasound-assisted extraction in 50% water content DES or IL at 5% solid loading with 50.8 W/cm2 power intensity at 363 K in 60 min. This improved extraction method can be economical, green and effective alternative to conventional solvent extraction for CURs.

Keywords: Curcuminoids; Solubility; Deep eutectic solvent; Ionic liquids; Hansen solubility parameters.

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Thermophysical properties study of protic ionic liquid 2-hydroxyethylammonium lactate for thermal energy storage systems

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Thermal energy plays an important role in the sustainable development of modern societies. Thermal energy storage (TES), as a kay component in different domestic and industrial processes and power generation systems, ensures power transmission capability and economic profitability. In this regard, ionic liquids can be used as potential candidates for thermal energy storage owing to their remarkable thermophysical properties. In this project, protic ionic liquid 2-hydroxyethylammonium lactate was synthesized. The synthesized ionic liquid is use in thermal energy storage systems, which has high thermal stability, easy and economical synthesis with suitable chemical and physical properties. In the following, thermophysical measurements such as heat capacity, surface tension, density, and speed of sound for pure ionic liquid at different temperatures were performed to evaluate the efficiency of these systems as thermal energy storage. The results of differential scanning calorimetry analysis show that the ionic liquid 2-hydroxyethylammonium lactate has a higher heat capacity than the other literature ionic liquids. Heat capacity also increases with increasing temperature. Efficient thermal energy storage systems have a sufficiently high heat capacity and thermal energy density. The ionic liquid 2-hydroxyethylammonium lactate with a high heat capacity and thermal energy density is recommended as an appropriate candidate for thermal energy storage.

Keywords: Thermal energy storage, Protic ionic liquids 2-hydroxyethylammonium lactate, Heat capacity, Thermal storage density.

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Green Separation of Azeotropic Mixture (Hydrocarbon + Alcohol) Using Deep Eutectic Solvent

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The separation of azeotropic mixtures is an “old” engineering problem that cannot be solved by simple distillation processes. One of the current ways to overcome this problem is to use other types of processes. Liquid–liquid extraction processes have been emerging as appealing alternatives because they do not require high amounts of energy, volatile organic compounds or high pressures[1]. A Deep eutectic solvent (DES) is a combination of a hydrogen bond acceptor (HBA) and a hydrogen bond donor (HBD), in which a mixture is formed, usually having much lower melting temperature than the components of the combination. DESs are advantageous because they can be easily prepared in high purity at low cost, their components are biodegradable and possess low toxicity. Moreover, most DESs are nonreactive with water [2]. In this work, the DES is tested as extraction solvent in the liquid–liquid separation of azeotropic mixture (hydrocarbon + alcohol) at T = 298.2 K and atmospheric pressure. Data for the binodal curve was determined by cloud-point titration method. Refractive index measurement was employed to determine the concentration of all species in each phase. The reliability of the experimental tie-line results was tested through the Othmer–Tobias correlation equation. Distribution coefficients and separation factors were evaluated over the immiscibility region. Finally, the experimental data were successfully correlated using the NRTL model. The results show the ability of this DES for extraction of alcohol from hydrocarbon.

Keywords: Azeotropic mixtures, Deep eutectic solvent (DES), Othmer–Tobias, NRTL model.

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Introduction and study of anodes (metal ions) in batteries and applications of nanotechnology in optimizing batteries

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Improving the properties of the anode, including increasing its capacity, is one of the essentials for improving battery performance. In this paper, high-capacity anodes with alloy performance are introduced, then the problem of fragmentation of these anodes and its effect on the life cycle is expressed. Finally, various cases are discussed. In this paper, electrode reduction at the anode, which is a nanoscale phenomenon, is described. The negative effects of this phenomenon on alloy anodes and how to remove it are described. These negative effects will be discussed by preparing suitable nanostructures[1].

Today, the use of carbon materials, especially synthetic graphite or the selection of highly ionized metals with higher energy capacity and voltage in discharge and charge modes is considered as an increase in efficiency and colometric energy in modern batteries in a negative state. . Lithium battery electrodes typically use a mixture of amorphous carbon and graphite to optimize properties such as power to energy ratio. In this research, it has been tried to investigate the increase of battery efficiency by selecting metals with high ionization power[2].

***Keywords**:* Optimizing batteries, Metal ions, Study of anodes

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Investigation of liquid-liquid equilibrium of ternary system (water + acetic acid + organic solvent) at *T*=298.2 K

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Liquid–liquid equilibrium (LLE) data for the ternary mixture of {water (1) + acetic acid (2) + organic solvent (3)} were determined at *T* = 298.2 K and atmospheric pressure. Cloud point method was used to obtain the solubility data and the acidimetric titration and refractive index methods were used to determine the tie-line data [1]. A type-1 LLE phase diagram was obtained for this ternary system. The reliability of the experimental tie-line results was tested through the Othmer–Tobias equation. The experimental LLE results were correlated with the UNIQUAC and NRTL models, and the binary interaction parameters were obtained [2]. Distribution coefficients and separation factors were obtained from the tie-line data in order to evaluate the capacity of the studied solvent.

Keywords: Ternary mixture, Acetic acid, Othmer–Tobias, UNIQUAC, NRTL.

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Study of liquid-liquid phase equilibria ternary systems of (water + acetic acid + styrene) at T=298.2 and 308.2: Measurement and modeling

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This study reports the liquid-liquid equilibrium (LLE) [1] data and ternary phase diagrams for the (water + acetic acid + styrene) at T = (298.2 and 308.2) K and under pressure of 101.3 kPa for the first time. The aim of this study is to scrutinize the partitioning of acetic acid from aqueous solutions by styrene. The cloud-point titration method was used to determine solubility curves data. The studied systems exhibit type-1binodal curves. The tie -line measurements were defined by acidimetric titration, the Karl-Fisher technique, and refractive index measurements. The distribution coefficients and separation factors were estimated over the immiscibility region. The validity of the experimental tie-line data were ascertained by applying the Othmer-Tobias and Hand correlations. The thermodynamic model of NRTL were successfully applied to fit the experimental tie lines and the model binary interaction parameters were determined [1].

Keywords: Liquid-liquid equilibrium, Phase diagram, Acetic acid, Benzyl acetate, Styrene Thermodynamic modeling.

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Excess molar volumes and excess isentropic compressibility's of binary mixtures of 3-Amino-1-propanol, N,N-dimethylacetamide and cyclohexanone at 298.15 K and ambient pressure

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Densities ρ, Speed of sound U, of binary mixtures consisting of 3-Amino-1-propanol, *N*,*N*-dimethylacetamide and cyclohexanone were measured at 298.15K for the liquid region and at ambient pressure for the whole composition ranges. The excess molar volumes V^E excess isentropic compressibility Δk_s were calculated by equations 1 - 3 from experimental data.

$$V_m^E = \sum_{i=1}^{N} x_i M_i(\rho^{-1} - \rho_i^{-1})(1),\ \ \Delta K_s = K_s - \sum_{i=1}^{2} x_i K_{s,i}^{\circ}(2),\ \ K_s = 1/\rho u^2\ (3)$$

The excess molar volumes and excess isentropic compressibility are positive over the whole composition ranges for binary mixtures of 3-Amino-1-propanol + *N*,*N*-dimethylacetamide and *N*,*N*-dimethylacetamide + cyclohexanone whereas is negative for 3-Amino-1-propanol + cyclohexanone. The excess molar volumes V^E and excess isentropic compressibility Δk_s magnitude for all binary mixture are as following: (3-Amino-1-propanol + *N*,*N*-dimethylacetamide): $0.05752 < V^E < 0.31478$, 1.68397E-09 < Δk_s < 1.03363E-08; (3-Amino-1-propanol + cyclohexanone): $-0.11144 < V^E < -0.5493$, -3.6738E-09 < Δk_s < -1.5502E-08; (*N*,*N*-dimethylacetamide + cyclohexanone): $0.00721 < V^E < 0.49662$, 4.28573E-09 < Δk_s < 2.11437E-08. The calculated data were satisfactory correlated by Redlich-Kister equation [1]. The results were analysed to discuss the effect of chain length, the orientation and number of OH group and the structural effect [2-3].

Keywords: Excess molar volume, Excess isentropic compressibility, 3-Amino-1-propanol, *N*,*N*-dimethylacetamide, Cyclohexanone

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Computational investigation of the functional monomer and solvent selection for molecular imprinting of propyl gallate

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Since the interactions between the functional monomer (FM) and template molecule (TM) affect the quality of the molecule identification sites and are related to the amount and mechanism of interactions in the pre-polymerization mixture [1]. Therefore, to produce a molecular polymer with high selectivity, it is necessary to study the physical parameters affecting these interactions [2-3]. In the present work, for the first time, the interaction process between n-propyl gallate and functional monomer in the preparation of molecularly imprinted polymer was performed based on computational studies. For this purpose, the optimal geometry, single point energy and binding energy were calculated from the density function theory (DFT) at the functional theory level of B_3LYP with a base set of 6-31G(d) [4]. Three functional monomers including acrylic acid, acrylamide, 4-vinyl pyridine were investigated and acrylamide was selected as the functional monomer. In order to investigate the environment and porous solvent, five solvents with different dielectric constants were discussed using the Polarizable continuum model (PCM), as a result toluene was selected as a suitable solvent in which synthesis can be performed [5]. The simulation results show that propyl gallate and acrylamide form a stable complex through hydrogen bonding which is the minimum binding energy in the of 1: 5 molars ratio and is the most stable complex.

Keywords: Functional Monomer, Template molecule, Molecularly imprinted polymer, DFT, PCM

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Permittivities and refractive indices for binary systems containing Dimethyl phthalate and Glycols at different temperatures

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The relative permittivity and refractive index of two binary systems containing a phthalate ester (Dimethyl phthalate) and Glycols (Diethylene glycol or Triethylene glycol) over the full composition range at T = (298.15, 303.15, 308.15) K and p = 0.1 MPa have been measured for the first time. In this study the role of intermolecular interactions and the constituent molecular structures on the dielectric, optical and structural properties of the binary liquid mixtures (Dimethyl phthalate + Diethylene glycol or Triethylene glycol) were studied and analyzed with various approaches [1].

Keywords: Dielectric, Relative permittivity , Diethylene glycol

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Activation of the methane C–H bond by Al- and Ga-doped graphenes: a DFT investigation

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Methane (CH_4) is the most important component of natural gas, accounting for more than 80% of its overall composition [1-2]. CH_4 is a potential candidate for use as a feedstock in chemistry due to the abundance of natural gas supplies [3]. However, because of the high chemical inertness of CH_4, such a goal remains a challenge for modern chemistry. Hence, one of the major objectives of current research is the conversion and use of CH_4 for the production of liquid and gaseous fuels [4]. The potential of Al- and Ga-doped graphene (Al–Gr/Ga–Gr) to activate the C–H bond of CH_4 by N_2O to generate methanol is explored using density functional theory calculations. Both surfaces have a higher affinity for capturing N_2O than CH_4. The oxidation of CH_4 starts with the decomposition of N_2O into N_2 and O_{ads} species, followed by a hydrogen transfer from CH_4 to O_{ads}, resulting in CH_3 and HO_{ads} species. Our results demonstrate that CH_3 combining with HO_{ads} to yield CH_3OH needs only 0.18 eV on Al–Gr, which is 0.11 eV lower than on Ga–Gr. The findings are comparable to those of other previous studies [6]. On the other hand, the competing CO oxidation reaction ($CO + O_{ads} - CO_2$) is inhibited over the Ga–Gr because of its greater activation barrier than the CH_4 oxidation process. These findings may provide valuable information for fine-tuning the catalytic activity of graphene-based materials in low-temperature partial oxidation of CH_4.

***Keywords**:* CH_4 activation, Density functional, Adsorption, CO oxidation, graphene

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New nanocomposite of $CuCo_2S_4$/Polyaniline on carbon cloth as a self-standing efficient electrode material for supercapacitors

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Supercapacitors are one of the practical technologies for electrochemical energy conversion and storage which have drawn tremendous attention due to their high power density, long cycle life and fast charge and discharge rates [1-2]. Developing new electrode materials to be used in supercapacitors has been the subject of many studies during recent decades [3]. In this work, $CuCo_2S_4$ nanosheets were grown on carbon cloth through hydrothermal route and then polyaniline conducting polymer was synthesized on the surface of nanosheets through chemical polymerization of aniline. $CuCo_2S_4$ nanosheets on carbon cloth were electrochemically active in a wide potential window of 1.2 V in Na_2SO_4 electrolyte with specific capacitance of 780 Fg^{-1} at a current density of 1 A g^{-1}. After composing these nanosheets with optimized amount of polyaniline, the electrochemical behavior was improved. Regarding the synergistic effect between polyaniline and $CuCo_2S_4$, the resultant $CuCo_2S_4$ /polyaniline nanocomposite demonstrated a wider potential range of 1.6 V and an improved specific capacitance of 920 Fg^{-1} at a current density of 1 A g^{-1}, which is significantly higher compared to that of bare $CuCo_2S_4$ nanosheets. A Symmetric supercapacitor applying as-prepared $CuCo_2S_4$ /polyaniline as both anode and cathode was assembled which demonstrated extended operating potential window (1.8 V) and delivered high energy density of 32.5 Wh kg^{-1} and power density of 900 W kg^{-1}. According to obtained results, the as-prepared nanocomposite exhibits improved electrochemical performance and can be considered as a promising candidate to be used in energy storage devices.

Keywords: $CuCo_2S_4$, Polyaniline, Composite materials, Nanostructured materials, Supercapacitor

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Ca coated B_{40} fullerene: A promising material for CO_2 storage and separation

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The natural greenhouse effect refers to a process in which certain gases in the Earth's atmosphere (known as greenhouse gasses) retain the Sun's heat. Since the early 20th century, human activities such as the use of fossil fuels and deforestation have drastically altered the atmospheric concentration of greenhouse gases, notably CO_2 [1-2]. Porous materials such as covalent organic frameworks [3] 1metal organic frameworks [4], and zeolites [5], are the most promising and competitive options for CO_2 capture. Density functional theory calculations were used to investigate the adsorption behavior of Ca coated B_{40} fullerene toward CO_2 molecules. It was found that Ca atoms are unlikely to form clusters on B_{40}. CO_2 molecules can be effectively adsorbed on the Ca coated B_{40}, as evidenced by large negative adsorption energies and significant charge transfer effects. Each Ca atom on B40 may adsorb four CO_2, with average adsorption energy of -0.54 eV which falls within the range proposed for an ideal CO_2 adsorbent. Furthermore, Ca coated B_{40} exhibits high selectivity for CO_2 from CO_2/N_2, CO_2/H_2, and CO_2/CH_4 gas mixtures.

***Keywords**:* CO_2 storage, Separation, B_{40}, Adsorption, DFT

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Methane oxidation into methanol catalyzed by TM-anchored $C_{24}N_{24}$ nanoclusters (TM = Fe, Co and Ni): A DFT study

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Global warming and air pollution are among the most important challenges of the current century. During the past decades, the combustion of fossil fuels in different stationary power sources and automobiles has led to an increase in the amount of air pollutants [1-2]. One of the possible strategies to overcome this problem is to find alternative and efficient energy sources. Methane (CH_4) is the chief constituent of natural gas, which is regarded as an attractive clean energy carrier due to its highest H to C ratio of any fossil fuel [3-4]. DFT calculations are used to explore catalytic reaction pathways for oxidation of methane (CH_4) into methanol (CH_3OH) over transition metal (TM)-anchored $C_{24}N_{24}$ fullerenes (TM@$C_{24}N_{24}$; TM = Fe, Co and Ni). The results indicate that TM@$C_{24}N_{24}$ fullerenes provide a reaction site for the adsorption of N_2O, leading to its dissociation into N_2, and an oxygen moiety (O_{ads}) adsorbed on the TM atom. Then O_{ads} reacts with CH_4 to form CH_3* and OH* moieties co-adsorbed on TM@$C_{24}N_{24}$. The reaction barrier for the $CH_4 + O_{ads} \rightarrow CH_3OH$ process is 0.72, 0.60 and 0.50 eV for TM = Fe, Co and Ni, respectively.

***Keywords**:* CH_4 oxidation, Fullerene, N_2O, DFT, Mechanism

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Sc-functionalized porphyrin-like porous fullerene for CO_2 storage and separation: A first-principles evaluation

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It is widely recognized that air pollution and climate change are the most pressing challenges affecting our planet. Massive amounts of greenhouse gases have been released into the atmosphere throughout the decades as a result of urbanization, rapid population expansion, and increased human energy dependency on fossil fuels [1]. In recent years, there has been a lot of interest in capturing and storing carbon dioxide (CO_2) on porous materials as an efficient method for decreasing the adverse effects of this greenhouse gas on the environment and climate change [2, 3]. The electrochemical reduction of CO_2 into useful chemicals such as methanol, formic acid, and methane has generated significant interest as an alternative; yet, this method requires active catalysts for effective operation [4, 5]. The current work introduces a Sc-decorated porphyrin-like porous fullerene ($Sc_6@C_{24}N_{24}$) as an efficient material for CO_2 capture, storage, and separation using density functional theory calculations. While CO_2 is physisorbed over pristine $C_{24}N_{24}$, the addition of Sc atoms on the N_4 sites of $C_{24}N_{24}$ greatly enhances CO_2 adsorption energy. Each Sc atom in $Sc_6@C_{24}N_{24}$ may adsorb up to three CO_2 molecules, resulting in a gravimetric density of 48%. Moreover, temperature may be used to modulate CO_2 adsorption/desorption over the substrate. The Sc-decorated $C_{24}N_{24}$ fullerene exhibits a lower affinity for adsorbing N_2, CH_4, and H_2 molecules than CO_2. As a consequence, this material might be considered for purifying CO_2 molecules from CO_2/N_2, CO_2/CH_4, and CO_2/H_2 mixtures. This study also sheds light on the nature of the Sc-CO_2 interaction as well as the underlying mechanism of selective CO_2 adsorption on Sc decorated $C_{24}N_{24}$.

***Keywords**:* CO_2 storage, Fullerene, DFT, Separation

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Electrochemical investigation of hollow micro-assembled $CuCo_2S_4$ nanoparticles composed with polyaniline

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Concerns related to rapid depletion of fossil fuel resources has made scientists seek and develop new alternative energy production technologies. In this regard, fuel cells, batteries, and supercapacitors have been developed as energy conversion and storage devices on the basis of electrochemical energy conversion [1-2]. $CuCo_2S_4$ is a well-studied promising electrode material for energy storage devices[3]. Here, by composing this bimetal sulfide with polynaniline, we have successfully increased its electrochemical performance. First, through facile solvothermal method $CuCo_2S_4$ nanoparticles were synthesized in hollow sphere structures which are in the range of 500-600 nm. They exhibit excellent capacitive behavior with specific capacitance of about 839 Fg^{-1} at current density of 1 Ag^{-1} in three-electrode configuration. Next, aniline was polymerized on surface of these micro-sized hollow spheres through oxidative polymerization which led to form an electrochemically improved nanocomposite and the specific capacitance is increased to about 1120 Fg^{-1} at current density of 1 Ag^{-1}. This superior capacitive performance can be attributed to the hollow core–shell structure of the obtained nanocomposite. The assembled symmetric supercapacitor device based on as-synthesized $CuCo_2S_4$/PAni nanocomposite demonstrated a wide working potential of 2 V in 1 M Na_2SO_4 which could reach a high energy density and power density of 44.16 Wh kg^{-1} and 1 kW kg^{-1}, respectively.

Keywords: $CuCo_2S_4$ nanoparticles, Polyaniline, Micro-hollow structures, Nanocomposite materials, Supercapacitor

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Thermodynamic study of electrolyte mixture with L-Serine in aqueous solutions at T = 298.2 K

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Amino acids are the basic building blocks of proteins, and are widely used in several fields such as pharmaceutical, chemical, and food industries. They have an important role in metabolism of organism. Hence, the study on some processes such as separation, purification, and concentration of these biomolecules is very important [1-2]. Various methods have been studied for separation and purification of amino acids usually; these methods are carried out in the presence of electrolytes [3]. Among the experimental techniques, the potentiometric method is more used to study the thermodynamic properties of electrolyte solutions. The cell potential method presents advantages such as rapidity, stability, and relative simplicity to generate experimental data with regard to the other methods [2, 4]. In recent years, multi-component electrolyte systems such as (NaCl + serine + water) [2] and ($CaCl_2$ + serine or proline + water) [5] were studied and some experimental data were reported. In this work, the thermodynamic properties of the quaternary (KCl + KNO_3 + L-Serine + water) system, determined using the potentiometric method, were reported. The potentiometric measurements were performed in aqueous solution containing 5% mass fraction of L-Serine, over total ionic strengths from 0.0100 $mol \cdot kg^{-1}$ to 3.0000 $mol \cdot kg^{-1}$ at T = 293.2 K and P = 0.1MPa. Different series of the salt molal ratios r ($r = m_{KCl} / m_{KNO3}$= 1, 2.5, 5.0, 7.5, 10.0) and single salt KCl and KNO_3 solution in aqueous solution containing 5% mass fraction of L-Serine were used for the potentiometric measurements. The potentiometric measurements were performed on the galvanic cells of the type: (a) K−ISE | KCl (m_A), L-Serine (5%) | Ag−AgCl, (b) K−ISE | KNO3 (m_B), L-Serine (5%) | NO3-ISE, (c) K−ISE | KNO_3 (m_B), L-Serine (5%) | Ag−AgCl, and (d) K−ISE | KCl (m_1), KNO_3 (m_2), L-Serine (5%) | Ag−AgCl. The K-ISE was prepared in our laboratory using the ionophore treated by carbon nanotubes. Thermodynamic properties were implemented using the Pitzer ion interaction model. Subsequently, unknown parameters were determined and utilized to calculate the mean activity coefficients of the system under investigation.

Keywords: Activity coefficient, Potentiometric method, Pitzer, L-Serine

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Aggregation of Eosin B in Presence of Urea solutions as Additives

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Eosin dyes are an important group of fluorescent materials which have significant photophysical properties that make them suitable for many applications. They are most common to stain the cytoplasm in histology because their acidic sites can bind to basic components of a cell, mainly proteins located in the cytoplasm. It can also be used to stain collagen and muscle fibers for examination under the microscope [1]. The word eosin comes from the Greek word "EOS", which means magic. The aggregation of these dyes in different environments is an important phenomenon that considerably affects their spectral properties [2]. The combination of molecules depends on several parameters such as the dye concentration and structure, solvent environment, pressure and temperature. The aggregation can make the emission spectra to become lower [3].

To investigate the effect of additives on the dye properties, we used urea as a water structure-breaker additive in the dye solutions and studied the changes in UV-Vis spectra of the dye through the water-additive and dye-additive interactions [4]. In this work, the self-association phenomena of eosin B is studied in the presence of urea as a neutral additive, using the UV-Vis absorption spectral data.

Keywords**:** Eosin B, Self-association, Urea, UV-Vis Absorption spectra.

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Efficient hydrogen storage on Al decorated $C_{24}N_{24}$: a DFT study

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Fossil fuels currently provide the majority of the world's energy. However, their use is directly related to significant environmental issues such as air pollution and the greenhouse effect [1-2]. As a result, there is a significant need for new renewable energy supplies. In this regard, hydrogen has long been acknowledged as a solution to our energy issues, as its combustion produces only water as a byproduct [3]. H_2 storage and capture are critical components in the development of clean and sustainable hydrogen energy [4-5]. The current work investigates the H_2 adsorption properties and storage on the Al-decorated porphyrin-like small porous $C_{24}N_{24}$ cluster using density functional theory calculations. Each Al site in the $Al_6C_{24}N_{24}$ cluster can adsorb up to five H_2 molecules, with an average adsorption energy of -0.30 eV. The impact of temperature and pressure on the hydrogen storage capacity of Al-decorated $C_{24}N_{24}$ clusters is also studied. A Kubas type mechanism and electrostatic interactions are found to be essential in the adsorption of H_2 molecules on the Al-decorated $C_{24}N_{24}$. According to our findings, $Al_6C_{24}N_{24}$ has a gravimetric density of 7.1 wt% H_2. These findings demonstrate that the Al-decorated $C_{24}N_{24}$ may be a potential candidate for reversible H_2 storage under normal conditions.

***Keywords**:* Hydrogen storage, $C_{24}N_{24}$, Metal- decorated, DFT

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Extraction of work from motions related to the degrees of internal freedom of molecules

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Every thing thet happens in the universe, from the vital processes within a bacterium to the most complex computations in advanced upercomputers made by eletrons, atoms, molecules and their movements between energy levels, or energy level changes. It is done by analyzing the energy exchange between quantum systems and the einironment [1-5]. Quantum thermodynamics has recently flourished, enhanced by highly controlled quantum experiments, the availability of powerful numerical methods, and the development of new theoretical tools such as unbalanced thermodynamics and quantum information theory that describe inequal oscillations which is used for the purposes such as better understanding of heat in quantum systems in the field of quantum and the design of new experiments, thermodynamic quantum exploration using nuclear rotation, molecular degrees of freedom and etc. Quantum states and energy levels belonging to molecular vibrations as well as inhibited rotation around chemical bonds can be used as a means of extracting or storing energy. The processes of extraction, transfer, and exchange of energy and heat in quantum motors designed based on degrees of internal molecular freedom can be used to transmit, store, and information process. Quantum motors designed based on the degrees of internal freedom of molecules can be used to transfer molecules and materials through interfacial space, thus model can be used to predict the equilibria phase of fluids and condensed matter. We can stimulate above processes and designed quantum motors by network methods and specify(identify) the critical states of the case-comment and use it them for their control.

Keywords: Quantum thermodynamics, Quantum machines, Work and heat, Internal degrees of freedom, Internal energy levels

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Modeling the flotation process of line-2 of Sungun copper complex using Design Expert 12 software

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Flotation is widely used to separate different minerals , which depend on the drifting difference,This method combines the minerals with value through chemical and chemical reactions [1-5]. In Songun Copper Complex, this method is used for concentration copper. In this work, Designe Expert 12 software was used to model the flotation process of phase 2 of Sungun copper complex. Based on the parameters of chemical injection rate, grade and tonnage of the input feed were performed based on research and entered into Designe Expert 12 software as experimental parameters. Recovery was selected as the answer to the experiments. Total flotation circuit recovery with Design Expert 12 modeling equal to 93.30% and Optimal Consumption amount of 8.12 g/t Z11, 12.52 g/t Flomin, 5.43 g/t A70 and 5.34 g/t A65 when the input feed tonnage and the input feed grade were respectively 107.83 t/h and 0.9%, was obtained as a mode optimal using Designe Expert 12 software.

Keywords: Flotation, Designe Expert 12, Modeling, Sungun Copper

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Preparation of a Magnetic Nanocomposite for the Removal of Methylene Blue from Aqueous Solutions: Synthesis, Characterization, and Investigation of Different Parameters

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In the present study, a magnetic nanocomposite was synthesized for the removal of methylene blue from aqueous solutions. In the first step, magnetite nanoparticles were synthesized via co-precipitation method and then, they were modified with 3-aminopropyltriethoxysilane (APTES) and acryloyl chloride, respectively.

Itaconic acid and 2-hydroxyethyl methacrylate were then copolymerized in situ and grafted on the modified nanoparticles to prepare the final nanocomposite. The prepared nanocomposite was used as the adsorbent to study the removal of methylene blue dye from aqueous solutions. According to the obtained results, the nanocomposite showed high adsorption efficiency toward the dye within 15 minutes. Different parameters were investigated and optimized such as pH, adsorbent amount, initial concentration of the dye, and contact time. Moreover, the nanocomposite was characterized by different methods such as FT-IR, VSM, TGA, XRD, and FE-SEM analyses [1-5].

Keywords: Magnetic nanocomposite; Methylene blue; Dye removal; Aqueous solutions

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Molecular dynamics simulation (dimethyl-tert-butyl-sililoxy) and (triethyl-silyloxy) piroxicam, investigation of their lipophilic property and comparison with the original drug.

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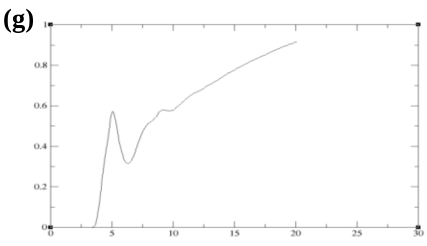
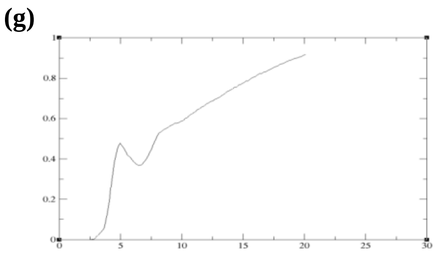
Piroxicam is a painkiller and its main use is to reduce or stop pain. This drug has anti-inflammatory effects in osteoarthritis. This drug is used to treat many diseases such as headaches and toothaches, leg pain,and piroxicam reduces the production of prostaglandins by controlling cyclooxygenase, thus showing its effectiveness in reducing and eliminating pain. Piroxicam is a phenolic drug. These drugs are difficult to pass through the lipid barrier, and the presence of lipophilic groups, such as organosilicon, will increase this property, that is, increase the property of the drug, so the introduction of these groups will modify the property of the drug. For this reason, we did this work with various silyl groups [1].Molecular dynamics simulation (MD) is knowledge that combines biological sciences, chemistry, and methods and uses a variety of computer-mathematical algorithms [2].The theoretical part is related to the simulation of molecular dynamics in which piroxicam and the derivative of dimethyl tert-butyl silyloxy piroxicam, each separately in three boxes (the first box contains pure water, the second box contains pure octanol, and the third box contains a mixture of water and octanol), were simulated. After examining energy indices, hydrogen bonding, diffusion coefficient, RDF, and SDF, it was found that the interaction between the drug and its silylderivative in a box containing a mixture of water and octanol was close to the state where the drug and its silylderivative were in the pure octanol box.



RDF spectra silyl derivative with water oxigen



RDF spectra silyl derivative with water hydroxyl

Keywords:Piroxicam, Prodrug, Silyl derivative, Lipophilicity

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Synthesis and characterization of two different Zr-Melamine coordination compounds; coordination polymer and MOF via solvothermal method

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Coordination polymers (CPs) and Metal-Organic Frameworks (MOFs) as their subsets, have attracted a lot of attention because of hybrid inorganic and organic nature that enables tuning of structure and structural properties [1, 2]. In this work we synthesized a CP and a MOF based on Zr(IV) and melamine as building blocks. By varying the metal/ligand ratio, solvent type, solvents ratios and adjusting the pH, we obtained two new structures. Synthesis was performed via hydrothermal method. In both structures, the solvent was a mixture of methanol-DMF and the molar ratio between the metal/ligand, temperature and reaction time were the same. The only difference was in the ratio between the solvents and modulator. In the first synthesis, formic acid was added to the reaction mixture as a part of solvent and a modulator, which changed the ratio of solvents and led to the CP structure. The second synthesis without formic acid led to the MOF structure. The EDX results confirmed the presence of Zr and ligand's atoms in both structures, but their percentages were different. The IR spectrum of the two structures were different, indicating the ligand-metal were differently bonded together. PXRD results also showed different crystal structures for each case. The results obtained of BET analysis illustrates 6 m^2/g specific surface area, 3.35 nm mean pore diameter and 5×10^{-3} cm^3/g total pore volume. These results for the MOF were respectively; 260.11 m^2/g, 2.47 nm and 16×10^{-2} cm^3/g. SEM microscopy indicates that particles size of both structures are under 100 nm, but they have different morphologies. CP and MOF respectively have rod-like monoclinic and orthorhombic morph. These results indicate that solvent and modulator have significant effect on the structure of synthesized materials.

Keywords: Coordination Polymer, Metal-Organic Framework, Zirconium, Melamine

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Synthesis and characterization of Zr-bistetrazole metal-organic framework, study efficient RB19 dye adsorption

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Metal-organic frameworks (MOFs) are assembly of inorganic nodes with organic linkers that have porous nature. Because of their highly tunability in structure, porosity and stability, they have vast variety of applications. For the first time Omar M. Yaghi introduced the term MOF for these coordination compounds [1-2]. Zirconium based MOFs have high water stability over a wide range of pH and for this reason they are desirable for applications in aqueous media such as electrochemical sensors, water splitting and CO_2 reduction or pollutants adsorption [3]. In this work we synthesized a new MOF based on Zr(IV) with 5,5′-bistetrazole linkers via hydrothermal method. The EDX results confirmed the presence of metal and linker atoms in the structure. To synthesize this structure, different metal and linker ratios were examined. Water, DMF and MeOH solvents were examined, only synthesis in aqueous media produced porous crystalline structure and were confirmed via powder X-ray diffraction (PXRD), but in DMF or a combination of DMF and MeOH, as solvent, the structures were amorphous and did not show porosity. We studied different synthesis temperatures in aqueous media from 85 °C to 140 °C, and the best crystallinity were observed in 130 °C. The best time for synthesis was 96 hours. The synthesis was performed in the various pH range from 2 to 7, and for adjusting the pH, NH_4OH and HCl were used. Variation of pH has significant effect on the sharpness of the PXRD peaks and the best results were observed at pH 4. In other pH values, the structures did not show much porosity. The material was used to study the adsorption of RB19 dye, for which briefly 0.02 g of MOF immersed in 100 ml 10 ppm RB19 solution, after an hour, it completely absorbed by the material.

Keywords: Zirconium, 5,5′-bistetrazole, Metal-Organic Framework, Reactive Blue 19

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Densities and derived thermodynamic properties study for the binary mixtures of acetonitryle+ dichloroethane, tetrachlorethan at temperature range of 293.15-303.15 K: Experimental results and application of the Prigogine–Flory–Patterson theory

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The thermodynamic and transport properties of liquids and liquid mixtures have been used to understand the molecular interactons between the components of the mixture and also for engineering applications concerning heat transfer, mass transfer and fluid flow. In the present work, densities, ρ, and viscosities, η, for binary mixture of ($x1$ acetonitryle +$x2$ dichloroethane) and ($x1$ acetonitryle +$x2$ tetrachlorethan) have been measured at atmospheric pressure and in the entire composition range. These quantities have been used to calculate excess molar volumes, V_m^E. These excess and deviation quantities have then been fitted to the Redlich– Kister equation [1]. The obtained correlations were used to calculate the other thermodynamic functions such as thermal expansion coefficient, α, and its excess value, α^E, and isothermal coefficient of excess molar enthalpy $(\partial H_m^E/\partial P)_{T,x}$. Results of such calculations were used for interpreting intermolecular interactions that exist between molecules of the binary mixture, qualitatively. The Prigogine-Flory-Patterson (PFP) theory has been successful in prediction the volumetric properties of various kinds of binary mixtures [2]. In this theory, excess thermodynamic properties of a binary mixture are separated into three contributions: the interactional contribution which is proportional to the interaction parameter, χ_{12}; free volume contribution which arises from the difference between size of two components; and pressure contribution which depends on the internal pressure and reduced volume of the components. In this work, we have investigated the PFP theory as a method to predict the V_m^E of these binary mixtures. Results of these calculations were used for interpreting intermolecular interactions that exist between molecules of the binary mixture. The densities of these binary mixtures were measured over the temperature range and over the entire composition range. Data of the excess molar volumes for these binary mixtures were calculated from the values of the experimental density. The calculated excess molar volumes using the PFP model are comparable with experimental values [3,4].

Keywords: Binary mixture, Excess molar properties, Density, acetonitrile, PFP model

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Thermophysical properties study for the binary mixtures of (acetonitrile+ dichloroethylene, or tetrachloroethylene) at different temperature

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In the present work, viscosities, η, for binary mixture of ($x1$ acetonitryle $+x2$ dichloroethylene) and ($x1$ acetonitryle $+x2$ tetrachloroethylene) have been measured at atmospheric pressure and in the entire composition range. These quantities have been used to calculate viscosity deviations, $\Delta\eta$. These deviation quantities have been fitted to the Redlich–Kister equation [1]. The obtained correlations were used to calculate the other thermophysical functions such as the excess free energy of activation for viscous flow ΔG^{*E} have been calculated. The aim of this work is to provide results for the characterization of the molecular interactions in these mixtures. Viscosities of the binary mixtures under study were measured and their deviations were calculated as a function of composition and temperature. The results of such calculations show that viscosity deviations are negative over entire composition range at all temperatures for all of the binary mixtures, and become less negative with increasing temperature. This effect confirms this deduction that the attractive interactions between components of the mixtures make weaker with increasing temperature and then they can flow easer with lower viscosity [2].

Air tight stopper bottles were used for the preparation of the mixtures. The mass of dry bottle was first determined. The less volatile component of the mixture was introduced in the bottle, and the total mass was recorded. Subsequently, the other component was added, and the mass of bottle including two components was determined. Each mixture was immediately used, after it was mixed by shaking. All the weightings were performed on an electronic digital balance (AB 204-N Mettler) accurate to $\pm1\times10^{-5}$g. The uncertainty in the mole fraction is estimated to be lower than $\pm1\times10^{-4}$. Conversion to molar quantities was based on the relative atomic mass table of 2006 issued by IUPAC [3]. The uncertainty in the excess molar volumes estimated to be $\pm1\times10^{-4}$ cm^3.mol^{-1}.

Viscosity was determined using an Ubbelohde viscometer which was fixed in a water bath and the temperature was controlled with a precision of ±0.01 K. The flow times were taken by using a digital chronometer model of KENKO KK-5898 with a precision of ±0.01 second [4,5].

Keywords**:** Binary mixture, Excess molar properties, Density, acetonitrile, PFP model

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Densities and derived thermodynamic properties study for the binary mixture of (Acetophenone+choloroethylene) at different temperature

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In the present work, densities, ρ, for binary mixture of (Acetophenon+dicholoroethylen, tricholoroethylene) have been measured at atmospheric pressure and in the entire composition range. This quantity have been used to calculate excess molar volumes, V_m^E. This excess and deviation quantity have then been fitted to the Redlich– Kister equation [1]. The obtained correlations were used to calculate the other thermodynamic functions such as thermal expansion coefficient, α, and its excess value, α^E, and isothermal coefficient of excess molar enthalpy $(\partial H_m^E/\partial P)_{T,x}$. Results of such calculations were used for interpreting intermolecular interactions that exist between molecules of the binary mixture, qualitatively. The densities of the pure components and their binary mixture were measured with an Anton Paar DSA 5000 Oscillating U-tube densitometer, and the uncertainties were estimated to be within $\pm 1\times10^{-2}$ kg m^{-3}. The temperature in the cell was regulated to ±0.01K with a solid state thermostat. Each mixture was immediately used, after it was mixed by shaking. All the weightings were performed on an electronic digital balance (AB 204-N Mettler) accurate to ±0.1 mg. The uncertainty in the mole fraction is estimated to be lower than $\pm 1\times10^{-4}$ [2].

The excess molar volumes of binary mixture are negative within the entire composition range and become less negative with increasing temperature from (298.15 to 318.15) K. The increase in the magnitude of the $\bar{V}_{m.i}^E$ values with increasing temperature can be attributed to the decreasing importance of hydrogen bonding with increasing it. Results of these calculations were used for interpreting intermolecular interactions that exist between molecules of the binary mixture. If interactions between unlike molecules are stronger than those exist between like molecules, as a consequence negative V_m^E will be observed, other factors that affect the volume are molecular shape and size of components in the mixture [3].

Keywords: Binary mixture, Excess molar properties, Redlich- Kister correlation, Density

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Densities and derived thermodynamic properties study for the binary mixtures of (2-hydroxy ethylammonium formate + Aminopropanol) at different temperature with application of the PFP theory

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Study of ionic liquids (ILs) as solvents has received an increasing attention in the last years from fundamental and applied points of view [1]. ILs has been used for reducing or eliminating the hazards from volatile organic solvents, solvents in analysis, synthesis, catalytic reactions, and separation processes. ILs have been accepted as “green-chemicals” which excited both the academia and the chemical industries due to their unique properties, and are liquids wide temperature range including room temperature. To design any process involving ILs on an industrial scale, it is necessary to know some thermo physical properties such as viscosity and density [2-3]. In this work, the thermodynamic properties for the binary mixtures of 2-hydroxy ethylammonium formate with Aminopropanol (AP) and isobutanol have been investigated. We have measured densities, ρ, for the binary mixture of {$x_1$2-hydroxy ethylammonium formate +x_2Aminopropanol} and {*2-hydroxy ethylammonium formate* +$x_2$ethanoamine} at atmospheric pressure in the temperature range of (293.15 to 338.15) K and in the entire composition range. The excess molar volumes, $V_{\mathrm{m}}^{\mathrm{E}}$, partial molar volume, $\bar{V}_{m,i}$, excess partial molar volume, $\bar{V}_{m,i}^{E}$, partial molar volume at infinite dilution, $\bar{V}_{m,i}^{*}$, apparent molar volume, $\bar{V}_{\varphi,i}$, the excess thermal expansion coefficients, α^{E}, isothermal coefficient of excess molar enthalpy $(\partial H_m^E/\partial p)_{\mathrm{T,x}}$, were calculated from the experimental values of densities . These data were correlated with the Redlich- Kister equation. The excess molar volumes of both binary mixtures are negative within the entire composition range and become more negative with increasing temperature from (298.15 to 318.15) K.

Keywords: Ionic liquids, Excess molar properties, Redlich- Kister correlation, PFP theory

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Synthesis of hydroxyethylammonium-based ionic liquids (ILs) with carboxylate anions and investigation of physicochemical properties of binary systems including ILs with alkanolamine at different temperatures

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Study of ionic liquids (ILs) as solvents has received an increasing attention in the last years from fundamental and applied points of view [1]. ILs has been used for reducing or eliminating the hazards from volatile organic solvents, solvents in analysis, synthesis, catalytic reactions, and separation processes. ILs have been accepted as “green-chemicals” which excited both the academia and the chemical industries due to their unique properties, and are liquids wide temperature range including room temperature. To design any process involving ILs on an industrial scale, it is necessary to know some thermo physical properties such as viscosity and density [2,3]. In this work, the thermodynamic properties for the binary mixtures of IL with Aminopropanols have been investigated. We have measured densities, ρ, for the binary mixture of x_1IL+x_2Aminopropanols at atmospheric pressure in the temperature range of (293.15 to 338.15) K and in the entire composition range. The excess molar volumes, V_m^E, partial molar volume, $\bar{V}_{m,i}$, excess partial molar volume, $\bar{V}_{m,i}^E$, partial molar volume at infinite dilution, $\bar{V}_{m,i}^*$, apparent molar volume, $\bar{V}_{\varphi,i}$, the excess thermal expansion coefficients, α^E, isothermal coefficient of excess molar enthalpy $(\partial H_m^E/\partial p)_{T,x}$, were calculated from the experimental values of densities . These data were correlated with the Redlich- Kister equation. Excess molar volumes for binary mixture of {x_1IL + x_2AP} shows ne negative values at the opposite extreme. With increasing temperature, it increases. We can observe that the excess molar volumes present a minimum at $x_1 \approx 0.65$ to 0.75 for this system. The strength of ion-dipole interaction between the ILs and the solvent is in agreement with the increasing order of the absolute values of V^E. The increase in the magnitude of the positive V^E values with increasing temperature can be attributed to the decreasing importance of hydrogen bonding with increasing temperature. If interactions between unlike molecules are stronger than those exist between like molecules, as a consequence negative V^E will be observed.

Keywords**:** Ionic liquids, Excess molar properties, Redlich- Kister correlation

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First-principles study of the effect of Sc doping on the Structural, Electronic, and Optical properties of Zr_2CO_2 Nanostructure

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Other two-dimensional (2D) materials, such as transition metal dichalcogenides, monochalcogenides, and monoelemental 2D semiconductors, have garnered increased attention in theoretical and practical disciplines since the discovery of graphene and intensive investigation of its remarkable features [1]. Furthermore, due to their fascinating physicochemical features that distinguish them from their bulk counterparts, 2D transition metal carbides and carbonitrides (MXenes) have gained much attention [2]. MAX phrases are commonly used to make MXenes. The principal predecessors for MXenes are MAX phases, which have the chemical formula Mn+1AXn (M: an early transition metal, A: an element from the group of 13 or 14, X: carbon or nitrogen, and n = 1, 2, 3, or 4) [3].

The computational analyses are based on Density Functional Theory (DFT) and projector augmented wave (PAW) potentials, as implemented in the Vienna ab initio simulation package (VASP) [4], which includes hybrid approaches. Compared to pure DFT computations, hybrid techniques often improve the precision of estimated band gaps. The Monkhorst– Pack technique was utilized for structural optimization and static self-consistent calculations, and the k-points of 11*11*1 and 13*13*1 were obtained automatically. The cut-off energy is set to be 520 eV. The optical absorption properties of the 2D semiconductor photocatalyst were explored using the analysis of dielectric constants (ε) at a specific frequency. The Heyd- Scuseria-Ernzerhof (HSE06) hybrid functional with 11*11*1 k-point mesh was employed. The VESTA code [5] was used to investigate the atomic structures.

The influence of the doping element Sc on the structural, electrical, and optical characteristics of Zr_2CO_2 nanostructure was investigated using first-principles calculations based on the density functional theory in this study. Sc doping, on the other hand, had the opposite effect: it increased flexibility while reducing some strength. It is inferred that there is an apparent association between orbital hybridization and the charge transfer of electronic properties by examining the electronic structure. This research provides a theoretical foundation for understanding the doping mechanism in Zr_2CO_2 nanostructures and a potential method for improving MXene performance.

Keywords: Density functional theory (DFT), Structural, Electronic, Optical, Nanostructure.

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Computational Studies and Tuning the Electronic and Optical Properties of Y_2CF_2 and Sc_2CF_2 Monolayers Using Biaxial Strain Effect with GGA-PBE and HSE06 Functionals

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Optical and electronic studies of solid materials, especially semiconductor materials, have been currently considered among the most important research topics. Using hydrofluoric acid (HF) solution and above method, the transition metal carbides, from MAX phase family, e.g., Ti_3AlC_2,Ti_2AlC, and Ta_3AlC_3, can be exfoliated into 2D layers, so called MXenes [1]. The MAX phase are a family that has a chemical formula of Mn+1AXn where n = 1, 2, or 3, “M” demonstrates a transition metal, “A” denotes A group (mostly groups 13 and 14) elements, and “X” can be carbon or nitrogen [2]. During the etching process, the A atom in the MAX phase is displaced by O, F, and/or OH, resulting in the formation of functionalized MXenes. Several methods for the modification of the electronic structures of 2D materials have been developed, e.g., doping atoms, applying gate voltages, electric fields, or external strains. Applying strain is considered to be a feasible way due to the excellent mechanical flexibility of MXenes. In this study, the electronic structure, optical properties, and bandgap tuning under compressive and tensile strain (CTS) of 2D Y_2CF_2 and Sc_2CF_2 are investigated herein using density functional theory (DFT) calculations. All calculations were performed with both GGA-PBE [3] and HSE06 functionals [4]. It is observed that with the HSE06 functional the amount of band gaps Y_2CF_2 and Sc_2CF_2 nanostructures increases. The results reveal that the band gaps of 2D Y_2CF_2 and Sc_2CF_2 nanostructures can be tuned by applying CTS. The covalent bonding between the atoms become stronger under compressive strain. To investigate the optical properties, the absorption spectrum and percentage reflectivity of these structures along the x and z directions are calculated using the real and imaginary parts of the dielectric function. Upon applying 2%, 4%, and 6% compressive strain, the number of absorption peaks increases in the visible region along the x direction. These tunable electronic and optical properties of semiconductors of 2D Y_2CF_2 and Sc_2CF_2 make them as candidates for the design of optoelectronic devices and in nanodevice applications.

Keywords: MXene, Two-dimensional, Density functional theory (DFT), Bandgap tuning, Compressive and tensile strain (CTS).

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Molecular Engineering of Compounds Based on Novel 2D Nanoparticles to Application in Water Splitting Process: A DFT Study

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The growing use of fossil fuels has prompted the development of new energy generation systems that are more sustainable and have less negative environmental consequences. Massive carbon dioxide (CO2) emissions and global environmental concerns have resulted from the large consumption of fossil fuels. Because of its limitless supply, solar energy is regarded as one of the most promising choices. Photocatalytic water splitting could be crucial in future renewable energy systems since solar energy can be directly converted into chemical energy in hydrogen. An ideal photocatalyst must have the following criteria: (1) The conduction band minimum (CBM) must be larger (more negative) than the hydrogen reduction potential (H^+/H_2) for a photocatalyst to work. The water oxidation potential (H_2O/O_2) should be lower (more positive) than the valence band maximum (VBM) [1]. (2) Second, for a semiconductor to be employed as a photocatalyst, the minimum bandgap is 1.23 eV.

MXenes are a new class of 2D transition metal carbides/nitrides that are created by selective chemical etching of "A" from MAX phases, where M is a transition metal, A is an IIIA or IVA element, and X is C or N [2]. Hydrogen created by the direct splitting of water using a semiconductor photocatalyst in the presence of sunlight is seen as a viable alternative to fossil fuels and a potential solution to serious environmental issues.

We look at some two-dimensional nanostructures from the MXene family in this research. One of the main goals of our study is to look at techniques for finding photocatalysts for the water-splitting process. We do this by calculating the structural, electrical, and optical properties of these 2D MXenes and then combining them. According to our findings, it is a suitable and promising photocatalyst for the water-splitting process. We use the Vienna ab initio simulation package (VASP) [3] for this project. Because the GGA-PBE [4] consistently underestimates the band gap, a computationally more expensive Heyd–Scuseria–Ernzerhof (HSE06) hybrid functional [5] has yielded accurate values that match tests in a wide range of systems. As a result of this research, we see that nanostructures Hf_2CO_2 and Zr_2CO_2 are suitable photocatalysts for the process of water splitting.

Keywords: MXene, Photocatalyst, Water splitting, Density functional theory (DFT), Hybrid functional

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Epoxy coating with super corrosion protection containing 2-mercaptobenzothiazole modified ZnO with core shell structure as anticorrosion pigment

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Corrosion of the metallic structures has undesirable effects on the industry and daily life in both economically and safety points of view [1]. Organic coatings were extensively used for protecting purposes in the corrosive media [2]. Epoxy (EP) coating which has low cost, good barrier properties, and good adhesion is preferred to other organic coatings [3].

In this study, 2-mercaptobenzothiazole modified ZnO with the core-shell structure (ZnO@PANI@MBT) was synthesized by layer by layer (LBL) method and characterized successfully by fourier transform infrared spectroscopy (FTIR), scanning electron microscopy (SEM), thermogravimetric analysis (TGA), Zeta potential, raman spectroscopy and dynamic light scattering (DLS) techniques.

Different weight percentages of pure ZnO nanoparticle and ZnO@PANI@MBT core shells (0.5,1,2 wt.%) were embedded into epoxy and coated on mild steel. The corrosion protective performance of coatings were studied by electrochemical impedance spectrometry (EIS) in saline electrolyte (NaCl 3.5 wt.%, 65 ℃). The EIS study indicated that epoxy resin with the 1 wt.% addition of ZnO@PANI@MBT core shell nanoparticles had higher corrosion protection and lower permeability to water penetration. Also, using modified ZnO nanoparticles with the core shell structure as anti-corrosion pigment increased the hydrophobicity of epoxy coatings. The highest coating corrosion resistance (R_{coat}) after 200 h immersion time in saline electrolyte was obtained in the presence of 1 wt.% ZnO@PANI@MBT (4.8×10^{8} Ωcm^{2}) which is higher than that of epoxy/pure ZnO coatings ($R_{coat} = 9.2\times10^{6}$ Ωcm^{2}) and net epoxy ($R_{coat} = 9.1\times10^{3}$ Ωcm^{2}). The water uptake amount of epoxy/ZnO@PANI@MBT 1 wt.% was 1.04 time smaller than epoxy/pure ZnO and 1.90 time smaller than net epoxy after 200h immersion.

Keywords: Epoxy, Core shell, ZnO, corrosion inhibitor, layer by layer synthesis.

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Boosting Solar Vapor Generation by a Bio-based 3D Evaporator for Solar Desalination

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Interfacial solar vapor generation (ISVG) is a promising and cost-effective way for seawater desalination. This technology uses a photothermal converter to absorb sunlight and convert it to heat-to-vapor. However, there are still challenges to be faced in embracing these new technologies. Efforts to find suitable structures and photothermal materials having high evaporation rate, high efficiency, low-cost, eco-friendly, self-floatable and salt rejecter, are to be continued. 3D structure design is the new approach for boosting the evaporation rate and efficiency of ISVG evaporators. To date, various structures for ISVG have been proposed, based on 2D and 3D designs [1-3]. Here, we introduced an elaborate structure with bio-based materials, with both warm and cold evaporation surfaces. In this work, a 3D modified bio-based floatable assembly (3D-MBFA) is suggested as an environmental-friendly, efficient, self-floating, and salt-rejection solar vapor generator based on the modified wicking fabric and sunflower stem. Thermal management and high light absorption are crucial for the structure of solar vapor generation**.** The utilized superhydrophilic wicking fabric as acts as both porous substrate of solar absorber and water transporter to the evaporation region. The wicking fabric was coated with cross-linked calcium alginate incorporation Au nanoparticles. Meanwhile, the sunflower stem with its inherent wonderful characteristics, such as low thermal conductivity, water transportation ability and self-floatability, causes heat localization, water supply to the surface and high evaporation yield of the 3D-MBFA for solar steam generation. Overall, by using the 3D-MBFA, a high evaporation rate of 3.2 kg m^{-2} h^{-1} at 1 Sun illumination is obtained.

Keywords:Wicking fabric, Sunflower stem, Photo-thermal, Solar desalination, Au nanoparticles

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Preparation and Characterization of poly (O- Toluidine-Carbon nano tube) Nano films and Study of optical properties

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In this study, nano films were prepared from poly (O-toluidine) (POT) and the structural, optical and electrical properties were studied, and then POT was mixed with nanomaterial (Multi-walled Carbon Nanotubes) (MWCNT) in certain proportions of the size to form nano-membranes With distinctive characteristics. Properties: The solution is deposited on the bottles by spin coating method (2000 r/m in 10 seconds), the prepared membrane samples by determining their crystalline nature by X-ray diffraction, and studying the surface morphology of the deposited films using scanning electron microscopy (SEM) and atomic microscopy (AFM), studying the optical properties by obtaining the absorption and transmittance spectrum in the UV visible regions as a function of wavelength to find the optical energy gap as well as the refractive index, as well as the extinction coefficient and the dielectric constant. It included the study of the electrical properties of the final films, which included electrical conductivity, as well as the study of testing overlapping films such as solar cells and gas sensors to know the characteristics of the current voltage, the packing factor, the efficiency of the solar cell and then the sensitivity in different conditions such as the temperature test. The optical properties of the prepared thin films were studied, including absorption spectrometry recording for wavelengths (300-800 nm), and it was found that the absorption (A) and extinction (K) coefficients increased with increasing rates from (MWCNT) (90:10, 80:20, 70:30). , 60: 40, 50: 50) and the energy gap values are reduced, which leads to an improvement in the optical properties.

Keywords: Multi-walled carbon nanotubes, Morphology, Absorption, wavelengths

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Molecular insight into deep eutectic solvent based on choline chloride and caprylic acid by molecular dynamics simulation

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Economic storage of thermal energy is a key issue for technologies that use solar energy [1]. Fatty acids have excellent chemical stability and non-toxicity used for the purpose of phase change materials (PCMs) [2]. The less volume change of FAs during phase transition could lead to the introduction of them as great candidate in the preparation process of eutectic solvents [3]. Deep eutectic solvents (DESs) are prepared from a combination of hydrogen bond donor (HBD) and hydrogen bond acceptor (HBA) that have natural origin [4]. Information about the microscopic structure of eutectic mixtures can help to design new solvents. Molecular dynamics simulation (MD) is a useful tool to achieve the structural properties. In this work, the structural properties of the eutectic mixture of choline chloride salt (Ch^+ Cl^-) and caprylic acid (CAP) were investigated at 353 K.

Assessed structural properties include the non-bonded energy between species, the radial distribution functions (RDFs) the Hydrogen bonding network between species and spatial distribution functions (SDF). Structural properties of the binary mixture of CAP/ Ch^+ Cl^- with a molar ratio of 1: 3 showed a decrease in the strong interaction between CAP molecules in the binary mixture than those in the pure state. The analysis of the atom-atom RDFs and Spatial distribution functions (SDF) of the eutectic mixture was indicated the hydrogen atoms that dependent on the hydroxyl group of CAP molecules are surrounded by chloride anions (see Fig.1). The non-bonded energy revealed that the presence of choline chloride salt leads to a significant disruption of the intermolecular interaction between CAP molecules. In general, the results of this work are presented evidence that interactions between chloride anions and the H atom of the carboxyl groups of caprylic acid play a key role in the formation of eutectic solvents based on CAP and Ch^+ Cl^-.

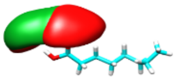

Fig.1. Spatial distribution functions (SDFs) of the components of the binary mixtures at 353 K. Green isosurfaces correspond to Ch+, red isosurfaces are chloride anion.

Keywords: Deep eutectic solvents, Caprylic acid, Choline chloride, MD simulation, Structural properties.

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Molecular dynamics simulations of menthol and Palmitic acid deep eutectic solvents: Investigation of structural properties

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Deep eutectic solvents (DES) are prepared from a combination of hydrogen bond donor (HBD) and hydrogen bond acceptor (HBA) each of which has a melting point above that of the mixture [1]. In 2003, the term Deep Eutectic Solvent was initially used for the mixture combination of choline chloride and urea by Abbott et al [2]. These compounds are widely used in comparison with volatile ionic liquids due to their biocompatible and less toxic components and low cost of synthesis [3]. DES fields of applicability and ILs are overlapped in the chemical and pharmaceutical industries as solvents. The prediction of the microscopic structure of eutectic mixtures can help to design new solvents and expand their application in the industries. Molecular Dynamic Simulation is a complementary tool to provide insights into the structure of these versatile solvents [4]. In this work, a new class of DESs including menthol (MEN), as HBA, and Palmitic acid (PLA), as HBD, were investigated to understand effective interactions in the formation of the eutectic mixture (HBA: HBD; 3:1). For this purpose, the interaction energies between HBA and HBD and structural properties such as atom-atom radial distribution functions (RDFs), the hydrogen-bonding network between species, and spatial distribution functions (SDFs) were computed at 353 K. RDFs were calculated to investigate the relative distribution of molecules in the considered systems. Furthermore, this analysis was used to obtain the hydrogen bonds between MEN and PLA molecules. The peak of the MEN -- PLA RDF observed at 2 Å showing a strong attractive interaction or hydrogen bonding between the H atom of the hydroxyl (—OH) group of MEN molecules and the O atoms of carboxyl (−COOH) group of PLA. The results of SDFs are presented evidence that the maximum densities of PLA molecules were found near the O atom of the hydroxyl group of MEN in the binary mixtures. In general, the probable cause of the distribution decrease of menthol molecules around the reference molecule is interactions between the carboxyl groups of FAs and the hydroxyl group of MEN.

Keywords: Deep Eutectic Solvents, Palmitic acid, Menthol, MD Simulation, Structural Properties.

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Theoretical study of interaction between gabapentin drug and Si-doped graphene nanostructure toward designing of suitable nanocarrier for drug delivery

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Controlled and targeted drug delivery method prevents the toxicity of the drug, its destruction and repeated use. Biocompatibility and drug loading capacity are important properties that are considered as Drug delivery for the required materials. In recent years, the unique chemical and physical properties of carbon nanostructures have led to many advances in various fields, including chemistry and pharmacy. Graphene is one of the carbon nanostructures that has been considered by researchers in the effective absorption and release of various drugs [1]. Due to the cross section of graphene, it can be used as a biological carrier in drug delivery. Silicon in the body strengthens the body's immunity and improves tissues, so graphene contamination with silicon improves its function as a nanoparticle in the body [2]. Gabapentin, also known as Neurontin, is an anticonvulsant that is primarily used to treat minor seizures and neuropathic pain, and in 2019, it was the tenth most widely used drug in the United States. In this study, using a theoretical study, the interaction between gabapentin and silicon graphene plate (graphene-silicon) and the formation of a stable complex between them was investigated. Silicon-coated graphene was used as the drug delivery [3]. The study was based on the theory of density function of method 6-31g(d)/mo6 2x and using Gaussian 09 software. The adsorption energy and electronic structure of the gabapentin / graphene-silicon system were calculated. Gabapentin from the nitrogenous part with the desired drug delivery with absorption energy equal to -18.497 kcal/mol bonding distance 2.947 Angstrom was also measured from the oxygen part with silicon-impregnated graphene drug delivery with adsorption energy -27.887 kcal/mol and bond distance 2.238 Angstrom was examined. The electron charge distribution also indicated the association of electron clouds between the drug and the nanostructure. The results showed that a strong bond was established between gabapentin and graphene-silicon and the formed complex was thermodynamically stable. Due to the possibility of forming a stable complex, bread graphene-silicon is predicted to be a suitable carrier for the delivery of gabapentin to target cells.

Keywords: Drug delivery, Gabapentin, Graphene doped silicon, Density functional theory

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Cadmium Selenide quantum dot nanocomposite hydrogel based on carboxymethyl cellulose as a photocatalyst and adsorbent for removal of dye from water solution: kinetic and thermodynamic studies

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Hydrogels are three-dimensional hydrophilic polymers that are used for many applications [1]. The hydrogel network can be used as template for the controlled synthesis of nanoparticles such as quantum dots [2]. Quantum dots (QD) are semiconductor nanostructures with applications in many fields including photocatalysis, adsorption, and solar cells industries [3]. In this research, the hydrogel based on carboxymethyl cellulose and acrylic acid were prepared by using radical polymerization method, and then cadmium and selenide ions were loaded in the network of hydrogel. Then, removal of cationic dyes by using the nanocomposite hydrogel was examined. The Cadmium selenide quantum dot nanocomposite hydrogel (CdSe QD-NCH) was characterized by Fourier transform infrared spectroscopy (FT-IR), thermal gravimetric analysis (TGA), scanning electron microscopy (SEM), transmission electron microscopy (TEM), and Photo-luminescence (PL) analysis. The size of the quantum dots was estimated about 5 to 10 nm by TEM. Different studies were shown that CdSe QD-NCH has a significant potential for adsorption of cationic dyes such as crystal violet, and malachite green. The results showed that with increasing temperature, the ability of adsorption of the adsorbent increases. The highest adsorption efficiency was obtained at pH in the range of 6-7. The results of reusability test showed that the nanocomposite hydrogel has the ability to use at least five times without significant changes in adsorption. The CdSe QD-NCH showed photocatalytic activity in the presence of UV light. Kinetic and thermodynamic studies revealed that the pseudo-second-order model matches with the experimental data and Langmuir adsorption isotherm fits the results perfectly.

Keywords: CdSe Quantum Dot, Nanocomposite hydrogel, Carboxymethyl cellulose, Photocatalyst, Dye.

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Kinetic study of doxorubicin drug release from nanocomposite hydrogels containing calcium phosphate entrapped in calcium alginate

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Recently, a lot of attention has been paid to nanoparticles as carriers for drug delivery and slow and controlled drug release [1]. Nanoparticle carriers improve drug operation and reduces side effects by changing the pharmacokinetics of the drug [2-3]. The aim of this study is to synthesize a nanocomposite hydrogel based on carboxymethyl cellulose and investigate the ability of drug delivery of this compound. The kinetics and thermodynamics of the release of Doxorubicin were also studied. The nanocomposite hydrogel was synthesized by loading the hydrogel with calcium chloride and sodium phosphate. Then, the nanocomposite hydrogel and doxorubicin were mixed and entrapped into the calcium alginate beads. Designing this slow-acting system reduces damages of doxorubicin, while increasing bioavailability and toxic effects against cancer cells. To ensure hydrogel formation and loading of the drug, Fourier transform infrared spectroscopy (FT-IR) and thermal gravimetric analysis (TGA) were characterized. Scanning electron microscope (SEM) and transmission electron microscopy (TEM), were used to examine the morphology of the surface of the nanocomposites and to determine the size of the nanoparticles, respectively. The results showed that the nanocomposite hydrogel significantly increases the loading of doxorubicin and its slow release. Increasing the initial concentration of calcium chloride also reduces drug release. The optimum conditions were obtained at pH=4 and 45 °C. According to the kinetic patterns, drug release follows the Korsmeyer–Peppas model.

Keywords**:** Nanocomposite hydrogel, Doxorubicine, Carboxymethyl cellulose, Calcium alginate

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Removal of MB dye from aqueous solution using biochar prepared from orange peel

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Dye are the first known pollutants in industrial wastewater, and various industries such as food processing industries, paper, cosmetics, leather, textiles, printing and pharmaceuticals discharge large amounts of wastewater containing dyes with toxic compounds into the environment [1], and it is estimated that 50,000 tons of organic dyes are disposed of annually worldwide [2]. Dyes are toxic, mutagenic and carcinogenic due to the presence of compounds such as aromatic amines in their structure. Therefore, it is necessary and essential that wastewater containing paints be treated before entering the environment and the amount of paint in them be reduced and removed. There are several methods for removing dye from aqueous solutions, among which, the adsorption method due to advantages such as low economic cost, flexibility in the process, lack of sludge production, ease of process, high speed and efficiency have been highly regarded [3]. In the present study, biochar prepared from orange peel was used as an adsorbent to remove MB dye from aqueous solution. FTIR analysis was used to the characteristics of the prepared biochar, which showed that there are functional groups -OH, C-H and C = O in the structure of biochar. In the MB dye adsorption process, the effect of temperature parameter in the range of 25-50 °C was investigated. The results showed that with increasing temperature, the process efficiency decreases and the adsorption process is exothermic. Also, the value of entropy and enthalpy parameters was determined to be negative, which indicates that the process is spontaneous and exothermic.

Keywords: Biochar, Adsorption, Dye, Temperature

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Synthesis of Magnetic Nanocomposite based on Metal Organic Framework ($ZIF\text{-}8@SnO_2@CoFe_2O_4$) as a Novel Adsorbent

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In this study, $ZIF\text{-}8@SnO_2@CoFe_2O_4$ nanocomposite was synthesized by hydrothermal method and has been used as an efficient adsorbent for the removal of nickel ions from aqueous solution and in addition, the antibacterial performance of this nanocomposite has been investigated. The FT-IR results (Fig. 1) indicate that the peaks at 2920 and 1421 cm^{-1} are belong to the C-H and C = N bonds of the imidazole ring, respectively. The peak at 431 cm^{-1} was also related to the Zn-N bond stretch. As can be seen from FE-SEM images (Fig. 2), SnO_2 nanoparticles have an almost colloidal structure due to its high affinity for aggregation (23–46 nm). The image of $CoFe_2O_4$ show a strong tendency for the nanoparticles to bind, largely due to the high surface area and magnetic tension between the nanoparticles. Also, the FE-SEM image of ZIF-8 have a spherical shape (3–50 nm). Magnetic sensitivity results demonstrated that $CoFe_2O_4$ and $ZIF\text{-}8@SnO_2@CoFe_2O_4$ with saturation magnetization (M_s) value of 22.22 and 7.21 emu g^{-1} would have a fast magnetic response. The X-ray diffraction spectrum (Fig. 3) for $CoFe_2O_4$, SnO_2 and ZIF-8 indicating a crystalline spinel, tetragonal and cubic sodalite-associated structure, respectively. $ZIF\text{-}8@SnO_2@CoFe_2O_4$ has a porous structure (23–46 nm) and SnO_2 and $CoFe_2O_4$ particles are doped at its surface, however, the porous structure of the ZIF-8 substrate is almost preserved [1,2]. The highest removal of nickel ions (50 ppm) by $ZIF\text{-}8@SnO_2@CoFe_2O_4$ (20 mg) after 120 min were found to be 75% at pH of 6. The results of antibacterial properties of nanocomposite for Escherichia coli and Staphylococcus aurous had minimum inhibitory concentration of 2.5 and 1.25 $mg.ml^{-1}$ and minimum lethal concentration of 5 and 2.5 mg. ml^{-1}, respectively.

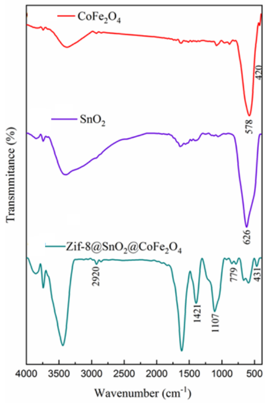

Fig. 1. FT-IR Spectra

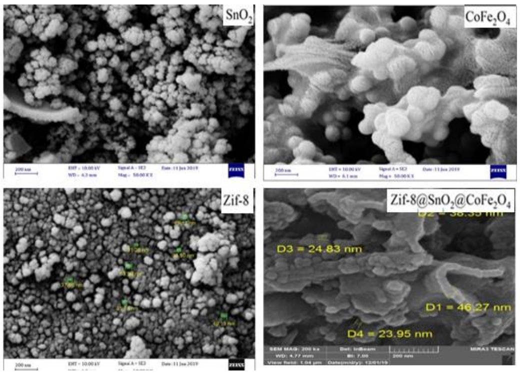

Fig. 2. FE-SEM image

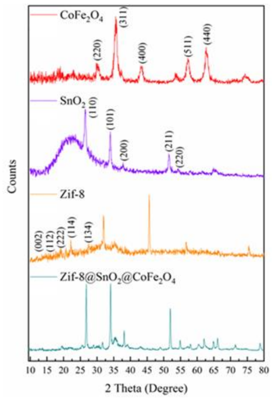

Fig. 3. X-Ray diffractogram

Keywords: Magnetic ZIF Nanocomposite, Antibacterial, Adsorbent

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Oxidation of carboxymethyl cellulose with hydrogen peroxide in order to adsorb Cr (III) from tannery waste water

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The leather industry is one of the most lucrative and at the same time the most environmental polluting industry in the world. Raw hide is imported and transformed into leather. The most important materials in the convertion of hide to leather is chromium sulfate, which contains trivalent chromium (Cr (III)) [1]. Unfortunately, not all chromium is consumed and about 20-30% of it enters the waste water. Cr (III) is less toxic, but under some conditions it converts to more hazardious Cr (VI) [2]. One of the most suitable methods for removing this metal is the adsorption method. In this method, chromium ions are adsorbed by electrostatic or covalent bonds [3].In recent years, natural polymers like carboxymethylcellulose (CMC), have attracted much attention. CMC has a higher solubility than cellulose, but still its solubility is not suitable for environmental applications [4]. Oxidation can modify natural polymers. The resulting functional groups, especially carboxyl groups, are highly suitable for reaction with Cr (III) [5]. Therefore, in this study CMC was first oxidized using the hydrogen peroxide as oxidizing agent. The results of FT-IR analysis and titration showed that with increasing the concentration of hydrogen peroxide from 30% to 100%, the amount of carboxyl groups is increased from 1.26% to 3.42%. Then, this adsorbent was used to adsorb Cr (III) from the tannery waste water. A batch adsorption process was carried out with different adsorbent dosage, and contact time. The results of the analysis showed that using oxidized CMC, the adsorption of chromium reached 90%.

Keywords: Oxidation, Carboxymethyl cellulose, Hydrogen peroxide, Cr (III), Waste water

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Optimization of Sodium Sulfate Purification using Sodium Sulfide complexer and Hydrogen peroxide reagent based on the Taguchi method

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Today, the industry of recycling lead-acid batteries is one of the well-known industries due to its widespread use. Sodium sulfate, as one of the products of the lead acid battery recycling process, is produced from desulfurization of battery sludge or neutralization of battery acid [1] . Due to the nature of the lead acid recycling process, sodium sulfate contains significant amounts of heavy metal elements such as lead and iron and is of very low value. In this study; heavy metal deposition based on sulfide precipitation was used to remove lead and iron heavy metals from sodium sulfate [2] . The precipitation process using excess sodium sulfide and oxidation of excess sulfide with hydrogen peroxide was used. Experimental design based on Taguchi method was used to reduce the number of required experiments [3] . Sodium sulfide content, hydrogen peroxide content, pH and residence time were selected as design parameters at four levels and 16 different experiments were designed based on the L16 array. Analysis of the results based on analysis of variance showed that all selected parameters were effective for the removal of lead metal and the concentration of lead in solution could be reduced from 400 ppm to a maximum of 1.5 ppm.

Keywords: Lead-acid battery recycling, Sodium sulfide, Oxygenated water, Taguchi design method, Analysis of varianc

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Activated carbon synthesis from raisin production wastes and its application in methylene blue removal from aqueous media

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East Azerbaijan Province is one of the major dried fruit poles in Iran. Raisin production is one of the important provincial products and one of the active industries in the province. Raisin factories face a waste problem. Major raisin plant wastes can be classified into four categories: fracture wastes, stem and spike wastes, laser wastes and raisins. All of these wastes are carbon rich materials. In this study we attempted to synthesize activated carbon from raisin wastes. For the synthesis of activated carbon, a chemical activation method using zinc chloride as activating agent (1:1 mass ratio). After synthesis of activated carbon from various wastes and optimization of parameters such as type of activating agent, ratio of activating agent, carbonization temperature and carbonization time, the best conditions for activated carbon synthesis were selected [1].

In order to evaluate the efficiency of the synthesized activated carbon, a methylene blue dye removal test was performed as a model. The parameters affecting the efficiency of the method were optimized. Optimal conditions for the removal of methylene blue using activated carbon including neutral pH, ambient temperature and the amount of adsorbent 0.01 g per 10 ml of solution with a concentration of 20 mgL^{-1}, in which case the removal efficiency is more than 99 Percentage is obtained. The adsorption capacity is about 20 mg g^{-1} and the quasi-synthetic reaction is quasi-second order . According to thermodynamic studies the endothermic reaction is spontaneous and with increasing entropy. The dye adsorption mechanism on the adsorbent also follows the Langmuir isotherm, which indicates the uniformity of the adsorbent surface and the adsorption of the monolayer. Finally, in order to compare the performance of synthetic activated carbon, the removal rate of the synthesized sample under optimal conditions was compared with the commercial activated carbon sample of Merck, Jacobi and activated carbon from almond skin. The results showed that synthetic activated carbon can compete with commercial samples [2].

Keywords: Activated carbon, Raisin waste, Chemical activation, Remove

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Poly (N-vinyl imidazole) nanocomposite hydrogels as an efficient Acid dyes and Ni(II) ion adsorbent from aqueous systems

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Synthetic dyes and heavy metal ions are categorized as main pollutants in wastewater that need careful treatments prior to discharging. However, the adsorption method exhibited great strengths owing to its low energy consumption, high efficiency and ease of operation [1]. They offer some flexibility in terms of swelling kinetics, surface characteristics such as charge, functionality, fast diffusion process, large area, controllable pore structure, thermo-stability and interesting acid/base properties [2]. Two series of pH-sensitive poly (N-vinyl imidazole)/NGQD nanocomposite hydrogels (PVI/NGQD) were synthesized successfully via an in-situ polymerization approach. In the first series, the polymerization was carried out with different feeding ratios of VI and MBA (N, N′- methylene-bis-acrylamide) in the presence of NGQDs (0.3-1.0 wt%) (PVI/NGQD-1). The second series was prepared using VI and DIL (3, 3′ -divinyl-1, 1′ (1, 6-hexanediyl) di-imidazolium dibromide) (PVI/NGQD-2) as a synthesized crosslinker in the presence of NGQDs. The synthesized PVI/NGQD nanocomposite hydrogels were characterized by FT-IR, TGA, XRD, EDS and SEM. Thereafter, the removal of Acid dyes (Acid Red, Acid Bblue and Acid Yellow dyes) and Ni(II) ion from water through the prepared hydrogel network was examined. We examined the influence of pH, contact time and initial concentration of the metal ions on the adsorption capacity. Furthermore, the adsorption isotherm and kinetics were also studied to evaluate the behaviour of the nanocomposite hydrogels.

Keywords: Nanocomposite hydrogels, N-doped graphene quantum dot, N-Vinyl imidazole, Dyes, Heavy metal ions

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Proteolysis of wheat gluten to enhance functional properties and compare different digestion methods

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Recently, new sources of food proteins are needed because of increasing global demand. Wheat gluten can be an economical and diverse alternative to animal proteins as nutrients [1]. The expanding utilization of wheat gluten in food and non-food industries has been limited by lack of some desirable functional properties, such as solubility and emulsifying ability. Consequently, wheat gluten have been hydrolyzed by physical, chemical and biochemical methods [2]. The objective of this present research is to compare various wheat gluten hydrolysis methods; therefore, the modification of wheat gluten is made by mild acid treatment (hydrochloric acid), a commercial proteolytic enzyme (papain) and microbial proteases. The hydrolytic efficiency of these techniques on wheat gluten also compared. Moreover, wheat gluten hydrolysates (WGHs) had superior solubility (>60%) over a pH range 2-12. The molecular mass of peptides released during hydrolysis was in the range of 5-15 kDa and determined by SDS-PAGE and size exclusion chromatography on Ultrahydrogel linear. The results showed that with the increasing of degree of hydrolysis (DH) values, there occurred a large amount of smaller polypeptides and Papain represent best for the preparation of products with the maximum DH 31.2%.

Keywords: Wheat gluten, Protein, Hydrolysis

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Investigation of the kinetic behavior of methylene blue dye adsorption process from aqueous solution using bio-charcoal prepared from tea waste

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Dyes are one of the main causes of water pollution caused by human activities. Synthetic dyes are highly toxic and one of the most resistant environmental pollutants that have deadly and dangerous effects on the lives of humans, plants and other animals in the environment [1]. Dyes due to entering the human body and other living organisms can cause diseases and illnesses such as severe irritation of the eyes and skin, nausea and stomach pain [2,3]. Therefore, it is necessary to remove dyes from the aqueous solution and the environment, because it is dangerous to humans and other living organisms. In the present study, biochar was synthesized from tea waste and investigated as an effective and low-cost adsorbent for removing MB dye from an aqueous solution. In the present study, the effect of various parameters such as pH, temperature, contact time, and adsorbent dose on the initial dye concentration of 10 mg/l was investigated. The maximum efficiency of the adsorption process (93.25%) was determined in pH 10, adsorbent dose of 2 g/l, contact time of 80 minutes, and temperature of 25 °C. To investigate the kinetic behaviour of the MB dye adsorption process, pseudo-first-order and pseudo-second-order models were used. The results showed that the quasi-quadratic kinetic model has more ability to describe the kinetic behavior. The thermodynamic study was showed that the adsorption process is spontaneous and exothermic and it can be stated that biochar from tea waste can be used in removing dyes from aqueous solutions.

Keywords: Adsorption, Biochar, Tea waste, Aqueous solution, Dye

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Synthesis of two-dimensional hematene nanosheets by exfoliation methods and its applications for photocatalytic degradation of tetracycline

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Hematite (α-Fe_2O_3), is a stable crystalline phase of iron oxide, which has a low cost and simple preparation method. Exfoliation of hematite, on the other hand, remains a challenge due to its low yield and time-consuming [1]. In this paper, we described two preparation methods of novel two-dimensional non-van der Waals hematene (2DHm) nanosheets including ultrasound-assisted liquid-phase exfoliation (US-Hm), and chemical-assisted liquid-phase exfoliation (CH-Hm), which were obtained from bulk hematite. The photocatalytic activity of 2DHm nanosheets was evaluated to the decomposition of tetracycline. To investigate the physical and chemical properties of the exfoliated samples, various advanced analyses were used. The single, double, and triple-layered structures of 2DHm were confirmed by SEM and TEM analyses. Also, the formation of hydroxyl radicals ($^{\cdot}OH$) on the surface of 2DHm nanosheets was approved using the o-phenylenediamine [2]. No significant loss was observed in the photocatalytic activity of the 2DHm nanosheets even after three consecutive runs.

Keywords: 2D layered materials, Hematite, Exfoliation, Hematene nanosheets, Photocatalyst

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Synthesis of La-doped NiAl LDHs nanocomposite as a highly efficient visible-light-driven catalyst for degradation of an emerging pollutant

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In this study, La-doped NiAl-layered double hydroxides (LaNiAl-LDHs) were synthesized by a chemical co-precipitation method. The as-synthesized samples were characterized by various solid and liquid characterization methods, and evaluated for the decomposition of antibiotic under visible light irradiation. Antibiotics are persistent and resistant emerging pollutants in an aqueous solution [1]. Under the optimum condition, the photocatalytic activity of La-doped NiAl LDH was higher than NiAl LDH. By doping rare earth ions into the LDHs, the charge separation was enhanced. In addition, the vacant d-orbitals of rare earth elements and the distortion of the lattice may contribute to the surface charge injection process, which is of great importance for the photocatalytic reaction [2]. The effect of the addition of various gases and scavengers was evaluated. The GC-MS analysis was employed to verify the generation of some intermediates during the photocatalytic reaction. The chemical oxygen demand (COD) was analyzed to evaluate the mineralization of the probe pollutant. Furthermore, the reusability and photostability of the nanocomposite was examined.

Keywords: Advanced oxidation process, Photocatalyst, Layered double hydroxides, Lanthanide, Doped

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Fabrication of $Cu_3V_2O_7(OH)_2$/Polyvinyl alcohol based nanocomposite as a new conducting membrane for Low-temperature proton exchange membrane fuel cell

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Fuel cells are promising energy conversion systems that can meet this energy need. One of the essential components in Proton exchange membrane fuel cells (PEMFCs) is the proton exchange membrane. Membranes used in PEMFC must have high proton conductivity, low fuel crossover, thermal/chemical stability, high mechanical strength, and low cost [1]. PVA stands out because of its high hydrophilic character, nontoxic chemical composition, easy modification, and good film-forming properties. Furthermore, it has the disadvantages of high water uptake and low mechanical stability. Hence it cannot provide all desired membrane properties alone. It is required to adjoin proton sources into the PVA to increase hydrophilicity and proton conductivity. Additive materials are used to increase the chemical, structural, and mechanical properties together with the performance of the polymer membranes. This improvement is associated to effective hydrogen bonding interactions in the membrane matrix [2-3]. The mixed metal oxides are known as proton carrier, which are promising materials for devices such as fuel cells. The hydrogen bonding interactions increase in presence of oxygen grope of nanoparticles. mixed metal oxide structures can be used as hygroscopic materials to improve humidity sensing performance. Due to the proton conduction mechanism of these materials upon interaction with water, they are well-known as positive ionic conductors [4-5]. In this project, new nanocomposite membranes based on polyvinyl alcohol (PVA) and copper hydroxide vanadate ($Cu_3V_20_7(OH)_2$) were prepared with the aim of increasing proton conductivity and improving the mechanical and thermal stability of PVA membranes by using the solution casting method. Proton conductivity measurements were performed at 80 and 95% humidity. The nanocomposite membrane showed higher proton conductivity than the pure PVA membrane due to the presence of vanadium copper hydroxide nanoparticles in the membrane matrix. The highest values of proton conductivity at 75°C and 90% humidity for nanocomposite membranes containing 0.5wt.% of copper hydroxide vanadium nanoparticles was obtained 63 mS/cm. The prepared nanocomposite membrane showed higher thermal and mechanical stability than the pure PVA membrane.

Keywords: Proton conductivity, Nanocomposite, Polyvinyl alcohol, Proton exchange membrane fuel cells

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Facile preparation of 2D-biotene by mild solvent thermal exfoliation process from biotite clay

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Since graphene's exodus, layered materials' exfoliation to two-dimensional (2D) nanosheets has attracted much attention. The primary layered materials are composed of weak van der Waals interlayer forces and strong intralayer bonds[1]. Biotite (BTT) or black mica ($K(Mg,Fe)_3AlSi_3O_{10}(F,OH)_2$) is one of the members of mica clays, which has stronger interlayer forces, like highly ordered pyrolitic graphite[2]. In this study, thermal and facile exfoliation of BTT intercalated compounds were combined. In this procedure, BTT was first intercalated in a mixture of H_2O_2 and H_2SO_4 and then was exposed to a rapid heat treatment at 900 ^oC. During these steps, BTT was expanded, afterward, it was exfoliated in an organic solvent to obtain 2D-biotene (BTN) nanosheets. This study has improved synthesis method for producing few-layered BTN nanosheets that are cost-effective, reproducible, and scalable. By this method, BTN nanosheets with reduced thicknesses of 56 nm were obtained, while the specific surface areas were increased by 4 times.

Keywords: Biotite, Clay, 2D-biotene, Mild solvent thermal, Exfoliation

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Synthesis of Nitrogen-Rich Graphitic Carbon Nitride by Thermal Treatment Method and its Use for Improving the Performance of Ultrafiltration Membranes

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Wastewater from the textile industry consists of a variety of complex chemicals, including dyes, detergents, greases, oils, sulfates, solvents, heavy metals, and other inorganic salts, depending on the process regime. Textile wastewater treatment is very challenging due to high temperature, high pH, high oxygen demand and low biodegradation. In addition, it also contains high concentrations of inorganic salts and azo dyes that pose serious risks to human health and the environment [1]. Ultrafiltration (UF), a pressure-based process, has been well developed and used in various industrial applications. UF is often used as pretreatment before reverse osmosis (RO) and nanofiltration (NF) [2]. Despite excellent maintenance performance, there are still problems that limit its widespread use, the biggest known problem being membrane clogging. Membrane clogging may affect the performance of the filtration process, leading to reduced performance and increased energy consumption, which remains a major challenge in filtration processes [3].

In the present study, an attempt was made to improve the performance of ultrafiltration membranes by adding nitrogen-rich graphite carbon nitride (g-C_3N_5). g-C_3N_5 was synthesized by 3-amino-1,2,4-triazole (3-AT) and NH_4Cl by thermal modification. Ultrafiltration membranes with different concentrations of g-C_3N_5 (0-1 wt.%) were fabricated by phase inversion method. Distilled water and protein filtrations were performed to evaluate the performance of the ultrafiltration membranes with different concentrations of additive. According to the results, it was found that the water flux and protein flux of the membranes increased with the addition of g-C_3N_5 indicating lower fouling of these membranes. The prepared membranes were characterized by contact angle measurement, scanning electron microscopy (SEM) and atomic force microscopy (AFM).

Keywords: Graphitic carbon nitride, Thermal treatment, Ultrafiltration

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Extraction of alumina from low-grade Jajarm's bauxite by sintering method

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The components of low grade bauxite is 31% silica, 33.9% alumina, 14.8% iron oxide and 10.7% loss on ignition. Due to the high silica content of this type of bauxite, it cannot be processed by Bayer method. Therefore, sintering method with limestone and sodium carbonate was used for selective extraction of alumina. Experimental design was performed by surface response method (RSM) using box behnken design. Selected parameters are temperature, mass ratio of sodium carbonate to bauxite (S/B), mass ratio of limestone to bauxite (L/B) and mass ratio of carbon to bauxite(C/B). The maximum amount of extraction of alumina from low-grade Jajarm bauxite by sintering method is 61.97%, which is obtained in the optimal values of the parameters as follows: (S/B) = 0.5, (L/B) = 1.19, (C/B) = 0 and T= 1000 °C. The experimental results showed that carbon has a negligible negative effect on recovery of alumina from bauxite. Sodium carbonate increases alumina extraction yield [1]. Limestone increases alumina recovery by about 1.19 times the weight of bauxite and then reduces the recovery. The optimum temperature is about 1000 °C. The thermograms of each material and their binary and triple mixtures (carbon, limestone, bauxite) show two endothermic peaks at about 600 °C and 1000 °C, The first peak is related to the change of crystalline structure of bauxite and the second is related to the decomposition of limestone and evolving of carbon dioxide. The endothermic reduction peak of iron oxide is not seen in thermograms, which indicates that carbon does not react with iron oxides. This is also confirmed in the results of experimental design modelling, which indicates the negligible role of carbon in the process and the lack of need for carbon. In 27 run experiments, the mixture of materials powder was transferred to a platinum crucible and heated in a muffle furnace at temperatures determined by the experimental design. The soaking time was 20 minute. The sintered material was pulverized. The resulting powder was leached by 100 mL of alkaline solution for 30 minutes at a stirring speed of 300rpm. Extracted aluminium from leaching stage was analysed by atomic absorption spectrometry.

Keywords: Sintering, Alumina,Atomic Absorbtion,Box behnken

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Fabrication of polyethersulfone ultrafiltration membranes with simultaneously enhanced permeability and antifouling performance by impregnating with 2D-biotene

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According to the huge population increase, water shortage is one of the most critical problems in many parts of the world. Contamination of water from agricultural residues, industrial waste, and sewage intensifies this challenge [1]. Due to producing high-quality water, high efficiency, low cost, and operation simplicity, membrane-based technologies have acquired wide acceptance among the diverse approaches that have been developed [2]. In this work, one or few-layer-biotene (E-BIT) was prepared by liquid-phase exfoliation of bulk biotite (B-BIT). The successful preparation of E-BIT was further verified via scanning electron microscope (SEM), transmission electron microscopy (TEM), X-ray powder diffraction (XRD). This nanoadditive was utilized to improve the properties of polyethersulfone (PES) polymeric membrane. E-BIT blended membranes with various quantities (0-2 wt%) were prepared via the phase inversion method. The fabricated membranes' morphology was investigated by applying atomic force microscopy (AFM) and SEM techniques. Contact angle analysis was applied in order to confirm the improvement of the membranes' hydrophilicity in the E-BIT presence. 1 wt% E-BIT blended membrane illustrated permeability enhancement of 198.8 L/m^2 h, and high pollutants removal of bovine serum albumin (99%), reactive red 195 (98%), reactive green 9 (93%), reactive blue 19 (88%), with emproved flux recovery ratio of 73%.

Keywords: Biotite, Clay, 2D-biotene, Ultafiltration, Mix matrix membrane

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Using synthesis gas exiting the biochar producer system to reduction of iron oxide wastes resulting from cooling stage of steel ingots

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One of the most important features of sustainable development is the use of technologies with an environmental approach. Environmentally, green steel production is highly recommended, because fossil fuels are still the primary source for reducing agent in the steel industries [1]. Also, recycling various wastes such as agricultural wastes can be a priority for any government, both environmentally and economically [2]. Therefore, the research aims at evaluating the performance of a combined system of 1) biochar producer system as a supplier of synthesis gas (syngas) as a reducing agent and 2) reduction system of iron oxides. One of the byproducts of biochar production by rotary kilns is synthetic gas, which is usually used as an auxiliary fuel on site. In this work, the designed continuous rotary kiln was used to produce biochar, which also used greenhouse waste as feed. The existing hot syngas is heated to over 900ºC and then enters the small-scale rotary kilns where it reacts with the iron oxide waste to produce direct reduced iron (DRI). The results showed that the syngas exiting the biochar producer system contains approximately 87.6% H_2+CO, 2.1% CO_2, and 10.3% CH_4. The H_2/CO ratio is about 1:6, which is the same as used in a natural gas-based Midrex plant after reformation and has a suitable efficiency on reducing the iron oxide wastes.

Keywords: Syngas, Biochar, DRI, Fe_2O_3, Environment.

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The inhibitive effect of naphthalene-based azo-azometin as corrosion inhibitor of mild steel in 0.1 M HCl solution: Design, performance and electrochemical studies

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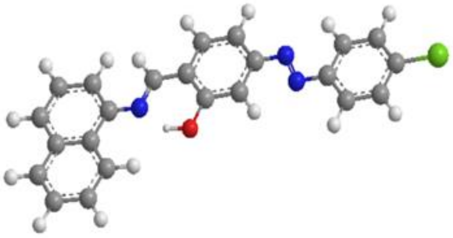
In a recent paper, a naphthalene-based azo-azometin inhibitor of 4-((4-chlorophenyl) diazenyl)-2-((naphthalen-1-ylimino)methyl) phenyl, HL, has been prepared by reaction of 1-(3-formyl-4-hydroxyphenylazo)-4-chlorobenzene with 1-naphthylamine in EtOH [4]. The HL was characterized using NMR, FT-IR and Uv-Vis spectroscopic methods. The inhibitive effect of HL was investigated as corrosion inhibitor of mild steel in 0.1 M HCl solution using weight loss, polarization and electrochemical impedance spectroscopy techniques [1]. The effects of time, temprature and concetration of HL on corrosion rate of mild steel was also investigated [3].The scanning electron microscopy, SEM, study of steel in HCl medium indicated that the inhibition is the result of the adsorption of HL on the mild steel surface and blocking of the active sites. The presence of N and O atoms, heterocyclic and aromatic rings, increase the inhibition effect of HL [2].



Schem. 1. The Structure of HL

Keywords: Inhibitor, Corrosion, Acidic environment, Ggravimetric, Polarization impedance

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Introducing a novel technology for landfill leachate treatment

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As a developing country, the population, urbanization and industrialization are growing rapidly in Iran. Landfill leachate (LFL) that is dark effluent resulting from decomposition of municipal solid waste (MSW) contains high amounts of organic matter, recalcitrant compounds [1] and emerging contaminants [2]. If it is not properly collected and treated, it causes a critical problem to environment [3]. Currently, various processes are used for LFL treatment, such as chemical, physicochemical, biological, etc., each of which has its limitations. But evaporation is the only treatment technology available today that actually rids the water component from water-based waste streams. It can, reduce the total volume of leachate to less than 5% of original volume. However, current evaporation methods still have limitations such as high cost and sediment production, etc. In the present work, the designed process consists of two following parts: 1) the thin film evaporation column and 2) the continuous rotary kiln. The results showed that the process reduced the total volume of the leachate to less than 2% of initial volume. Also, the BOD and COD content decreased significantly.

Keywords: LFL, MSW, Thin film evaporator, Pollutant, Environment.

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Lipase-Tween 80 as an interfacial activated biocatalyst for biodiesel production

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Biodiesel is a renewable energy source, which is produced through transesterification reactions [1]. Despite great attention to develop enzymatic biodiesel production, there are serious obstacles to the industrial development of it such as its cost and slow reaction rate. Along with disadvantages, there are several advantages for enzymatic biodiesel production. Higher purity of fuel and glycerol is known as the most important achievement of enzymatic process [2]. In this study, performance of four different fungi for lipase production was investigated and Aspergillus niger was selected as enzyme source. Lipase production were optimized using experimental design and the optimized factors were determined as pH 5, temperature 30 °C, Potato Dextrose Broth (PDB) 3 % w/v, olive oil 1.50 % v/v, with maximum lipase activity of 42.8 ± 0.51 U/mg. In order to interfacial activation of the lipase, effect of surfactants was studied. Therefore, surfactant-enzyme aggregates were used as biocatalyst for transesterification reaction. Effects of factors on biodiesel yield were studied too. The yield was 96.41 ± 1.20 % at the optimized conditions (methanol/oil molar ratio (5.50:1), enzyme concentration 19 % v/ w, Tween 80 concentration 19 mg L^{-1}, temperature 40 °C and reaction time 46 h).

Keywords: Biodiesel, Transesterification, Aspergillus niger, Interfacial activation

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Cotton/Fe_3O_4@SiO_2@$H_3PW_{12}O_{40}$ a magnetic heterogeneous catalyst for biodiesel production

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This research aims to design and prepare a new magnetically recoverable catalyst based on agro-wastes. For this purpose, cotton waste was selected and its application in the preparation of magnetic catalysts (Cotton/Fe_3O_4@SiO_2@ $H_3PW_{12}O_{40}$) used for the production of biodiesel, which is based on heteropoly acid (HPA), was investigated [1, 2]. Magnetic cotton powder with high dispersibility, porosity and magnetism were prepared by the co-precipitation method and covered by silica using tetraethyl orthosilicate (TEOS) to form Cotton/Fe_3O_4@SiO_2. Finally, the nanostructured catalyst was prepared by impregnation of phosphotungstic acid (HPW). The proposed catalyst was characterized by X-ray diffraction (XRD), Fourier transform infrared spectroscopy (FT-IR), Field emission scanning electron microscopy (FESEM) equipped with Dispersive Energy X-ray spectroscopy (EDS), Thermo gravimetric analysis (TGA), The Brunauer-Emmett-Teller (BET) surface area analysis, Barrett-Joyner-Halenda (BJH) pore size and volume analysis and vibrating sample magnetometer (VSM). The results showed the Keggin structure of the catalyst. The performance of the proposed core-shell nanocomposite to catalyze transesterification reaction was evaluated and optimized by response surface methodology (RSM). According to the results, 3 wt. %, 3.5 h, 12:1 and 70°C were found as optimum values for catalyst dosage, reaction time, the molar ratio of methanol to oil and reaction temperature, respectively. The production yield was higher than 90% for three runs. On the fourth attempt, the catalyst performance was decreased slightly to 85.5%. The used catalyst was characterized by FT-IR, XRD, EDS and FESEM for leaching studies. The quality of the biodiesel product was tested according to the standard procedures defined by the American Society for Testing and Materials (ASTM) and European Union (EU).

Keywords: Waste cotton, Biodiesel, Transesterification, Heteropoly acid, Heterogeneous catalyst

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Lipase immobilization on Rubber-$Fe_3O_4@SiO_2$ nanoparticles as biocatalyst for biodiesel production

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The purpose of this work is to develop a magnetically recyclable immobilized lipase for biodiesel production to meet the need of green and clean production [1, 2]. Magnetic Rubber-Fe_3O_4 nanoparticles were prepared with coprecipitation method and covered with SiO_2 to form the core–shell Rubber-$Fe_3O_4@SiO_2$ nanoparticles. Then the nanoparticles were modified with glutaraldehyde for functionalization of the surface to aldehyde groups. The functional groups, structure, morphology and magnetic susceptibility of synthesized and modified Rubber-$Fe_3O_4@SiO_2$ magnetic nanoparticles were characterized by FTIR, XRD, SEM, TGA, and VSM techniques. It was observed that the lipase was immobilized on the nanoparticles successfully from the Fourier transform infrared spectra. The immobilized lipase on Rubber-$Fe_3O_4@SiO_2$ nanoparticles was characterized and compared to free enzyme. The immobilized lipase displayed higher relative activity in Compare with the free enzyme, the immobilized one showed higher thermal stability, especially at high temperature. Thus, the prepared lipase was proved to have the advantages like higher relative activity, better stability, broader pH range and easy to recovery. These results suggest that immobilization of lipase on Rubber-$Fe_3O_4@SiO_2$ nanoparticles has the potential in biodiesel production. A fatty acid methyl ester (FAME) conversion of 94.89% could be achieved by lipase immobilized on Rubber-$Fe_3O_4@SiO_2$ magnetic nanoparticles under optimized conditions. The FAME conversion remained greater than 80% even after reusing the catalyst for 5 reactions.

Keywords: Biodiesel, Transesterification, Magnetic biocatalyst, Lipase immobilization

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Rubber-$Fe_3O_4@SiO_2@H_3PMo_{12}O_{40}$ as Heterogeneous catalyst for biodiesel production

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The aim of this research is to develop magnetically recoverable Heteropoly acid (HPA) based catalyst (Rubber-$Fe_3O_4@SiO_2@H_3PMo_{12}O_{40}$) for biodiesel production. Magnetic Rubber powder with high dispensability, porosity and magnetism were prepared by co-precipitation method and covered by silica using TEOS to form Rubber-$Fe_3O_4@SiO_2$. Finally, nanostructured catalyst was prepared by impregnation of phosphomolybdic acid (PMA)[1, 2]. The proposed catalyst was characterized by X-ray diffraction (XRD), Fourier transform infrared spectroscopy (FT-IR), Scanning Electron Microscopy (SEM) equipped with Dispersive Energy X-ray spectroscopy (EDS), Thermo gravimetric analysis (TGA), The Brunauer-Emmett-Teller (BET) surface area analysis and vibrating sample magnetometer (VSM). The results showed the Keggin structure of the catalyst. The performance of the proposed core-shell nanocomposite to catalyze transesterification reaction was evaluated and optimized by response surface methodology (RSM). According to the results, 3 w/w %, 3h, 12:1 and 69°C were found as optimum values for catalyst dosage, reaction time, molar ratio of methanol to oil and reaction temperature, respectively. The production yield was higher than 85 % for four runs. At the fifth try, the catalyst performance was decreased slightly to 78.87%.

Keywords: Biodiesel, Transesterification, Heteropoly acid, Heterogeneous catalyst

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Rapid fabrication of the 2D close-packed colloidal crystals at the air-water interface for Nanosphere Lithography

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An easy and fast way to fabricate large-scale close-packed colloidal monolayers is to directly apply polymer nanospheres at the air-water interface. Thus, 2D colloidal crystals are formed by self-assembly that can be transferred to any substrate [1]. In this study, we show that different factors play crucial roles in the fabrication of 2D close-packed colloidal crystals such as the components of the liquid phase, the polymer solution, and also the way of adding the polymer solution to the liquid phase. It is shown that the use of 0.1 mM sodium dodecyl sulfate (SDS) is an anionic surfactant that emulsifies, puffs, accelerates dissolution and foaming, and then counteracts the repulsive force between poly (methyl methacrylate) (PMMA) nanospheres. Therefore, it makes the polymer nanospheres come together in a hexagonal lattice as monolayers [2]. Also, it is proved that adding propanol or ethanol to the polymer solution with specified concentrations can have a great effect on the dispersing of the polymer nanospheres on the surface of the liquid phase. Furthermore, it is also revealed that injecting a small amount of the polymer solution on a hydrophilized tilted glass substrate at a specific angle that is partially inside of the liquid phase, can facilitate the fabrication of monolayers on the air-water interface. Then, 2D colloidal crystals can be transferred to various substrates such as silicon and glass using different methods. In our experiment, the monolayers are transferred on a tilted substrate that is placed inside of the liquid phase, under the monolayer using the liquid discharge with a controlled rate [3]. The proposed monolayers of polymer nanospheres can be used as a mask in Nanosphere Lithography (NSL) that can be applied to fabricate metal nanoparticle arrays with different shapes and morphology on substrates which is promising for a wide range of applications.

Keywords: Colloidal crystals, Nanosphere lithography, Poly (methyl methacrylate), Self assembly, Air/Water interface.

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Activation energy of thermal degradation of Styrene based polymers using the Kissinger kinetic model

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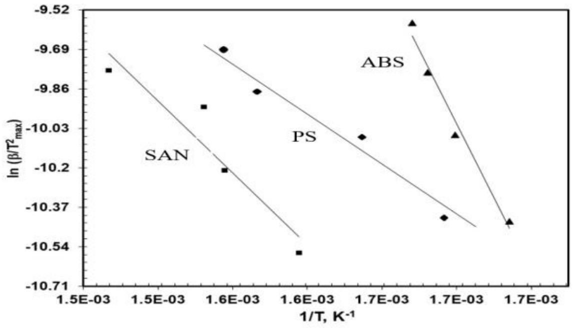
Abstract: In this study, the kinetic analysis of degradation of some different polymers in nitrogen medium has been studied using Kissinger method and the results have been compared with each other. Also, the degradation activation energy of these polymers was determined using the Iso-conversion method [1]. In this research, kinetic models related to different degradation mechanisms have been used. Thermal gravimetric method has been used for thermal degradation studies [2]. Experiments are usually performed under non-isothermal conditions. The activation energy was determined by using the reaction mechanism fitting method [3]. There was a relationship between degradation rate and activation energy, wherein quick degradation rate income low quantity of activation energy. The kinetic model determines the kinetic parameters, in the conversion range. It was concluded that the model-free methods, could be used for determining the dependency of activation energy on conversion. Also the most degradation reactions are not simple one-step processes and consist of multiple steps during degradation process.



Schem1.The Kissinger Model Used for Some Polymers

Keywords: Activation energy, Kissinger model, polymers, Thermal degradation

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The thermodynamic parameters of different polymer/blowing agents systems determined by the magnetic suspension balance (MSB).

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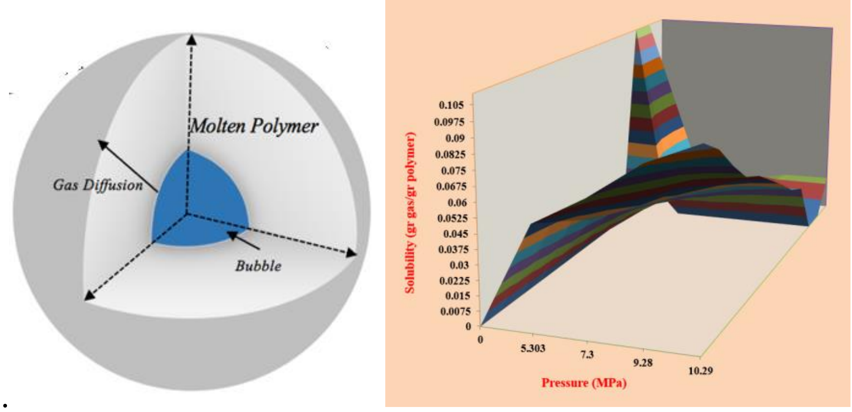
Abstract: In this work, the MSB system and equation of state was used for calculating the thermodynamics parameters like, solubility and diffusivity of different gases in polymer matrices. For determining the specific volume of polymers with blowing agents, the Sanchez-Lacombe (SL) equation of state was used which the chemical potential gradient of any gas was found from numerical calculation using the SL equation [1]. Fick’s second diffusion law was used for determining the diffusion coefficients [2]. The effect of different conditions on the solubility and diffusivity of blowing agents in the samples was examined. The results show that the solubility was increased by saturation pressure increment. Also it was disscused that the thermodynamics parameters were affected by the temperature increment. The diffusivity was increased with increasing of the pressure and temperature. The solubility data was corrected with the SL eqution and the diffusivity value was determined by fitting the Fick law equation on experimental data. The schimatic view of gas diffusion and the dependency of solubility on pressure were shown in Schem 1.



Schem. 1. The Schimatic View of Diffusion (left Schem) and the Solubility Versus Pressure (right Schem)

Keywords: Thermodynmic parameters, Solubility, Diffusivity, Blowing agents

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Temperature and pressure effects on the cellular structure of amorphous polymer foams produced by the batch foaming technique

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The production of cellular polymer foams has been well-known recently because of their various applications like thermal insulation, furniture and automotive industry [1]. In this study the amourphous polymers with two different blowing agents (CO2 and n-pentane) were foamed via the batch foaming system. The system contains a high-pressure stainless steel vessel, pressure gauge and temperature controller. The thermodynamic instability in polymer/gas system could be provided through a rapid pressure release or temperature increment. The effect of different foaming conditions, like temperature and pressure on the foaming process, were investigated. The morphological study was investigated for samples by using the scanning electron microscopy (SEM) [1-2]. The cell density was decreased with increasing of the temperature and increased by the pressure in foams, respectively. The results also show that the temperature, and using two blowing agents, could control the final cellular structures of polymer.

Keywords: Cellular structure, Amorphous polymers, Batch foaming technique.

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Effect of Magnetite Nanoparticles on Iron Deficiency Anemia

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The biosynthesis of nanoparticles by using microorganisms develops as an ecofriendly method for nanoparticle synthesis because of its cheap, simple and non-toxic. Iron supplement drugs such as ferrous sulfate is the most used drug for treatment of iron deficiency anemia, but this supplement report that can yield undesirable side effects. The nanoparticles are synthesized in this study were iron oxide and chitosan – iron oxide nanoparticles. The dose of nanoparticles has more bioavailability compare to ferrous sulfate. Furthermore, both doses of nanoparticles cause lower inflammation than ferrous sulfate and more efficiently restored of serum iron, ferritin and transferrin to normal range.

According to the following, we was suggested the mechanism of Fe_3O_4 entered to the erythrocyte as figure in research content:

- Coating with chitosan by formation chelating agent with iron.
- Increased the levels of Malondialdehyde (MDA), Ferritin, Total Antioxidant Capacity, Serum iron.
- Decrease the level of Transferrin.
- Increase of Conductivity of erythrocytes.
- Alteration of RBC shape band in UV-visible scan.
- Changing in Electrophoresis of erythrocytes bands.

Keywords: Iron deficiency anemia, Ferrous sulfate, Nanoparticle, Chitosan

A Molecular Imprinted Polymer based on Graphene Quantum Dot as an Intelligent Drug Delivery System

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Molecularly imprinted polymers (MIP) have attracted much attention in pharmaceutical fields due to their distinct advantages. In recent years, it has been found that these MIP-based drug delivery systems (MIP-DDS) can improve the therapeutic efficacy of the drugs as a new strategy for delivering therapeutic agents with desired controlled release and/or targeting efficiency. When MIP are used as the carriers, sustained drug release can be achieved due to the specific selectivity and affinity of MIP to template molecules, which make MIP to be a promising drug delivery system [1,2]. An intelligent MIP-DDS can be obtained by employing functional materials, including magnetic, pH sensitive, temperature sensitive, photo sensitive and bio-macromolecule sensitive materials. Graphene quantum dots (GQDs), a monoatomic thickness structure similar to that of graphene, have unique optical properties and retain many of the electrical and mechanical properties of graphene, have many applications in bioimaging and drug delivery [3]. In this regard, the aim of this study was to preparation of a chitosan-based molecular imprinted polymer for anticancer drug using the sol-gel method. Also, graphene quantum dot (GQD) was prepared by the pyrolysis of citric acid (CA), and was incorporated into chitosan through electrostatic interactions and H-bonding. The nonimprinted polymer (NIP) was prepared and used as a control, during the whole experiment. The physicochemical and morphological characteristics of the prepared sytems were investigated using FTIR, XRD, TGA and SEM analyses. Afterwards, the performance of product as an anti-cancer carrier was examined through in-vitro drug relaeses experiments. Results showed the influence of GQDs content on the system property. The specificity of the prepared system into drug was indicated by an acceptable imprinting factor. From the in vitro drug release studies, the prepared MIP system exhibited an excellent controlled drug release profile without burst release.

Keywords: Molecular imprinted polymer, Drug delivery, Graphene quantum dot

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Preparation of Inorganic-Organic Hybrid Materials as Anticancer Drug Carriers

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Inorganic-organic hybrid materials possess multi-functionalities with noteworthy properties due to the combination of their counterparts. These materials may find significant application in biomedical technology, specifically in drug delivery process [1]. In this regard, micro and mesoporous inorganic products, such as zeolites, have been largely used as adjuncts to polymeric substances in a variety of forms, such as composites, blends, and hydrogels for drug delivery [2, 3]. The objective of this study was to develop an inorganic-organic hybrid material based on zeolite and alginate for sustained release of an anticancer drug to improve its half-life. For this purpose, first drug was loaded on zeolite pores by soaking and mixing procedures. Then, hybrid hydrogel beads, composed of zeolite-drug core coated with alginate shell were prepared by using in-situ gel preparation technology. The prepared drug delivery system was characterized by Fourier transform infrared spectroscopy (FT-IR), X-ray diffraction (XRD), and scanning electronmicroscopy (SEM) analyses. By in vitro experiments the effects of zeolite contents and pH of the release media on the release rate of the drug were investigated. According to the results, the inorganic-organic hybrid hydrogels showed an improved encapsulation efficiancy (EE) and drug loading content (DLC). The swelling of hydrogels showed a pH-responsiv behavior in three buffer media. Finally, in vitro drug release studies revealed the delivery of anticancer drug with a controlled manner.

Keywords: Inorganic-organic hybrid, Zeolite, Drug delivery

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Modification of self-cleaning alumina coatings by Polydimethylsiloxane

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One of the biggest day-to-day problems facing communities is cleaning up pollution at multiple levels [1]. The purpose of this research is to create a coating [2], self-cleaning and removing the defects of the previous generation of these types of coatings [3], as well as to increase durability, maintain cleanliness and reduce production costs and the use of self-cleaning films[4]. In this study, alumina coatings were used for their durability. Also, polymeric Polydimethylsiloxane were used to increase the efficiency of these films . X-ray diffraction patterns (XRD) for the phase detection of used components in thin films, scanning electron microscope (SEM) for surface morphology, optical microscope (OM) and contact angle goniometer (CAG) for measuring the hydrophobicity ability were used to characterize formed thin films. The results of various analysis as well as the examination of the contact surface angle equal to 2 degrees are proof that a coating with superhydrophobic and self-cleaning properties has been created.

Keywords: Self-cleaning, Alumina, , Polydimethylsiloxane

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Application of amorphous UiO-66 and NH_2-UiO-66 metal organic frameworks in gas separation membrane

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In the present research, amorphous UiO-66 and NH_2-UiO-66 metal organic frameworks (aMOFs) were fabricated by typical solvothermal [1] method and the following ball milling process. After characterizing prepared aMOFs, they were inserted into polymer matrix containing polyethersulfone, polysulfone and polyvinylpyrrollidone with weight percent ratio of 40:40:20, respectively. The fabricated mixed matrix membranes (MMMs) were analysed by FT-IR, SEM, TGA, XRD and DSC techniques and their gas separation performances were also evaluated by constant volume/variabe pressure method in three upstream pressure of 3, 5 and 7. The best outcome was related to the MMM containing NH_2-UiO-66 at 7 bar in which CO_2 permeability and CO_2/CH_4 selectivity of 8.69 barrer and 75.56 were achieved, respectively.

Keywords: Gas separation, Membrane, Amorphous metal organic framework

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Comparative study of kinetic and electrical energy consumption of paraquat herbicide removal process in aqueous solution using UV/TiO_2NP/KPI and UV/TiO_2NP/KPS as advanced oxidation processes

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In this study, the kinetic and electrical energy consumption of UV-C irradiation/TiO_2 nanophotocalysise (TiO_2NP)/potasium persulfate (KPS) and UV-C irradiation/TiO_2 nanophotocalysise (TiO_2NP)/potasium periodate (KPI), as advanced oxidation processes (AOPs) for removal of paraquat (PQ) herbicide in aqueous solution have been comparaded. Removal kinetic of PQ was assessed under the optimum conditions ([PS]=400 mgL^{-1}, [TiO_2NPs]=150mgL^{-1}, and [pH]in=6 for UV/TiO_2NP/KPS process and [PI]=90 mgL^{-1}, [TiO_2NPs]=125 mgL^{-1}, and [pH]in=6 for UV/TiO_2NP/KPI process) for 30 mgL^{-1} of the herbicide initial concentration at 25°C, based on pseudo-first-order equation both processes and the kinetic constants are 0.0299 min^{-1} for the PS process and 0.0604 min^{-1} for the PI process. The electrical energy consumption was estimated to be about 481.60 $kWhm^{-3}$ for the PS process and 238.41 $kWhm^{-3}$ for the PI process.

Paraquat is a nonselective contact herbicide and is used as the third most widely herbicide in the world [1,2]. The United States Environmental Protection Agency (USEPA), classified paraquat dichloride as a restricted use pesticide due to high acute toxicity to animals and people with the acute oral toxicity of 4,4-bipyridyl with an LD_{50} value of 40-200 mg/kg body weight [3]. Nowadays, heterogeneous photocatalytic degradation in the presence of nanostructure catalysts and inorganic oxidants such as $S_2O_8^{2-}$ and IO_4^- as one of the advanced oxidation processes (AOPs) intensively studied as the most environmentally friendly and promising techniques for the degradation of recalcitrant organic pollutants in water by powerful oxidants especially hydroxyl radicals or superoxide radicals [4-8].

Keywords: Paraquat herbicide removal, Advanced oxidation processes, Kinetic study, Electrical energy consumption.

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Development of MoS_2-based nanocomposite membrane for effective removal of direct red 23 dye

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Nowadays, technologies related to membrane processes have received particular attention due to their low level of energy consumption, lack of contamination, eco-friendly, and ease of conversion to larger scales [1]. Nanofiltration (NF) is a membrane separation process that is in the range of ultrafiltration (UF) and reverse osmosis (RO) in terms of performance and pore size. NF membranes are widely used in various fields such as desalination of seawater, water softening, removal of heavy metal ions from drinking water, and textile effluent treatment due to their advantages such as relatively low operating pressure, high permeability, good recovery, and appropriate rejection of multivalent ions, and small organic molecules [2,3].

In the present study, the molybdenum disulfide/oxidized carbon nanotubes (MoS_2/O-CNTs) nanocomposite was initially synthesized using the ultrasonic-hydrothermal method. Next, the MoS_2/O-CNTs nanocomposite was employed to modify the surface of polyethersulfone (PES) membranes. PES membranes were fabricated via a facile and affordable phase inversion method. Afterward, to stabilize the MoS_2/O-CNTs nanocomposite on the surface of PES membranes, the membranes were immersed in a polyvinyl alcohol solution. The dead-end filtration system was utilized to evaluate the membranes' performance. The outcomes showed that the MoS_2/O-CNTs nanocomposite membrane with a mass ratio of 10:1 could reject 95% of direct red 23 dye, similarly to the MoS_2 membrane. Simultaneously, the nanocomposite membrane had a permeation flux of 7.7 L/m^2 h bar for direct red 23 dye, almost 1.5 times more than the MoS_2 membrane.

Keywords: Nanofiltration, MoS_2, Wastewater treatment, Dye separation, Polyethersulfone membranes

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Extraction of alumina from Nepheline Syenite assisted by carbon

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Alumina extraction from nepheline syenite was investigated using carbon. Selected parameters for alumina extraction from nepheline syenite are reaction temperature, soaking time and carbon content [1]. The experimental design was done by box Behnken design (BBD) by Minitab version 18 software to investigate the effect of effective parameters on alumina recovery from nepheline syenite and to determine the optimal point of alumina recovery. A mixture of nepheline syenite powder and graphite was heated in the temperature range of 1000 °C to 1200°C [2]. The heated mixture was leached by a 300 g/L sodium hydroxide solution for 30 minutes while stirring at 400 rpm. Finally, the amount of extracted alumina was determined by the atomic absorption spectrometric method. The maximum and minimum recovery of alumina was 82.1% and 8.85% of the alumina in nepheline syenite respectively [3]. It was found that the most important factor affecting alumina extraction is the temperature square. Some parameters such as carbon, temperature×carbon and temperature, are respectively other important factors, and the soaking time parameter is the least important.The P-value of the obtained model was 0.001 and the Lack-of-Fit of the model was 0.800 [4]. The maximum alumina extraction predicted by the obtained model is 84.24%, which is achieved ata temperature of 1109 °C, a soaking time of 54 minutes and a weight ratio of nepheline to the carbon of 2.

Keywords: Carbon, Nepheline syenite, Alumina, Atomic sbsorption, Box behnken

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Evaluation of electro-Fenton removal of doxycycline from polluted water via carbon-cloth cathode

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Pharmaceutical contaminants are one of the most acute problems in modern life. The most important reason of the study and control of pharmaceutical contaminants in the environment is the entry of these contaminants into the food cycle and their high resistance to degradation, which leads to many environmental and medical hazards [1, 2]. Over the past decades, several methods have been reported to remove contaminants from polluted water. Among the studied methods, advanced oxidation processes (AOPs) has received more attention by researchers and scientists [3]. Electro-Fenton (EF) is one of the AOPs methods which is safe and low-cost due to the in-situ production of H_2O_2. It takes place at room temperature and pressure. This method is capable of completely mineralizing the organic pollutants if all the effective factors are optimized [4].

In the present study, electro-Fenton (EF) process was applied to remove doxycycline (DOX) antibiotic from polluted water via carbon-cloth and platinum electrodes as cathode and anode, respectively. Raman spectroscopy, X-ray diffraction, atomic force microscopy, scanning electron microscopy, mapping, energy dispersive X-Ray, and cyclic voltammetry analyses were performed to investigate the carbon-cloth cathode. The effect of operational parameters in EF, including current intensity (mA), initial pH, initial DOX concentration (mg/L), and process time (min) on the DOX removal efficiency was investigated via the response surface methodology. According to the results, the maximum DOX removal efficiency were obtained at a current intensity of 200 mA, initial DOX concentration of 40 mg/L, pH = 3, and reaction time of 120 min. Finally, the intermediates of DOX removal and the amount of DOX mineralization were determined via gas chromatography-mass spectrometry analysis and total organic carbon analyses, respectively.

Keywords: Carbon-cloth cathode, Doxycycline, Electro-fenton

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Removal of doxycycline from contaminated water through anodic oxidation process using Ti/RuO_2–IrO_2 anode

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The expansion of cities and industries has led to the production of increasing amounts of domestic and industrial wastewater. Pharmaceuticals are one of the main groups of organic pollutants in water resources [1]. Antibiotics as group of high-consumption pharmaceuticals are widely used in the treatment of medical and veterinary infections, and about 15% of all pharmaceuticals usage belong to this group [2]. Advanced oxidation processes (AOPs) are known as a reliable method for the removal of pollutants. AOPs include processes in which hydroxyl radicals react with the contaminant as a strong oxidant, causing complete degradation or the production of biodegradable intermediates. AOPs have been considered as a clean method due to their high efficiency, low cost, ease of processing and availability of reagents [3]. Anodic oxidation (AO) is one of the most widely used methods of AOPs [4].

In this research, AO method was used to remove doxycycline (DOX) antibiotic from contaminated water via Ti/RuO_2–IrO_2 anode and active carbon cathode. Raman spectroscopy, X-ray diffraction, atomic force microscopy, scanning electron microscopy, mapping, and energy dispersive X-Ray analyses were performed to investigate the Ti/RuO_2–IrO_2 anode. Ti/RuO_2–IrO_2 anode electrochemical behaviour was investigated by cyclic voltammetry analysis. The effect of operating parameters, including current intensity (mA), initial pH of solution, initial DOX concentration (mg/L) and process time (min) on the DOX removal efficiency was investigated using the response surface methodology. The results showed that the optimal values for the variables of current intensity, pH, initial DOX concentration and process time were 400 mA/cm^2, 3, 20 mg/L, and 120 min, respectively. Using gas chromatography-mass spectrometry analysis, DOX removal intermediates were detected and the DOX mineralization efficiency was determined by total organic carbon analysis.

Keywords: Anodic oxidation, Doxycycline, Ti/RuO_2–IrO_2 anode

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Fabrication of Quantum Dot Sensitized Solar Cells Photoanode Based on TiO_2 Inverse Opal and Enhancement of its Performance by Lanthanide Doping

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Quantum dot-sensitized solar cells (QDSSCs) have attracted a great deal of attention in the field of solar cell fabrication due to their excellent optoelectronic properties[1]. Studies have shown that proper engineering of structures can effectively help absorb light, transfer charge and improve the efficiency of solar cells. Photonic crystals with physical properties such as slow light effect, light trapping, and photonic bandgap increase the efficiency of solar cells, and photonic bandgap inhibits light propagation in a certain wavelength range due to Bragg diffraction[2]. Rare intermediate metals such as Er^{3+}, Yb^{3+}, and Tm^{3+} can absorb electromagnetic waves in the low-energy infrared wavelength region, and emit electromagnetic waves in the visible region at higher energies, a process called upconversion[3]. Metal lanthanide elements due to the displacement of the emission from the infrared wavelength region with less energy to the visible region with more energy and the deposition of these nanoparticles on the surface of photonic crystals due to the different refractive index in the structure of photonic crystals, improves the emission displacement in Nanoparticles are doped intermediates in the photonic crystal structure. In this work, by doping lanthanides to the structure of inverse opal and depositing QDs by sillar method on TiO_2 inverse opal and measuring current intensity and voltage, we observed the current from 8 mA to 10 mA with dopping Er^{3+} and the voltage to 670 mV increased.

Keywords: Solar cells, Quantum dots, Inverse opal photoanode, Quantum efficiency, Lanthanide doping.

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Inhibitive effect of synthesized 2-(((1H-3-tetraazole) imino) methyl)-4-bromophenol as a corrosion inhibitor for mild steel in hydrochloric acid medium

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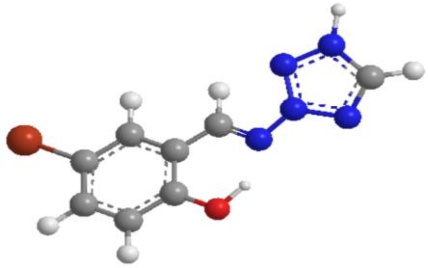
In this research, adsorption of 2-(((1H-3-tetraazole)imino)methyl)-4-bromophenol (HTIMB) on mild steel (MS) surface in 0.5 M HCl solution and its corrosion inhibition effect was studied. The HTIMB was synthesized from the reaction between 3-amino-1-hydrogen-1,2,4-triazole and 5-bromo-2-hydroxybenzaldehyde in EtOH, Fig. 1. The prepared compoun was characterized using standard spectroscopic methods(1H NMR, FT-IR and Uv-Vis) [1,2]. In order to determine the corrosion parameters in the metal-soluble interface and to evaluate the corrosion kinetic parameters and thermodynamic performance of the adsorption, the adsorption surface and the inhibition effect of the compound on the steel were investigated. for this purpose, a series of techniques, such as potentiodynamic polarization, gravimetric techniques, electrochemical impedance spectroscopy (EIS), atomic force microscopy (AFM) and scanning electron microscopy (SEM) were used [3,4]. The results showed that as the concentration of HTIMB was increased the inhibition of mild steel in acidic environment was also increased. Also, as the temperature of acidic medium was reduced the corrosion inhibitive ability of HTIMB was increased. The SEM and AFM studies in HCl medium indicated that blocking of the active sites of mild steel was increased by adsorption of HTIMB on the steel surface.



Schem. 1. The Structure of HTIMB

Keywords: Inhibitor, Corrosion, Mild steel, Gravimetric, adsorption, impedance, Active sites

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Measurement of chloride in colored water of the radiator with a conductometer

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It is not possible to measure chloride in colored samples of radiator water by Mohr method[1]. A conductivity meter was used to measure chloride in these samples[2]. First, one milliliter of sodium with a concentration of 0.2 normal was added to the samples[3]. The pH of the samples was then adjusted between 7 and 9. 0.3 g of sodium hydrogen bicarbonate was added to the samples. The samples were then filtered with blue-band filter paper. Then the amount of electrical conductivity of the samples was measured and recorded. Silver nitrate was added to the samples until. The process of electrical conductivity increased rather than decreased. Finally, the chloride concentration of the samples in the range of 20 to 500 mg/Lit was measured with acceptable accuracy. These results were measured and confirmed by ion-selective chloride electrodes. To ensure this method, three samples of radiator water were mixed with a certain amount of chloride standard. And their chloride was measured seven times by the above method. The difference between the theoretical and experimental results was less than one percent.

Keywords: Chloride, Water, Radiator, Conductometer

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A process for the production of catalysts and the production of catalyst-based liquid propane gas

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A catalyst can be defined as a substance that accelerates chemical reactions by providing an alternative pathway for breaking and bonding [1,2]. Reduces the activation energy required to perform this chemical reaction. Catalysts are often specific for a particular reaction, and this is especially true for enzymes that catalyze biological reactions [3]. When the catalyst is soluble in the reaction medium, it is called a "homogeneous catalyst" and when the phase catalyst is separate from the reaction phase, it is called a "heterogeneous catalyst". In most cases, a heterogeneous catalyst is a solid catalyst from which gas or liquid reactors evolve, and as a result, the term "catalyst" is often used to refer to a heterogeneous catalyst [4]. The purpose of this paper is to prepare a catalyst that can produce carbon dioxide containing propane as a major component by reacting carbon monoxide with hydrogen; A process for the production of catalysts and a process for the production of liquefied petroleum gas with a catalyst [5].

Keywords: LPG, Propane, Catalysts, Synthesis, Recycling

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Synthesis of nanocomposite containing metal organic framework, graphene oxide and cobalt-zinc spinel ferrite for removing cationic blue 41 dye

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Up to date, researchers have focused on the tackle the problem of the water shortage crisis. The idea of making an efficient and stable adsorbent has been a topic of much thought to solve the problem of contaminated water. The aim of this study was to remove the cationic blue 41 (known as basic blue 41) from aqueous solutions by synthesis of a new nanocomposite. Iron-containing metal organic framework (NH_2-MIL-88(Fe)), magnetic cobalt-zinc spinel ferrite nanoparticles ($Co_{0.5}Zn_{0.5}Fe_2O_4$) and graphene oxide were nominated to synthesis the nanocomposite [1, 2]. The synthesized adsorbent was characterized using FT-IR, XRD, TEM, FESEM, elemental mapping, EDX, BET, VSM, and TGA techniques. The adsorption experiments were performed based on the suggestion of Central Composite Design and the operating conditions were optimized. Thus, the best removal was obtained 98.89% for an initial dye concentration of 10.0 mg·L^{-1} at temperature of 29.0 $^{\circ}$C, pH equal to 8.70 and adsorbent dosage of 0.0132 g·L^{-1}. Interestingly, the adsorption process was too fast and almost completed within 60 s as the kinetics study showed. The fractal-like pseudo-first-order (FL-PFO) equation was the best model to fit the experimental kinetics data. It was proposed that the nature of NH_2-MIL-88(Fe) along with π-stacking, H-bonding and coulombic attraction were dominant forces to adsorb cationic blue 41. Regeneration of the adsorbent was magnificently done by two different approaches; i) dye desorption using sodium chloride solution in the presence of ultrasonic waves (0.1 mol·L^{-1}, 5 ml, with contacting time of 5 min), ii) degradation of dye by hybrid advanced oxidation process involving Fenton and ultrasound. Indeed, due to the presence of iron cation in the structure of nanocomposite, it was possible to decompose dye using Fenton method [3]. Consequently, the regenerating of adsorbent was successfully accomplished for six cycles.

Keywords: Metal organic framework, Graphene oxide, Cationic blue 41, Adsorption, Ferrite

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Natural zeolite, a useful adsorbent for purification

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Environmental pollution is one of the major problems worldwide. Large amounts of pollutants formed during various industrial processes reach the ecosystem. Therefore, heavy metals, oils and other organic compounds are responsible for water pollution [1]. Heavy metals have been shown to have toxic effects on the environment. Zeolites, which belong to a wide range of materials, show that they are a promising adsorbent. Modified zeolite has been widely used to remove contaminants in water. Physical modification includes thermal modification and ultrasonic modification. Heat correction is generally produced by muffle furnace heating or microwave heating, high temperatures can reduce the resistance of the zeolite surface and improve its exchange absorption capacity [2]. In addition to single correction, there are combination corrections that combine several correction methods. Composite modification can be divided into three categories: ultrasonic composite modification, thermal composite modification, alkali / acid / salt composite modification. Because salt-modified zeolite has a good adsorption effect on phosphorus and ammonium, the use of salt-modified zeolite is common in CWs. Removal occurs within the first 30 minutes of contact and stabilizes rapidly, indicating that diffusion in the zeolite pores is a limiting factor for adsorption [3]. In the case of pollutants, heavy metals, dyes and ammonium are readily absorbed by zeolites at rapid kinetic speeds. However, for anionic species, such as phosphoric compounds and some heavy metals (such as chromium and arsenic), adsorption is impaired, due to electrostatic repulsion, but may be within certain pH ranges. Organic compounds, which are mainly hydrophobic, are removed using zeolites by modifying them with surfactants to form a hydrophobic layer on the surface of the zeolite, which increases its affinity with these compounds [4]. In this case, the dose of surfactant becomes an important variable that must be considered.

Keywords: Natural zeolite, Adsorbent, Refining, Effluent, Desalination

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Green synthesis of TiO_2@ZIF-8 nanocomposite for dye and pharmacological pollutant degradation from water

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Pollution from the evacuation of textile factories, industries, and pharmacies in water, is a serious environmental concern that is constantly growing. These pollutants have destructive effects of carcinogenesis and chromosomal mutations on humans and other living organisms, especially aquatic organisms. Various methods have been introduced to remove contaminants from the effluent. Photocatalytic methods are a subset of chemical methods, as one of the most important methods of wastewater treatment. Photocatalytic reactions are a series of chemical reactions in the presence of light and a photocatalyst to destroy organic and complex aromatic compounds, which ultimately produce non-toxic gases [1]. Recent studies have shown that organic-metallic frameworks (MOFs) have excellent removal capacity and degradability due to their multifunctionality, water stability, large surface area, good electron conductivity, adjustable pore size, and recyclability [2]. In this work, the photocatalytic performance of zeolitic imidazolate framework-8 (ZIF-8)/ titanium dioxide was evaluated. XRD, FTIR, SEM, and Raman analyzes were used to describe the synthesized nano materials [3]. Experimental data showed that the nanocomposite, due to the synergistic effect of ZIF-8 and titanium dioxide, showed a better contaminant degradation ability than its parents for anionic dye and doxycycline exposed to visible light. The degradation process followed zero-order kinetics. Also, the synthesized nanocomposite provided good stability and reusability in four times use.

Keywords: TiO_2@ZIF-8 nanocomposite, Zeolitic imidazolate framework (ZIF-8), Phohotocatalysis, Organic pollttant degradation

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The photocatalytic ability of the embedded graphene quantum dot in the zeolite imidazolate framework (ZIF-8) to remove pharmacological contaminants

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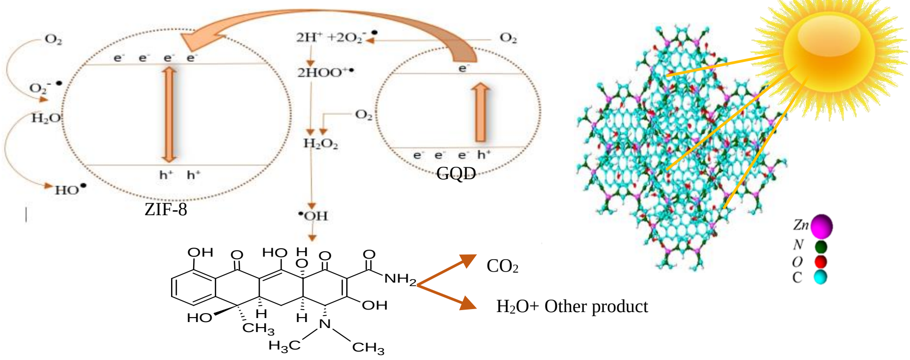
Water pollution is a critical concern for human health and the lives of other organisms, especially aquatic life. Therefore, finding methods to improve the situation and remove pollution is inevitable. Photocatalysis can be mentioned as one of the effective and practical methods of organic pollutants degradation. By reducing the width of graphene to 10 nm, graphitic plane to (<2nm deep), and restricting the movement of electrons, the effect of quantum restriction has occurred a new generation of the nanocarbon family, called graphene quantum dots (GQD) has emerged [1]. The combination of GQDs with ZIF-8 has the potential for rapid electron transfer, creating a stabilized and efficient photocatalyst. Herein, the photocatalytic performance of mentioned structure was compared to its parents and indicates favorable improvement for tetracycline degradation (Figure1). XRD, FTIR, SEM, BET, Raman, and HRTEM analyzes were used to confirm the structure of synthesized nanomaterial [2]. This photocatalyst is well compatible with pseudo-first-order kinetics and according to the studies performed provided good stability and reusability in three times use.

Keywords: Nanocomposite, Zeolitic imidazolate framework (ZIF-8), Graphene quantum dot (GQD), Phohotocatalysis, Pollutant degradation



Schem.1. Proposed mechanism of tetracycline degradation degradation

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Effect of different metal-organic framework morphologies on contaminants removal from the aquatic environment

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With the development of industries, emerging pollutants in the environment are increasing day by day. In particular, these contaminants in water can pose a serious threat to human life and other living organisms.Therefore, the removal of these pollutants has attracted widespread attention. Numerous methods have been proposed to achieve this purpose. Among all technologies, adsorption, with features: low cost, simple design, easy to use, no secondary pollution and energy saving can be selected as an effective method [1]. MOFs with high specific surface area, uniform porous structure and the ability to adjust the size and shape of cavities can be an excellent candidate for use in adsorption technology for wastewater treatment [2]. Herein, we synthesize a kind of metal-organic framework under various conditions. Finally, the resulting MOF was created with three different morphologies(rod, spindle and diamond like) that, despite the same chemical structure, showed different physicochemical properties even on dye adsorption [3]. In fact, the highest adsorption is seen in the morphology, which the crystalline surfaces have grown proportionately. Despite the different adsorption capacities of different MOF morphologies, all three morphologies are well compatible with the Langmuir isotherm and pseudo-second-order kinetic.

Keywords: Metal-organic framework, Different morphologies, Adsorption, Pollutant removal

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Removal of a textile cationic dye using Bentonite, ZnO nanoparticles and ZnO-modified bentonite as an adsorbent and photocatalyst in a separate and combined methods

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A research was carried out for the adsorption of Basic Red 46 (BR46) on bentonite as well as degradation of dye applying ZnO nanoparticles. Afterwards, the combinational method was evaluated using ZnO-modified bentonite for the complete removal of dye using adsorption and photocatalytic degradation.

At the first step, the adsorption performance of bentonite for the removal of BR46 was obtained and different isotherm models and kinetics studies were performed, as the maximum adsorption capacity of 624.48 mg g^{-1} was attained for the adsorption of BR46 on diatomite. The adsorption data were attempted by Langmuir and Freundlich isotherm models and the results were conformed to Langmuir isotherm model with the good correlation [1]. Moreover, pseudo-first-order and pseudo-second-order kinetics models were evaluated and results were found to conform to the pseudo-second order kinetics model [2].

At the second step, ZnO nanoparticles were synthesized using combustion method and the characterization of synthesized materials were carried out using Fourier-transform infrared spectroscopy, X-ray diffraction analysis and scanning electron microscopy. The photocatalytic properties of ZnO nanoparticles for the degradation of BR46 was studied using UV irradiation and the operational parameters and kinetics of degradation were investigated [3].

At the third step, ZnO-modified bentonite was prepared and the photocatalytic degradation was studied along with adsorption of dye. In this stage, decrease in UV-Vis absorption spectrum at different condition was investigated as well as complete mineralization of dye solution using total organic carbon analysis.

***Keywords**:* Photocatalysis, Bentonite, ZnO-modified bentonite, Adsorption

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Investigation of the kinetic behavior of crystal violet dye adsorption process from aqueous solution using bio-charcoal prepared from conifer cone

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The basic requirements to support healthy living are an unpolluted living environment and safe drinking water[1]. Among the various pollutants, dyes such as methylene blue (MB), rhodamine B (RhB), methyl orange (MO), methyl red and crystal violet are the most important industrial pollutants that are found daily in various industries such as textiles, cosmetics, leather, food, pharmaceutical industry, Paints, varnishes, pastes and paper are used and can enter the environment through the wastewater of these industries. this highly toxic dye can adversely affect all living organisms and human beings, causing many disorders ranging from allergic reactions in the skin, gastrointestinal tract, respiratory system, and cardiovascular system to more severe diseases such as genetic mutation and carcinogenicity[2]. Therefore, it is indispensable that wastewater containing dyes be treated before their release into the environment. One of the most effective methods of wastewater treatment is adsorption. Adsorption has been found to be superior to other techniques in terms of flexibility and simplicity of design, initial cost, insensitivity to toxic pollutants and ease of operation[3]. In the present study, biochar was synthesized from conifer cone and investigated as an effective and low-cost adsorbent for removing crystal violet dye from an aqueous solution. In the present study, the effect of various parameters such as pH, temperature, contact time, and adsorbent dose on the initial dye concentration of 10 mg/l was investigated. The maximum efficiency of the adsorption process (95.74%) was determined in pH 9, adsorbent dose of 1.5 g/l, contact time of 60 minutes, and temperature of 25 °C. To investigate the kinetic behaviour of the crystal violet dye adsorption process, pseudo-first-order and pseudo-second-order models were used. The results showed that the quasi-quadratic kinetic model has more ability to describe the kinetic behaviour. The thermodynamic study was showed that the adsorption process is spontaneous and exothermic and it can be stated that biochar from conifer cone can be used in removing dyes from aqueous solutions.

Keywords: Adsorption, Biochar, Aqueous solution, Dye

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Synthesis of new Crown ethers compound for water purification

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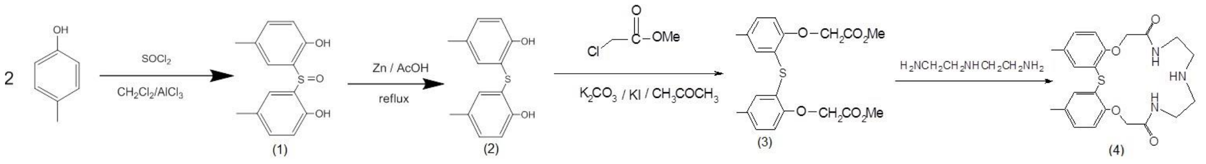
Crown ethers and their compounds have the property of complexing with metals, which is interesting in many fields and in topics such as environmental chemistry, metal extraction and separation, water treatment, nanotechnology, etc. Our aim of this research work is to prepare new diamidic macrocyclic compounds based on dibenzosulfide as receptors for metals, cations and also as components of nanomachines.

Prepared macrocycles can bond with metal ions due to having O and N atoms.
Crown ethers have the ability to form strong bonds with cations and form complexes, and this is due to the oxygen donor atoms being co-ordinated with the cation inside the ring. Crown ethers are effective in phase catalytic transfer because the outer surface of the ring is hydrophobic [1].

Their selectivity depends on the relative size of the cavity, the diameter of the cation, the number of donor atoms in the crown ring, the relationship between the donor atoms to the cation, and the cation charge [2]. Therefore, these compounds can purify water by absorbing heavy and dangerous ions from water.

The aim of this research work is to synthesize diamide macrocycles and related larite ethers. For this purpose, first sulfoxide (1) was prepared by the reaction of thionyl chloride with paracresol with 65% efficiency, then by reduction combination (1) was prepared with zinc powder and bisphenol acetic acid (2). Due to the reaction of bisphenol and methyl chloroacetate in the presence in dry acetone, methyl diester (3) was obtained by reflux with 98% efficiency. Diamide macrocycle (4), with efficiency 70% was prepared by amidation of methyl diester (3) and diethylene triamine and was crystallized by dry methanol. And Larith Ether due to the reaction of macrocycle of diamide with pentanoyl chloride in the presence of triethylamine and in dry dichloromethane solvent reflux was achieved with a yield of 74%.



The prepared compounds were identified by IR spectra, 1HNMR,3CNMR,mass spectrum.

Keywords: Crown ethers, Water purification

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Development of polyvinyl alcohol/polysulfone thin-film composite membrane modified with multi-walled carbon nanotubes

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In this research, multiwalled carbon nanotubes (MWCNTs) were used to modify the performance of the polyvinyl alcohol (PVA)/polysulfone (PSf) thin-film composite membrane for low-pressure desalination. In the first step, the mixed matrix PSf-based support membranes (16 wt% PSf) containing different content of the MWCNTs (0.01, 0.02, and 0.05 wt%) were fabricated using the phase inversion method. In the next step, the surface of the mixed matrix PSf membrane was coated by PVA using the dip-coating method using glutaraldehyde (GA) as the crosslinking agent [1]. In this method, the PSf-based support membrane was immersed in the coating solution containing PVA, and glutaraldehyde so that a thin layer of the solution was deposited on the surface of the membrane. Finally, the membrane was dried inside the oven. Thus, thin-film composite membranes (nTFC) were prepared. The performance of the fabricated membranes was assessed using the dead-end system to evaluate the pure water flux, salt removal, and protein rejection. According to the obtained results, removal of Na_2SO_4 salt by nTFC membranes containing 0.01, 0.02, and 0.05 wt% of MWCNTs were 79.3, 79.5, and 80.5%, respectively, and removal of NaCl salt by these membranes were obtained 40.5, 42.4 and 43.8%, respectively. However, the bare membrane showed lower rejection performance for Na_2SO_4 (74%) and NaCl (18%). Moreover, the pure water flux of the bare TFC membrane was increased from 29 L/m^2 h to 41, 52, and 61 L/m^2 h by introducing 0.01, 0.02. and 0.05 wt% of MWCNTs to the matrix of the PSf support membrane. As can be seen, the presence of the MWCNTs in the matrix of the support PSf layer can improve the desalination and permeability of the nTFC membranes [2]. In this study, the morphology and structure of all membranes were studied using scanning electron microscopy, atomic force microscopy, thickness measurement, and contact angle analyses. The results of contact angle analysis showed the positive effect of MWCNTs in increasing the hydrophilic properties of the nTFC membranes. It was found that MWCNTs improved the performance and properties of nTFC membranes.

Keywords: Nanofiltration, Surface modification, Polysulfone, Desalination, Multi-walled Carbon nanotubes

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Modifications made to the membrane shape and membrane modules of osmosis-based processes to improve the performance of the desalination process

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Commercialization of water desalination by membrane methods faces various challenges such as membrane type, draw solution, membrane module type and membrane fouling [1]. Various strategies have been implemented to overcome these challenges. Some of them are the use of spacers on both sides of the membrane, vibrating the membrane, membrane rotation, Dean vortex, pulsing the feed, air bubbling and changing the geometry and number of inlets of the membrane modules [2][3].

An optimized membrane chamber can reduce concentration polarization and membrane fouling among these methods. This research investigates different types of optimizations performed on the membrane module of the osmosis process. The results showed that the use of membranes with modified membrane shapes and the proper arrangement of spacers could reduce the effects of concentration polarization to an acceptable level and increase the permeate flux by more than 15%[4]. The results show that if an airfoil spacer is used, the water flux decreases along the membrane with a very slight slope (about 54% less than the base state). On the other hand, to reduce operating costs, process optimization and finding the type, number, size and location of spacers should be done by simulating the process with the help of the computational fluid dynamics (CFD) technique[5].

Keywords: Desalination, Osmosis, Membrane module, Computational Fluid Dynamics (CFD)

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Optimization of Experimental Conditions for Eco-friendly Preparation of Nano Silica from an Industrial Waste

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Extensive use of amorphous and crystalline silica (SiO_2) and nano-silica (n-SiO_2) in various industries, as well as the economic advantages is the reason for focus on their environment-friendly production from the industrial waste or side-products the environment [1]. Zircon ($ZrSiO_4$) as the principal source of zirconium (Zr) can be used commercially for manufacturing of zirconium carbide (ZrC), zirconium oxide (ZrO_2) and Zr sponge [2]. The modern production of ZrC is based on the carbothermic method, in which melted Zr is reduced with a carbon reducing agent (petroleum coke) in an electric arc furnace [3]. Generally, the reaction is carried out in a vertical reactor at about 2000 °C, producing of ZrC as the product, side-reactants *and side-products such as* SiO_2 and coke [4]. In this study, the industrial waste of the ZrC production process containg high percentage of SiO_2 was used to produce amorphous n-SiO_2 through an alkaline treatment followed by pH adjustment and filteration. The prepared n-SiO_2 was characterized by XRD, FT-IR, FE-SEM, TEM and EDXA techniques. Then, the effect of influencing parameters on the silica leaching process, including temperature, time and stoichiometric ratio of the raw-materials on the size, morphology and specific surface area of the prepared amorphous n-SiO_2 were investigated. The optimized conditions for an efficient extraction of SiO_2 (98%) were obtained to be 298K, 2h and NaOH/waste raw material weight ratio 9/10. Also, the effect of pH on the size and specific surface area of obtained n-SiO_2 was investigated. The Brunauer–Emmett–Teller (BET) specific surface area of the prepared n-SiO_2 was 472.51 m^2/g at pH 7. The results of dynamic light scattering (DLS) analysis exhibited that the average size of the obtained spherical n-SiO_2 was about 38.03 nm.

Keywords: Industrial waste, WPZF, Sodium silicate, Silica, Leaching

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Microreactor-assisted continuous synthesis of a quaternary ammonium

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Chemical manufacturing is conducted using either batch or continuous systems. Continuous systems have several advantages over batch systems, particularly in terms of productivity, heat-transfer and mixing efficiency, safety, and reproducibility. However, for over half a century, pharmaceutical manufacturing has used batch systems because synthesizing complex molecules such as active pharmaceuticl ingredients has been difficult to achieve with continuous systems. In order to exploit the entire advantages of continuous manufacturing, the separately developed unit-operations need to be integrated to form end-to-end systems from the raw materials to the final dosage forms [1-3]. Here we describe the continuous synthesis of a quaternary ammonium using three tandem glass microreactors. The microfluidic system is simple and stable with no purification in each step. Our results demonstrate that multistep (three steps in this study) chemical transformations for active phamaceutical ingredients' synthesis can proceed under microfluidics conditions, without separation of any intermediates, products, by-products, and excess reagents.

Keywords: Microreactor, Quaternary ammonium, Chemical synthesis

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Continuous synthesis of tertiary amines in microreactors

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Performing chemical reactions are of key operations in chemical industries. In the last decade, employing microreactors for performing organic-synthesis reactions has drawn much attention. The typical dimensions of microreactors are 10–500 μm. Because of the microstructure and high surface area–to–volume ratio, the microreactors have particularly excellent heat and mass transfer characteristics. In such reaction systems, almost every point has the same temperature; so the phenomenon of local overheating or overcooling is avoided. Compared with conventional macroscale reactors, the microreactors have excellent features such as fast heat and mass transfer, and short residence time. Such advantages would favorably affect reaction processes, and therefore the outcome has higher selectivity, yield, and product quality in many cases. Here we describe the continuous synthesis of a tertiary amine using glass tandem-connected microreactor, micro-extraction, and microscale phase separator. The tertiary amine is synthesized through mono-alkylation of a secondary amine, and the effect of few operating parameters such as temperature, residence time, and reactants molar ratio on the reaction yield was examined. It was found that yields up to 60% is obtained in mild reaction condition. Our results demonstrate that the platform is suitable for synthesizing other amine compounds through mono-alkylation reactions [1, 2].

Keywords: Microreactor, Tertiary amines, Chemical synthesis

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Fluoxetine degradation in aqueous media with homogeneous ferrous-assisted UV-LED/persulfate process

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Pharmaceutical compounds are considered as emerging environmental pollutants due to their persistence in the aquatic ecosystem even at low concentrations [1]. Fluoxetine is one of the antidepressants widely used in the past decade. This drug has been detected in surface waters due to imperfect destruction after therapeutic use [2]. In this study, the degradation of fluoxetine drug in aqueous solutions was investigated via the homogeneous photochemical process using potassium persulfate in the presence UV-LED irradiation. Persulfate oxidizing agent was activated with the emitted ultraviolet/visible light [3]. A falling film horizontally located light source photo-reactor was employed for conducting experiments. An array of 24 LED lamps (1 W with 395-400 nm wavelength) was utilized. The content was circulated by means of an external pump. Iron salts can be incorporated in this process favoring sulfate anion radical generation and the degradation efficiency [4]. The variation of degradation efficiency with persulfate concentration, Fe^{2+} concentration, pH, reaction temperature, and reaction time variables were investigated. The substrate concentration was followed by means of a UV-Vis spectrophotometer. The fluoxetine maximum wavelength is 226 nm. Under the found optimum conditions of persulfate concentration (100 mg/L), Fe^{2+} concentration (1 mg/L), natural pH (6.4) and temperature (40 ˚C), the pollutant was degraded to 71.1% after only 40 min treatment (fluoxetine initial concentration of 40 mg/L). Meanwhile, kinetic studies showed that degradation of fluoxetine follows a pseudo first-order reaction. In mechanism study, the free radical test indicated that both the sulfate radical and hydroxyl radical were involved in the reaction system, and further, the degradation products were explored by liquid chromatography-tandem mass spectrometry. The transformation pathways were proposed, being mainly the hydroxylation, breaking of the carbon-oxygen bond, defluorination of the $-CF_3$ to the carboxylic group, and ring-opening reactions. According to the results, the used homogenous UV-LED/PS/Fe^{2+} process could be a desired choice in the treatment of wastewaters containing recalcitrant drug pollutants like fluoxetine.

Keywords: Fluoxetine degradation, Persulfate activation, UV-LED, Ferrous ion, Mechanism

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Carbon nanotubes-incorporated Fe_3O_4/MIL-53(Cu) as novel Fenton-like catalyst for degradation of acid orange 7

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The potential of a novel magnetic Fenton-like catalyst Fe_3O_4/MIL-53(Cu)/CNT for the degradation of acid orange 7 has been evaluated. The supported iron-copper bimetallic catalysts, combining the advantages of immobilization and iron-copper synergy, have been developed and demonstrated to significantly increase the efficiency of Fenton-like processes [1]. Furthermore, introducing functionalized nanocarbons to heterogeneous Fenton catalysts with the electron donor property of the carboxyl groups on the surface of nanocarbons promotes the efficiency of catalyst over a wider pH range [2]. The satisfactory treatment of acid orange 7, as azo dyes involving aromatic rings, azoic linkages and amino groups [3], with high degradation efficiency of 84.6% has been obtained. The heterogeneous Fenton-like catalytic process in aqueous solutions was modeled and optimized employing Response Surface Methodology (RSM) based on Central Composite Design (CCD) regarding the influence of effective parameters of pH, nanocomposite dose and hydrogen peroxide concentration on the degradation efficiency as response. The predictability of proposed model has been confirmed with the close to unity regression coefficient (R^2=0.9985). The results of reduced quadratic model demonstrated that the highest degradation efficiency has been attained at optimum conditions of pH =5.78, nanocomposite dose (0.3 g/L) and hydrogen peroxide concentration of 1.5 mol/L. Moreover, the kinetics investigation revealed that the degradation reaction followed the first order with desired rate constant. Therefore, the efficient and fast degradation of acid orange 7 proposed utilizing the heterogeneous Fenton-like catalyst has confirmed its extensive applicability for the removal of various organic contaminant pH range.

Keywords: Heterogenous Fenton-like catalyst, Acid orange 7, Response surface methodology

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Degradation of oxycodone pharmaceutical in aqueous media using persulfate oxidant under visible light

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Pharmaceutical industries generate significant amounts of aromatic and chemical compounds that cause many environmental problems. Relevant contaminants include various drugs such as painkillers, antibiotics, cardiovascular drugs that most of them can be degraded by advanced oxidation process. In this study, the removal of the recalcitrant oxycodone pollutant, an industrially derived from opium compounds, was investigated using persulfate oxidizer under visible light. A vortex spiral reactor with a 150 watt visible lamp was used in this project. Sampling was performed every 10 minutes and was measured using UV spectrophotometer [1]. The effect of various factors in degradation process, including persulfate concentration, initial pH of the solution and reaction temperature was investigated. The oxycodone degradation efficiency could reach to 84.4%, during 60 min treatment, under the found optimal conditions of 150 mg/L persulfate, normal pH and temperature of 35 °C. In this process, 86.2% degradation was accomplished with hydroxyl radical and 13.8% with sulfate anion radical. The presence of conventionally found carbonate, bicarbonate and chlorine anions in water caused diminishing the oxycodone degradation. Further, presence of cations of intermediate metals caused stability and resistance of the contaminant against degradation. Kinetic study showed that oxycodon deletion followed a pseudo first-order reaction with the rate constat of 0.0299 min^{-1}. To determine the mechanism of degradation and identify the produced intermediates, liquid chromatography-mass spectrometry (LC-MS) analysis was performed [2]. Active radicals in the environment react with the pollutant and destroy its structure.

Keywords: pharmaceutical pollutant, oxycodone, visible light, Persulfate

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Reuse of paint sludge for the modification of bitumen and its effect on the physical properties of bitumen

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Refinery bitumen, which is the residue of crude oil distillation, is a thick, viscous fluid composed of heavy hydrocarbons. It is mainly made of bitumen for asphalt coatings in road construction and waterproofing in roof covering [1,2]. In some cases, it is necessary to change the physical and mechanical properties of bitumen, which is done by a suitable modifier. One of the most common modifiers is polymers. In recent years, recycling or reuse of polymers has also been considered, and in the case of bitumen modification, polymer wastes have been used to modify the properties of bitumen [3-5]. This study deals with the modification of bitumen by paint sludge and study the changes in physical and mechanical properties of bitumen. For this purpose, the paint sludge is first dehumidified and extracted solvent, and after pulverization, it is added to the molten bitumen with percentages of 1, 3 and 5. The mixtures were mixed well with a mechanical stirrer and homogenizer at 190 °C. The results of the analyzes showed that the degree of penetration of the modified bitumen showed a relative decrease of 60% and its softening point increased by 85% compared to the control sample. Frost breaking point also increased from -4 for control sample to +2 for sample 5% by weight of paint sludge.

Keywords: Bitumen, Paint sludge, Recycling, Physical properties

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The effect of cetyltrimethylammonium chloride surfactant on the structure and performance of PES membrane for filtration of pharmaceutical pollutants

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Pharmaceuticals compose a large group of medicinal human and veterinary compounds with a high consumption worldwide. The presence of these compounds in the environment corresponds to low concentration levels, its continuous input from wastewater treatment plants or direct discharge to natural riverbeds may represent a long-term potential threat for the aquatic and terrestrial ecosystems. Nowadays, membrane-based process as a significant solution for advanced physical wastewater treatment is playing sufficiently remarkable role in water industry due to its advantages including modular nature, which provide flexibility in designing, application possibility at very large or small scale, high quality of the filtered water, the almost slight footprint and in some cases less energy consumption [1]. NF separation process is considered as utilization of a high pressure-driven method with 0.5–10 nm of membrane pore size and 5–40 bar of operating pressures. Membrane fouling is one of the most significant concerns for membrane technology, which generally occurs in forms of foulant adhesion/ deposition. So various appropriate studies on membrane preparation have been dedicated to solve these problems and mitigate fouling phenomenon by using innovative modification techniques in order to fabrication of fouling resistant membranes. The objective of this work was to evaluate the effect a surfactant has on the nanofiltration process for removal pharmaceutical pollutant. CTAC was chosen for this study due to its potential application for removal organic contaminant. Therefor at first nanofiltration membrane of polyether sulfone using immersion method was synthesis Then by adding this surfactant, the membrane was examined for better removal of the toxic drugs[2].NF nanofiltration membrane was prepared via phase inversion process. Then, PVDF with a constant concentration of 18 wt.% was dissolved in DMAC as adorable solvent. CTAC also used as hydrophilic additive with different concentrations. A consistent casting solution was obtained for at least 5 h. In the next step, the shaped membrane held at room temperature for 24 h. The solution was cast on the glass plate using a film applicator and was immediately immersed in fresh distilled water to remove the remaining solvent. In this study, the effect of individual weight percentages of CTAC surfactant on the PES membranes performance revealed that all the PES/CTAC membranes indicated greater water permeability in comparison to the unmodified membranes and for the optimum modified PES membrane by 2wt% of CTAC additive, the highest pure water flux of 235.9 L/m2 h at 3 bar was reported which can be related to high hydrophilicity induced by CTAC surfactant. The fouling behavior assessment of the membranes by use of BSA solution indicated that all the PES/CTAC membranes in variable weight percentages, rejected the BSA protein more than 98% and superior fouling resistance properties were reported. The surfactant additive materials as a promising approach in order to modification of PES-based membranes have a considerable potential for fabrication of high-performance nanofiltration membranes

Keywords: Fouling resistance, Hidrophilyc additive, Nanofiltration membrane, Surfactant, Wastewater Treatment

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Hydrophilic cellulose and graphene oxide membranes for separation of alcohol-water mixtures

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Polyelectrolyte membranes of bipyridinium cellulose (BPC) and bipyridinium graphene oxide (BPGO) having a microporous polysulfone (PS) substrate were prepared and tested for the pervaporation dehydration of aqueous ethanol, isopropanol and butanol mixtures. BPC and BPGO membranes were characterized by Fourier transform-infra red spectroscopy (FT-IR), scanning electron microscope (SEM) and Thermogravimetric analysis (TGA) [1-3]. These membranes have high sorption and promising flux, especially at high alcohol concentration. The swelling degree of the membranes in water was significantly affected by the amount ratio between the alcohol and water [4]. However, for the membranes, the water sorption selectivity decreased considerably at high water concentration of water– alcohol mixtures because the membrane was highly hydrophilic. The BPC membrane showed total flux 981, 1980 and 2420 g/m^2 h and total flux of BPGO was 685, 1736 and 2123 g/m^2 h for 10 wt% ethanol, isopropanol and butanol mixtures at 60 ˚C, respectively. It was observed that this type of membrane was enough and achieved the highest flux and water sorption selectivity for separation of alcohol-water mixtures [5].

Keywords: Membrane, Polyelectrolyte, Separation, Hydrophilicity.

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Gold nanoparticle thin films' UV-Visible photoluminescence properties

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In this work, facile synthesis of gold nanoparticle thin films on a modified quartz substrate with UV-visible photoluminescence has been reported. The films are prepared by the centrifuge deposition of nanoparticles from a colloidal solution which has been synthesized by using the sodium citrate reduction of HAuCl4 in the water[1]. The adhesion of the gold nanoparticles on a quartz substrate is improved by oxidation with piranha solution and silanization with the 3-(trimethoxysilyl)-propylamine as shown by the atomic force microscopy (AFM)[2]. Subsequent annealing of the films at the temperatures of 600˚C for 1 hour has resulted in the pure crystalline nanogold thin layer with the localized surface plasmon resonance (SPR) peak of 522 nm. In addition, a sharp absorption peak is observed at about 242 nm (in the UV region) due to the gold nanoparticle interband transition[3]. The film scanning electron microscopy (SEM) reveals that Au nanoparticles are all sphere-shaped with an average radius range of 8-22 nm. The results of X-ray diffraction analysis (XRD) show that the films are well crystallized with the pure phases of gold. Performed X-ray photoelectron spectroscopy (XPS) analysis revealed the existence of the stable thin semi-conductive oxide layer in the phase of Au2O3 on the surface of the annealed thin films. At the applied excitation wavelength range of 220-260 nm, the films have shown a photoluminescence emission peak in the UV-Visible region at about 375 nm. This work suggests a simple pathway to fabricate nanogold thin film from colloidal samples maintaining stable optical properties for photonics and plasmonics applications[4].

Keywords: Gold nanoparticle thin film, UV-visible photoluminescence, Photonics and plasmonics applications.

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Evaluation of the inhibitory effect of phosphine-polycarboxylic acid copolymer to inhibit gypsum crystal growth under normal and high saturation conditions

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The Scale formations are responsible for lost efficiency, increased maintenance and operating costs in most industrial equipment and home appliances [1]. This phenomenon is promoted by the presence of dissolved salts in a supersaturated solution. So, high-proficiency and environmentally-friendly chemical scale inhibitors are much required [2, 3]. One of the inhibitors of the polymer scale that has recently shown good performance in this field is Polyphosphino Carboxylic Acid (PPCA) [4, 5]. In the present work, PPCA copolymer has been applied directly to inhibit the gypsum scale. All the kinetic studies and performance analysis of the scale inhibition were carried out by following the concentration of the heavy ion solutions such as calcium ion. The complexometric determination of the Ca^{2+} concentration showed that the PPCA (2.5 ppm) had 100% inhibition efficiency at a saturation index of 0.31 at room temperature and without pH regulation after 24 h. The Field Emission Scanning Microscopy (FESEM) images of the PPCA-inhibited and uninhibited samples illustrated that the typical gypsum microfibers are distorted and decreased in size considerably in the inhibited sample. At a still higher saturation ratio of 10 (saturation ratio of 1.47), the inhibition proficiency of PPCA decreased to 24% and 16% for two dosages of 10 and 2.5 ppm respectively which was credited to the upper ion activity coefficients at the very high ionic potency.

Keywords: PPCA, Gypsum, Calcium ion, Ion activity.

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Ultrasound-assisted catalytic activation of hydrogen peroxide on the chromium aluminum carbide MAX phase for degradation of an organic pollutant

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One of the critical problems all over the world that concerns environmental researchers is contaminated water with organic pollutants resulting in negative effects on the life of human beings [1]. In this study, the removal of dimethyl benzene-12-dicarboxylate as a model organic pollutant in contaminated water was investigated using the ultrasound/hydrogen peroxide/catalyst ternary system. The chromium aluminum carbide MAX phase was used as an efficient catalyst for the activation of the hydrogen peroxide under ultrasound irradiation. The synthesized MAX phase was characterized using X-ray diffraction, field emission scanning electron microscopy, and Fourier-transform infrared spectroscopy techniques. The effect of operating parameters including catalyst dosage (0-1 g/L) and pH (4-6) was investigated on the removal efficiency. Hydrogen peroxide (1 mmol/L) was efficiently activated in the presence of the optimum content of MAX phase (0.75 g/L) under ultrasound irradiation, resulting in the removal of 69% within 120 min of reaction time at the natural pH of the pollutant. Based on the results, the removal efficiency of dimethyl benzene-12-dicarboxylate was increased by decreasing the pH. Furthermore, the generated hydroxyl radicals in the ultrasound/hydrogen peroxide/catalyst ternary system were detected by a spectroscopic method using o-phenylenediamine as a probe. To the best of our knowledge, this research is the first report on using chromium aluminum carbide MAX phase for ultrasound-assisted activation of hydrogen peroxide. The results of this research introduce the MAX phase-based materials as an efficient catalyst in advanced oxidation processes.

Keywords**:** Dimethyl benzene-12-dicarboxylate; Ultrasound-assisted Catalytic activation; Hydrogen peroxide; Cr_2AlC MAX phase.

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Effect of preparation method on poly (vinylidene fluoride) scaffold morphological properties

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Piezoelectric materials are of great interest because of their ability to generate electrical signals in response to mechanical strain, which can have a positive impact on the growth, attachment and proliferation of osteoblastic cells. These materials can be used in preparation of bone tissue engineering scaffolds [1, 2]. Poly (vinylidene fluoride), PVDF, a piezoelectric polymer, is widely used in biomaterial applications [3]. In this study, we fabricated tissue engineering scaffolds based on PVDF using two different methods, solvent casting/particulate leaching (SC/PL) method and electrospinning method, and evaluated their morphological properties by scanning electron microscopy (SEM) and contact angle measurements. For SC/PL method, PVDF pellets were dissolved in dimethylformamide (DMF) at 15 wt.% under stirring at 60°C and NaCl particles were used as a pore forming agent. Also, the conditions for the preparation of electrospun fibers was evaluated by preliminary experiments and the optimal conditions were obtained as 15% for PVDF solution concentration, 17 cm for distance of the tip of the needle with the collector, an applied voltage of 17 kV and an injection speed of 0.5 ml/h. The results of SEM, showed a granular and porous surface with pore size of 5-10 μm for scaffolds fabricated by SC/PL method, as well as nanofibers with a diameter in the range of 100-500 nm for electrospinning method. In addition, from the contact angle results, the hydrophilicity of the nanofibers was more than the porous scaffold. Finally, it can be stated that scaffolds prepared by electrospinning method have sufficient morphological properties for use in bone tissue engineering.

Keywords: Poly (vinylidene fluoride), Solvent casting/particulate leaching, Electrospinning, Scaffold

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Sonocatalytic degradation of dimethyl phthalate using CoCr layered double hydroxide

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Organic pollutants generated by diverse industries contaminate the environment, leading to health problems and other issues[1]. Phthalates are synthesized in massive amounts to produce plastics, and consequently, a large amount of them have become widespread in environments due to extensive usage and production[2]. Among various treatment methods, advanced oxidation processes (AOPs) stand out because of their high-efficiency generation of reactive oxygen species, which can effectively degrade target pollutants. In recent decades, sonocatalysis has been used extensively as an AOP for degrading organic contaminants in water due to its ability to produce hydroxyl radicals that occur during the collapse of acoustic cavitation[3]. The semiconducting property of some layered double hydroxides (LDHs) makes them appropriate candidates to be used as a catalyst in AOPs for the efficient treatment of wastewater[4]. In this research, the effect of sonocatalytic activity of the CoCr LDH was studied. For this purpose, CoCr LDH was prepared via a facile co-precipitation method. The morphology and the structure of the synthesized LDH were analyzed using scanning electron microscopy, energy-dispersive X-ray spectroscopy, and X-ray diffraction. The high removal efficiency of 88.8% was obtained for sonocatalytic degradation of dimethyl phthalate (15 mg/L) in the presence of CoCr LDH (0.5 g/L) within 60 min of reaction. Moreover, the antibacterial effect of the synthesized catalyst against the Gram-positive bacterium Staphylococcus aureus (S. aureus) was evaluated with the colony-forming unit (CFU) method.

Keywords: Dimethyl phthalate, Sonocatalysis, Layered double hydroxide.

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Sonocatalytic degradation of a pharmaceutical pollutant on the Titanium Tin Carbide MAX phase

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In light of growing environmental concerns over antibiotic use, advanced technologies for removing antibiotics from pharmaceutical wastewater are required [1]. A new generation of efficient sonocatalytic water treatment systems could potentially solve such problems. In this study, we present a new type of nano-laminated material, titanium tin carbide (Ti_2SnC) MAX phase, that is prepared, characterized, and evaluated for its sonocatalytic activity. A variety of identification analyses including X-ray diffraction, scanning electron microscopy, and Fourier transform infrared were conducted to determine the physicochemical characteristics of the synthesized catalyst. The sonocatalytic degradation of oxytetracycline (OCT) in the aqueous solution with an initial concentration of 10 mg/L was investigated at various concentrations of the Ti_2SnC MAX phase. Among these, 1 g/L catalyst demonstrated high sonocatalytic performance and recyclability toward OTC degradation within 120 min at pH = 6.8 (natural) using an ultrasonic power of 150 W. Sonocatalytic performance of the catalyst was also investigated at pH ranges from 4 to 10. It was found to be primarily pH-independent, suggesting a wide range of catalytic activity. Ophenylenediamine was also used as a probe for determining the hydroxyl radical using a spectroscopic method. This work aims to develop an efficient and environmentally friendly wastewater treatment process using MAX-phase-based sonocatalysts.

Keywords: MAX-phase, Sonocatalysis, Antibiotic degradation

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Preparation of gelatin-based nanocomposite and evaluation of its properties for adsorption of chromium ions from aqueous solution

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Many heavy metals that are highly toxic for animals and human beings are discharged into the environment as industrial wastes, causing serious soil and water pollution [1, 2]. One of the most important and widely used heavy metals, chromium, is considered as a toxic and carcinogenic environmental pollutant. Among different methods, adsorption is one of the most economically favorable and technically feasible method to remove Cr (VI) from the solution [3]. In this study, batch adsorption system using a novel nanocomposite, gelatin/montmorillonite/polyaniline (Gel/MMT/ PANI) nanocomposite, was investigated to adsorption of Cr (VI) from aqueous solutions. The Gel/MMT/PANI nanocomposite was synthesized by chemical oxidative polymerization of aniline in the presence of gelatin-montmorillonite dispersion. The structure and morphology of the prepared nanocomposite was characterized utilizing Fourier transform infrared spectroscopy (FTIR), X-ray diffraction (XRD), scanning electron microscopy (SEM) and transmission electron microscopy (TEM). From the results the successful preparation of nanocomposite with intercalated structure was examined. Then, the removal of Cr (VI) ions from aqueous solution using the prepared adsorbent in a batch adsorption process was investigated. Based on the adsorption studies, the nanocomposite by high adsorption capacity can be used as an industrially viable, economical and successful product to removal of Cr (VI) ions from solutions.

Keywords: Chromium, Gelatin, Nanocomposite, Adsorption

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Removal of Methylene Blue-21 Dye from Aqueous Solution Using ZnO/SnO_2 nanocomposite

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The paint and textile industries produce large volumes of hazardous and toxic wastewater[1]. Adsorption processes are widely used in removing pollutants from wastewaters, particularly those that are not easily biodegradable such as dyes[2,3]. The photocatalytic degradation of methylene blue-21 (MB) dye in an aqueous medium was studied in dynamic mode using Zinc Oxide/ Tin(II) Oxide(ZnO/SnO2). Experiments were carried out under UV light irradiation as a function of a variety of operating conditions such as pH, initial dye concentration, feed flow rate, contact time, aeration, and presence of ethanol which acts as an inhibitor of OH° reaction. The best photo-degradation yield of MB dye was obtained in a basic medium, while that of MB 21 was reached in an acid medium. The initial concentration of dye solution and the photo-degradation efficiency are inversely proportional. Likewise, the feed flow rate and consequently the residence time in the dynamic photo-reactor significantly affect the performance of the process. Furthermore, the oxygen enrichment of the reaction medium improves the photocatalytic degradation of both studied dyes. However, adding ethanol has a negative impact on the oxidation process by the produced hydroxyl radicals OH°. The study of the efficiency of the photo-catalyst, after cleaning, highlights its stability after repeated use.

Keywords: Zinc Oxide/ Tin(II) Oxide, Methylene blue-21, UV-Vis, Adsorbent, Wastewater

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Synthesis and characterization of $BaFe_{12}O_{19}$ nanoferrites

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There is a huge demand to accurately determine the magnetoelectrical properties of particles in the nano-sized regime due to the modern IC technology revolution and biomedical applications[1,2] .In this work, ultrapure hexagonal $BaFe_{12}O_{19}$ nanoferrite was synthesized by a facile co-precipitation method. Formation of single phase was analyzed by using wide angle X-ray diffraction. Crystallite size was found to increase from 50 nm to 78 nm when annealing temperature increased from 800 °C to 1000 °C, respectively. Ferrimagnetic behavior with moderate value of saturation magnetization and coercivity were studied at room temperature with the help of vibrating sample magnetometer (VSM). The FTIR spectra confirm tetrahedral and octahedral sites in $BaFe_{12}O_{19}$ structure. The surface morphology was analyzed by scanning electron microscopy (SEM), which reveals that the particles are agglomerated into irregular shapes. Particle size was measured with transmission electron microscopy (TEM), which was in correlation with the already calculated size from x-ray diffraction (XRD) spectra.

Keywords: $BaFe_{12}O_{19}$, X-Ray Diffraction, Scanning Electron Microscopy

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Synthesis of nanoflower-like 2D-MoS_2/Polyaniline/3D-Ni-foam by a facile coating method: application in supercapacitor

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The demand for energy storage devices such as electrochemical capacitors (EC), rechargeable batteries, and so on, sometimes known as supercapacitors, has surged in recent years. Supercapacitors have been considered a suitable alternative to lithium-ion batteries due to their good stability, high capacity, fast discharge, etc [1]. Binary transition metals such as transition metal dichalcogenides (TMDCs) have attracted more in energy conversion and storage due to their unique layered structure [2-4]. MoS_2 is one of the transition metal dichalcogenides, which is widely used in several industries related to renewable energy, including solar cells, lithium-ion storage, supercapacitors, etc. It can be explained by the layer structure of MoS_2 that can improve storage in the charging process. In addition, 2-dimensional (2D) layer of MoS_2 improves the electron transfer process and ionic conductivity compared to other similar materials [5]. This study investigated the applicability of nanoflower-like 2D-MoS_2/polyaniline/3D-Ni-foam as a current collector for a supercapacitor. 2D-MoS_2/polyaniline nanocomposite were loaded onto nickel foam by a simple coating method. SEM, XRD, microscopic images, electrochemical impedance spectroscopy, and charge-discharge tests were used to identify the morphology, structure, conductivity, and capacity, respectively. The resulting composite had an 34.36 MF/g capacitance at a current density of 32.101 A/g in 1M KOH solution. Moreover, the high cyclic stability was happened by maintaining capacity at 2000 cycles. The results showed that the synthesized composite can be suggested as a suitable candidate in supercapacitors.

Keywords: Supercapacitor, MoS_2, Transition metal dichalcogenides, Ni-foam, Polyaniline

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Synthesis of open-cell flexible soy oil-based polyurethane foams: investigation of mechanical properties

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Recently, scientists have been working to discover a viable replacement for non-biodegradable products made from non-renewable resources due to environmental concerns. For example, the use of herbal oil-based polyols as producers in the production of polyurethane (PU) foams and sponges instead of petroleum-based polyols has been developed. PU foams have been used in a variety of applications, including packaging to furniture cushions, insulation to cleaning, etc. Depending on the polymer structure utilized for synthesis, these foams can be rigid, semi-rigid, or flexible [1-3]. Soybean oil-based polyol (SBOP) was successfully synthesized for the production of flexible PU foam in this research. Epoxidation with ring-opening reactions was being used to prepare epoxidized soybean oil (ESBO) in a single step. The parameter of reaction time for ESBO manufacturing was also evaluated, with the hydroxyl number increasing as the reaction time increased. Thereafter, an advanced thermal synthesis was used to generate SBOP. For comparison, foams were made by using a petroleum-based polyol and a 1:1 mixture of petroleum-based: soy oil-based polyol. 1H-NMR and FTIR spectroscopy had been used to confirm the chemical structure of the synthesized polyol. Microscopic photographs and tensile tests were used to assess the size and openness of the cells and study the mechanical properties. The tensile test results showed that the soy oil-based PU foam had become more resistant. According to investigations, soy oil-based foam had a much more regular cell structure, higher resistance, more open cells, and even a smaller average cell size than petroleum-based foam. As a result, the use of soy oil-based biopolyol to replace petroleum-based polyol is suitable for the production of flexible PU foams.

Keywords: Epoxidized soybean oil, Polyurethane foams, Soybean oil-based polyol, Petroleum-based polyols

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Reduction of pollution in Landfill leachate of Urmia city by using pozzolan

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Due to high pollution, the water produced in Landfill requires chemical and biological treatment methods. In general, landfill leachate contains organic pollutants, ammonium, halogenated hydrocarbons, heavy metals and inorganic salts, and one of the methods of leachate treatment is the use of silicate-based materials[1, 2, 3]. The purpose of this study is to reduce the contamination of Landfill leachate in Urmia city by using pozzolan mineral. In this regard, experiments were performed using pozzolan in 500 ml balloons and the test conditions consisted of a reaction temperature equal to the ambient temperature of 600 rpm. The minute distribution of pozzolan granulation was 45 microns and 500 nm with a solid weight of 10%. The results of the experiments show that in the granulation of 500 nm, better results have been obtained. Thus, the amount of ammonium in the tap water is reduced by 93% and the contamination is due to the presence of microbes, which before decontamination was 81 in a dilution of 10^{-18} It was reduced to 46 in a 10^{-3} dilution.

Keywords: Leachate, Landfill, Urmia, Reduction

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Optimization of the method for determining the amount of estrone and 17beta-estradiol in water sources and water ozonation conditions in order to remove these hormones

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The presence of endocrine disrupting chemicals in the environment and their adverse effects on human and animal health have attracted much attention in recent years. Estrogens are the most important endocrine disruptors and estrone (E1) and 17β-estradiol (E2) are the strongest if them. The aim of this study was to optimize the method for determining the amount of estrone and 17beta-estradiol in water sources and water ozonation conditions in order to remove these hormones. To evaluate the amount of E1and E2, high-performance liquid chromatography was used. The extracted samples using the optimized Halo fiber loaded with N-octanol solvent and then methanol solvent (as desorption solvent) were analyzed with a HPLC technique using a C18 column (250mm × 4.6mm, 5µm) at room temperature (25˚C), mobile phase of acetonitrile / water (80:20% v/v) in isocratic elution mode at a flow rate of 1 mL/min and UV detection at 280 nm.

To evaluate the effect of ozonation on the removal of the studied hormones, first the optimal ozonation conditions in terms of ozone gas concentration, ozonation time, pH and E1 and E2 hormones were calculated. According to the obtained results, ozone concentration of 4 mg / l, duration of 5 minutes, pH of 6 and initial concentration of solution of E1 and E2hormones up to 10 mg / l had the greatest effect. Eventually, ozonation under optimal conditions eliminated 90% of E1 and 95% of E2. Overall, the results of this study showed that ozonation under optimal conditions is a good way to remove these hormones from water.

Keywords: Estrone, 17β-estradiol, water, ozonation

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Preparation and characterization of magnetic Expanded graphite/epoxy-triazine nanoadsorbent and its application in the removal of malachite green

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Malachite green is a dangerous and highly toxic to human and aquatic organisms due to its mutagenicity, teratogenicity, carcinogenicity[1]. hence it is very important to remove this dye from effluent before discharging into the water bodies. the graphite-based materials which have reach surface areas and chemical stability, can be used as effectively as adsorbents for dyes removal from wastewater[2]. Expanded graphite is an excellent adsorbent due to its high porosity, large specific surface area, poor polarity, and its also is an eco-friendly compound. In this study epoxy-triazine modified Expanded graphite magnetic nanocomposite was synthesized and its application as an adsorbent to remove malachite green from aqueous solution was investigated. the features of obtained nanoadsorbent were characterized by FESEM,TEM, XRD, BET, FTIR techniques. the results showed that the nanoadsorbent was properly modified. the adsorption process was performed to study the factors affecting the adsorption including pH, contact time, initial dye concentration, temperature, amount of adsorbent. the optimum conditions were obtained as follows: pH=8, contact time=60 minutes, adsorbent dosage=0/075g, initial concentraion=200mg/lit, temperature=20°c. the adsorption data were fitted with Langmuir isotherm model and Pseudo-second order kinetic model. Based on parametrs obtained from thermodynamic studies, this process is endothermic and spontaneous.

Keywords: Nanoadsorbent, Expanded graphite, Adsorption, Malachite green.

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Synergistic antibacterial effects between the traditional antibiotics and the stable nanoemulsion of cinnamaldehyde and 1,8-cineol

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Essential oils (EOs) and their active compounds are gaining great interest as alternatives to synthetic antibiotics due to their antimicrobial activity [1]. Unfortunately using EOs have several drawbacks such as low solubility in the aqueous phase, instability, etc [2]. Encapsulation of EOs in suitable drug delivery systems such as nanoemulsion is an appropriate way for enhancing their bioavailability and increasing their biological activities [3]. In this research, a stable nanoemulsion from cinnamaldehyde and 1,8-cineol was produced using a sonicator. In continue, the antibacterial activity of the stable nanoemulsion was assessed against E. coli, P. aeruginosa and S. aureus using broth dilution assay. Also, the synergistic effects of the stable nanoemulsion and traditional antibiotics (chloramphenicol, amoxicillin and azithromycin) were analyzed and the fractional inhibitory concentration index (FICI) was determined. Our results revealed that the stable nanoemulsion of cinnamaldehyde and 1,8-cineol (particle size = 27.76 ± 0.37 nm) had noticeable antibacterial activity against selected microorganisms with the minimum inhibitory concentrations (MICs) values of 1,1 and 2 mg/ml against E. coli, P. aeruginosa and S. aureus, respectively. Calculation of the FICI revealed partial synergy of the nanoemulsion and azithromycin against E. coli and P. aeruginosa. This synergistic effect between nanoemulsion and traditional antibiotics can be a potential option to improve the effectiveness of antimicrobial agents.

Keywords: Synergistic effect, Nanoemulsion, Antibacterial action, Active compounds of Eos

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Physico-chemical properties and fatty acid profile of seed oil from *Citrus aurantium* L. comparison extraction methods

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Citrus aurantium L. seeds are normally waste products from fruit processing but they are a valuable source of certain pharmaceutical and nutraceutical compounds. Fatty acids, tocopherols, phytosterols are the source of bioactive compoundshe in citrus seed oil that have promising applications such as biodiesel, high nutritional value food and natural antioxidants [1-4]. This study was performed to determine and compare the physico chemical properties of of Citrus aurantium L. seeds oil extracted by cold pressing and n-hexan. The C. aurantium L. seed fatty acids profile was analyzed by GC-MASS, ^{1}HNMR و ^{13}CNMR. In this study the effectiveness of ultrasonic-assisted and influence of air pressure on extraction Citrus aurantium L. seeds oil by n-hexane was evaluated. The highest oil yields were obtained using ultrasound-assisted extraction (25%) compared to other methods. The five fatty acids, 9-oleic (18.07%), Linoleic (36.69%), palmitic (21.90%), stearic acid (6.6%) and 10-oleic acids (1.1%) were identified in this study.

Keywords: Citrus aurantium L. oil, Citrus aurantium L. seed, Pressurized extraction

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Investigating and comparing the antioxidant potential and total phenolic content of *Eryngium caucacicum* extracts

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Today, medicinal plants play a very important role in human health. Plants can be considered as a valuable source of a wide variety of secondary compounds [1]. Many medicinal plants contain large amounts of antioxidant compounds, such as polyphenols, which can play an important role in absorbing and neutralizing free radicals [2,3]. Eryngium caucacicum L. is a well-known medicinal plant belonging to the family Apiaceae. This biennial herb is used as food in Iran, Turkey, Kosovo, Spain, and Italy. It possesses numerous biological and pharmacological activities such as antibacterial, antifungal, antioxidant, antiinflammatory, antitumor activities [4]. In this study, after collection of the roots and leaves of Eryngium caucacicum from North of Iran, the methanol and ethyl acetate extracts were obtained, and then, their antioxidant potential and total phenol and flavonoid contents were investigated. The antioxidant potential was studied using DPPH assay and the total phenolic content was determined quantitatively using the Folin Ciocalteu reagent, with Gallic acid as the standard. Also, total flavonoid content was estimated using aluminum chloride method. The findings showed that the leaves methanol extracts had the highest total phenolic and flavonoid contents, and their values were equal to 70.94, and 35.62 mg/g extract, respectiely. Also, the antioxidant study indicated that the roots ethanolic and ethyl acetate extracts significantly exhibited antioxidant potential with IC_{50} values of 88.36 and 112.92 µg/mL, respectively. So, the results of this study could provide useful information to guide the application of Eryngium caucacicum parts in food and pharmaceutical fields.

Keywords: Antioxidant, *Eryngium*, Flavonoid, Phenol

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Essential oil constituents of Ziziphora tenuior collected from Northwest of Iran

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The genus Ziziphora belongs to Lamiaceae family being known as an aromatic medicinal plant. The Lamiaceae family has several species which are of great importance in pharmaceutical, food and cosmetic industry, as well as in traditional and modern medicine [1]. Ziziphora tenuior of this genus has been used extensively from ancient time until the now as folk medicines as well as herb in cooking. This plant is often used as remedy in Iranian folk medicine against various diseases such as insomnia, hypertension palpitations, sedative, infections, gastrointestinal problems, stomachic, and dysentery. Moreovor, it has been used as an cold treatment, carminative, analgesic, and to reduce fever and oedema [2,3]. In this study, the essential oil of the aerial flowering organs of wild Ziziphora tenuior, collected from Northwest of Iran, was obtained by hydrodistillation method and analyzed by gas chromatography (GC) and gas chromatography/mass spectrometry (GC-MS), and then the antioxidant potential was studied using 2,2-diphenyl-1-picrylhydrazyl (DPPH) assay. In total, 14 compounds (comprising 96.4 % of total essential oil) were identified, which the main identified compounds were pulegone and limonene. The antioxidant study showeh that the essential oil had antioxidant activity with IC_{50} walue of 84.3 µg/mL, and it can be due to the presence of monoterpenes such as pulegone and limonene, and several sesquiterpenes, and it is assumed that the contribution of minor and major compounds exhibited this activity and not only one or few active molecules.

Keywords: Antioxidant, Lamiaceae, Volatile oil, Ziziphora

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Evaluation the antioxidant activity of Myrtus communis at different phenological stages

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Antioxidants are compounds which have great importance to reduce oxidative stress and prevention of damage to biological molecules. Myrtus communis L., known as true myrtle, is one of the important aromatic and medicinal plants, and has been used by locals for its culinary and medicinal properties since antiquity [1]. This plant has many biological activities such as antimicrobial (antibacterial, antifungal and antiviral) and antioxidant [2, 3]. This plant cou;d have different capacities to produce antioxidant compounds at different phenological stages. To achieve their goal, breeders must consider the proper harvest time to reach the best yield for their target purposes, such as pharmaceutical, food, and cosmetic industries applications. For this reason, the antioxidant ativity was studied in different phenological growth stages of Myrtus communis. In vitro antioxidant activity was investigated in a dose-dependent manner 2,2-diphenyl-1-picrylhydrazyl (DPPH) method. Statistical analysis of this experiment showed that the antioxidant activity was significantly different in various phenological stages of this plant. The results indicated that the IC_{50} values in the vegetative stages, full flowering stage, early development of seeds stage, late-mature stages, and ripe seeds stage were 467, 509, 30, 764, and 847 µg/mL, respectively. So, the extracts obtained from early development of seeds stage had the highest antioxidant activity. In conclusion, the results of the present study could provide useful information to guide the application of Myrtus communis in food and pharmaceutical fields.

Keywords: Antioxidant, Medicinal plants, Myrtle, Phenological stages

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Comparing the total phenolic and flavonoid contents of Myrtus communis at different phenological stages

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Medicinal plants can be considered as a valuable source of a wide variety of secondary compounds, and the amounts of these compounds could be changed at at different phenological stages [1]. Myrtle (Myrtus communis L.) is a medicinal plant endemic to the Mediterranean area and it has been used by locals for its culinary and medicinal properties since antiquity [2]. It possesses numerous biological and pharmacological activities such as antibacterial, antifungal, and antioxidant [3,4]. This study investigated the polyphenol accumulation of Myrtus communis from the vegetative stage to the seed set stage. Plants were separated into leaves, stem, flowers, and fruits, and extracts were analyzed for total phenolic content (TPC), total flavonoid content (TFC). The analysis of TPC and TFC was done using the Folin Ciocalteu and aluminum chloride methods, respectively. The findings showed that the highest and lowest phenolic content were obtained in the ripe seeds stage (2840 µg/g dried sample), and full flowering stage (8 µg/g dried sample). The analysis of flavonoid content was showed that early development of seeds stage (14.37 µg/g dried sample) had the highest content, while the lowest amount related to full flowering stage (7.73 µg/g dried sample). The results of this study can be used as a guideline for grower to obtain the highest possible amount of desirable metabolites, beneficial in both food and pharmaceutical industries as well as their undeniable economical benefits.

Keywords: Flavonoid, Medicinal plants, Myrtle, Phenol

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Headspace-solvent microextraction with green solvent for determination the volatile compounds from Artemisia absinthium

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In this study, Headspace-solvent microextraction (HS-SDME) was developed for the extraction of volatile compounds using deep eutectic solvents (DESs) as extraction solvents [1]. HS-SDME was developed as a solvent-minimized extraction technique, but few studies have examined the applications of deep eutectic solvents (DESs) to the HS-SDME of essential oils compounds [2]. DESs, which were prepared by mixing choline chloride (ChCl) with p-Chlorophenol at different ratios [3], were applied to the extraction of three terpenoids from *Artemisia absinthium* by HS-SDME in this work. Then, headspace single drop micro-extraction (HS–SDME) was done that was connected to gas chromatography. HS-SDME is simple and rapid compared to heat reflux extraction. Moreover, DESs can be used in HS-SDME for the extraction of a range of volatile compounds.

Keywords: Headspace, Artemisia absinthium, Chlorophenol, choline chloride, deep eutectic

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Microwave assisted headspace single-drop microextraction for rapid analysis of volatile components from Achillea eriophora DC

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In this paper, a simple method based on gas chromatography–mass spectrometry (GC–MS) following microwave assisted headspace single-drop microextraction (MH-SDME) was developed for the determination of essential oil composition of Achillea eriophora DC. The MH-SDME parameters including the nature of extracting solvent, microwave power, extraction time, sample weight and microdrop volume were optimized. The method was compared with single-drop microextraction (SDME) and traditional hydrodistillation (HD). MH -SDME and HD -SDME techniques were successfully performed for the determination of volatile compounds in Achillea eriophora DC. 42 compounds were identified in Achillea eriophora DC using the proposed methods. Compared with HD and HD -SDME methods, MH-HS-SDME is an easy, rapid and efficient method for the analysis of essential oils in Achillea eriophora DC.

Keywords: microwave, Achillea eriophora DC, microextraction, gas chromatography

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A density functional theory (DFT) calculation of the cinchonidine geometry as natural product

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Cinchonidine, a natural cinchona alkaloid, is mainly found in the bark of the Cinchona tree. Cinchonidine has received a lot of interest in recent years due to its wide range of pharmacological actions [1]. Cinchonidine have a number of applications as pharmaceuticals for the treatment of malaria and cardiac arrhythmias [2]. DFT methods have been widely used as verification of experimental measurements for different systems [3]. In this study, cinchonidine was optimized at B3LYP/6-31++G(d,p) level using Gaussian09 software was and some parameters, such as E_{HOMO}, E_{LUMO}, gap energy (ΔE), electronegativity (χ), global hardness (η) were calculated. In the cinchonidine compound, LUMO orbitals (E=-1.50 ev) localized over the quinolin ring and HOMO (E=-5.68 ev) orbitals are localized over the azabicyclo ring. The electronegativity (χ) 3.59 ev value, global hardness (η) value of 2.09 ev, chemical softness (S) value of 0.23 ev and electrophilicity (ω) value of 3.08 ev for cinchonidine explain that cinchonidine with the appropriate softness value has the highest chemical reactivity. Also, this compound possesses dipole-dipole interactions (Dipole moment=4.15 D). The results of quantum calculations of cinchonidine revealed that this compound because of good chemical softness has high chemical reactivity and can be used as natural product for treat various diseases.

Keywords: Cinchonidine, DFT, Gaussian 09

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Extraction, identification and analysis of active compounds in the Rhus coriria

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There is a significant increase in the use of plant extracts by the food industry as a natural preservative. Fat oxidation and microbial growth in food can be controlled using plant extracts. Aqueous extract of sumac has a strong antioxidant and antibacterial activity against pathogens of natural foods, so the aqueous extract of the plant is used as an effective and natural preservative in food production. In industry, sumac seeds are suitable for the production of spice products. However, they are rich in linoleic and oleic acids, which are considered suitable conditions for the use of plant seeds as valuable raw materials for the oil industry. In this context, mixing sumac seed oil with olive oil for use in sumac salads and cooking is currently proposed. In this research work, the active ingredients of Iranian and Iraqi sumac were extracted with methanolic and aqueous methanol solution and were determined by mass spectrometry and high performance liquid chromatography (HPLC). In the continuation of research its phenolic, antioxidant and antibacterial substances were examined and then the structure of the products was determined by IR and NMR spectra.

Keywords: Rhus coriria, Antioxidant, Antibacterial activity, Extraction

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Geranium Essential oil and sun photoprotection

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Essential oils are volatile compounds that have been used since antiquity as local anesthetic, anti-inflammatory, antimicrobial, food flavoring agents and sedative [1]. Several herbs belonging to the genus Pelargonium graveolens are noted for their medicinal benefits in traditional system of medicine. This plant, Pelargonium, has various medicinal properties. They are rich source of monoterpenes, coumarins, sesquiterpenes tannins, cinnamic acids, phenolic acids, flavonoids, flavones and flavonols derivatives. Pelargonium-derived essential oil is used in perfumery, cosmetics, soaps, creams, aromatherapy products exhibit good antioxidant activity and has potential immune modulating effects no natural killer cells [2]. Rose geranium is a male-sterile cultigen and is therefore only propagated vegetatively. It is a popular plant due to its significant biological and pharmacological activities, including antiinfluenza, anticancer, antimicrobial, antioxidant, antineuroinflammatory, and antifungal activity [3]. The aim of this study is to investigate the photoprotection properties of Geranium essential oil in oil-in-water emulsions in the ultraviolet visible wavelength. The Geranium essential oil is mixed with the prepared emulsion. Thirty milligrams of emulsion exactly weighed were spread on PMMA plates over the whole surface (25 cm^2) using a finger coat to achieve a homogenous layer over the entire plate until a residual mass of 15 mg is obtained, a density of 0.6 mg/cm^2[4]. Three plates were prepared to be tested. Then, the transmission measurements were carried out using a Varian Cary 5000 UV/Vis/NIR Spectrophotometer. In this experiment, based on the results of UV absorbance, it shows that Geranium essential oil has UV absorbance in UVA = 12,70 ± 0.23 and in UVB = 9,41 ± 0.23. In this study, it finds that Geranium essential oil has the potential to use in sunscreen products.

Keywords: Geranium oil essential, photoprotection, sunscreen, skin

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Density functional theory study on the Epigallocatechin gallate natural product

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Epigallocatechin gallate (EGCG) is a natural phenolic compound found in many plants, especially in green tea, which is a popular and restorative beverage with many claimed health benefits such as antioxidant, anti-cancer, anti-microbial, anti-diabetic, and anti-obesity activities [1-2]. Density Functional Theory (DFT) is progressively becoming vital for the drug designing process. Since past few years DFT has appeared as a Quantum Mechanical (QM) method which is satisfactorily meticulous as well as competent to be employed in pharmaceutical studies [3]. In this study, EGCG was optimized at B3LYP/6-31++G(d,p) level using Gaussian09 software was and some parameters, such as E_{HOMO}, E_{LUMO}, gap energy (ΔE), electronegativity (χ), global hardness (η) were calculated. In the EGCG compound, HOMO (E=-5.97 ev) orbitals are localized over the trihydroxybenzoate group and LUMO orbitals (E=-1.84 ev) localized over the trihydroxyphenyl group. The electronegativity (χ) 3.91 ev value, global hardness (η) value of 2.07 ev, chemical softness (S) value of 0.24 ev and electrophilicity (ω) value of 3.69 ev for EGCG explain that EGCG with the appropriate softness value has the highest chemical reactivity. Also, this compound possesses dipole-dipole interactions (Dipole moment=3.51 D). The results of quantum calculations of EGCG revealed that this compound because of good chemical softness has high chemical reactivity and can implementable platform in the context of clinical development.

Keywords: Epigallocatechin gallate, DFT, Gaussian 09

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DPPH Radical Scavenging Activity of Hexane and Methanol Extracts of Mentha pulegium L. Aerial Parts

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Mentha pulegium L., commonly known as pennyroyal are widely used in traditional medicine, mainly for the treatment of various diseases like cold, flatulence, dyspepsia, sinusitis, food poisining and etc. This plant is a source of biologically and pharmaceutically active products such as essential oil and various extracts [1]. In this study the antioxidant effects of hexane and methanol extracts of Mentha pulegium L. aerial parts were examined using DPPH assays. Methanol extract indicated higher DPPH radicals scavenging activities than hexane extract. The methanol extract of Mentha pulegium L. leaves at the 100 µg/mL concentration exhibited 51.3 ± 3.6 % inhibtion. However, the hexane extract of Mentha pulegium L. leaves at the same concentration showed 16.1 ± 2.3 % inhibtion. Both the aforementioned extracts have significantly lower radical scavenging activity in camparison with BHT which showed 89.7 ± 3.4 % inhibtion against DPPH. The higher ability of methanol extracts against DPPH could be attributed to the existence of various compounds like flavonoids, phenolic acids [2]. These results are in agreement with several previous studies carried out with extracts of M. pulegium reported a close relationship between antioxidant activity and phenolic levels [3]. According to the obtained results it can be concluded that the Mentha pulegium L. could be used as potential sources of safe and inexpensive antioxidants to prevent oxidation in different products.

Keywords: Pennyroyal, Medicinal plants, Extract, Antioxidant activity

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Green Synthesis of Copper Oxide Nanoparticles by Walnut Leaves Extract and Evaluation of Extract effects on the Nanoparticles' Morphology and Size

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Development of reliable, nontoxic, environmentally friendly, cost-effective and easy-to-synthesize methods for the synthesis of nanoparticles is an important step in nanotechnology. The natural products can be used for the synthesis of NPs. The Walnut leaf contains numerous main bioactive compounds, such as phenolic compounds which can be effectively utilized as reducing and stabilizing mediators in the NPs Production. CuNPs were synthesized by the reduction of copper Sulfate using extract of Walnut leaves. The physical and chemical properties of green synthesized CuNPs were characterized by X-ray diffraction (XRD), scanning electron microscopy (SEM) and Fourier transform infrared (FT-IR). XRD patterns have been investigated for the detection of phase, size and structure of the crystal as well as the proof of CuNPs formation. SEM was used to morphology analyses and FT-IR analysis was used to checking different bonds. The Present study indicated that walnut leaf extract due to several natural compounds reduces copper ions and converts them into NPs and stables them.

Keywords: Copper Oxide, Nano Particle, Walnut leaves

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Encapsulation of polyphenol extract of *Melissa officinalis* by nano spray dry

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The bioavailability of herbal medicines is one of the most challenging parts of manufacturing these products. Due to the complex matrix of plant extracts and the diversity of phytochemicals, they complicate their absorption to increase the stability and bioavailability of effective extract materials. Various techniques used for encapsulation of herbal products. This process is usually done by formulating plant extracts with biopolymers and spray drying techniques. *Melissa officinalis* is one of the most important medicinal plants and due to the presence of secondary metabolites, it has antioxidant, analgesic and anti-eczema properties due to stress and therefore has many therapeutic functions. This study aimed to optimize the extraction process and investigate the effect of encapsulation on the stability and improvement of the medicinal properties of *M. officinalis* extract. Aqueous and hydro-alcohol extracts were prepared for this purpose. The content of rosmarinic acid quantified as the active ingredient was analyzed by the HPLC-UV method. Rosmarinic acid in different extracts was quantitatively and qualitatively determined and showed the highest amount of rosmarinic acid with 4.48 mg/g and 8.97 mg/g DW E, the highest amount of extraction yield of 10.8% belonging to the hydroalcoholic extract (70-30). The spray-drying method with natural polymers such as gum Arabic [1], maltodextrin [2], lecithin, and pectin encapsulates the hydroalcoholic extract. The physicochemical properties of obtained powder were characterized. The SEM and DLS results indicate the uniform distribution of particles and a suitable size (400 nm to 1000 nm). Powder production efficiencies were all within acceptable limits. Drug release studies are also underway. The results show that using the encapsulation method with a spray dryer is a promising method to improve the bioavailability and microstructures and the controlled release time of phenolic compounds.

Keywords: Melissa officinalis, Encapsulation, Spray drying, maltodectrin

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Overproduction of polyphenolic compounds of rosmarinic acid, coumaric acid and chlorogenic acid in the Saponaria officinalis hairy roots using titanium dioxide nanoparticles (TiO_2 NPs)

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Nanoparticles are being broadly used as a new generation of effective elicitors in biotechnology in order to stimulate the production of valuable secondary metabolites via inducing defense mechanisms. Phenols and polyphenols are a class of plant secondary metabolites recently drawing particular interest due to their broad spectrum of pharmacological effects. Rosmarinic acid (RosA) is an ester of caffeic acid and 3, 4-dihydroxyphenyl lactic acid. RosA's presence in medicinal plants, herbs, and spices is linked to beneficial and health-promoting effects. In plants, RosA is considered to be a cumulative defense compound, while in human, RosA has many biological activities, including antiviral, antibacterial, antioxidant, antimutagenic, and anti-inflammatory activities [1]. The extensive nanotechnology applications in hairy roots cultivation is a sustainable production foundation to produce such active elements. In this study, the effect of various concentrations of titanium dioxide nanoparticles (TiO_2 NPs) (0, 10, 20, 30, 50 mg L^{-1}) with two treatments (24 and 48 h) was examined on the rosmarinic acid, coumaric acid and chlorogenic acid in hairy roots of S. officinalis. The variance analysis shows significant differences between various concentrations of TiO_2 NPs and exposure times in terms of polyphenolic compounds production. According to the results, the maximum chlorogenic acid content (21.83 mg kg^{-1} FW) was obtained in 48 h exposure time of hairy roots with 50 mg kg^{-1} concentration. The minimum content of this compound (6.05 mg kg^{-1} FW) was observed in 48 h treatment with the concentration of 30 mg kg^{-1}. Treated hairy roots with the concentrations of 50 mg kg^{-1} (53.68 mg kg^{-1} FW) and 30 mg kg^{-1} FW (53.34 mg kg^{-1} FW) after 48 h exposure time produced the highest content of coumaric acid. The lowest coumaric acid content (32.65 m mg kg^{-1} 1 FW) was detected at 20 mg kg^{-1} of nano elicitor after 24 and 48 h. This research indicated that the rosmarinic acid content significantly increased in treating S. officinalis hairy roots with TiO2 NPs. The highest production and accumulation of rosmarinic acid rate (64.56 m mg kg^{-1} FW) was observed in 24 h treatment with the 50 mg kg^{-1} concentration of nanoparticle, which was 1.5 times more than blank samples. The lowest rate of rosmarinic acid (30.59 mg kg^{-1} FW) was obtained by the 48 h treatment of hairy roots with 50 mg kg^{-1} of nano elicitor.

Keywords: Elicitor, Nanoparticles, Polyphenolic compounds, Rosmarinic acid

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HPLC-Based Activity Profiling of the Endemic Iranian Medicinal Plant Helichrysum oligocephalum

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The Helichrysum genus, comprising over 600 species distributed mainly in Africa, Madagascar, Australasia, and Eurasia, has been used traditionally for the treatment of infections, digestive and hepatic disorders, colds, coughs, and wounds [1]. From phytochemical point of view, essential oils, sesquiterpenes, diterpenes, pyrones, benzofurans and various classes of phenolic compounds, including phloroglucinols, and flavonoids have all been reported. As an ongoing project, we are exploring the bioactive constituents of endemic Helichrysum species. In this study, we isolated and identified the active constituents of the endemic plant H. oligocephalum. The aerial parts of H. oligocephalum were collected from Mashhad (Iran) in May 2015 and a voucher specimen (13251) has been deposited at the Herbarium of Mashhad University of Medical Sciences. The dried aerial parts were milled and exhaustively percolated with methanol. The obtained methanol extract was dried under reduced pressure to afford solid residue and was then partitioned successively with dichloromethane (DCM), ethylacetate, and butanol solvents. The cytotoxicity of the fractions were evaluated by Alamarblue assay. The DCM fraction, as active cytotoxic fraction, was subjected to column chromatography on silica gel, using a gradient of n-hexane−chloroform [2]. Fractions 1−25 (F1−F25) were combined on the basis of TLC patterns. The active compounds were tracked with the aid of HPLC-based activity profiling. The activity profile of 15 5 min fractions were obtained. Of 25 fractions obtained from normal phase chromatography, 10 fractions F10-F20 contained the active constituents. The active fractions were further phytochemically analyzed by RP-HPLC. The purified compounds were identified by NMR and high resolution mass techniques. Ten compounds belonging to pyrones, phloroglucinol derivatives, and compounds containing both structural motifs have been isolated.

Keywords: Helichrysum, phloroglucinol, pyrone, cytotoxic

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Enrichment natural pigment from pomegranate juice: isolation by macroporous resin and characterization adsorption/desorption process

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Color plays an important role in human life and different industries, including food, cosmetics, and pharmaceuticals. Synthetic pigments in spite of providing variety in color, high yield and low price, always being a concern in different industries. For this purpose, natural pigments, due to their biologically and environmentally safe feature, attracting a considerable attention to using them in the food products [1]. Anthocyanins (ACNs) are water-soluble natural pigments responsible for producing various colors in flowers, fruits, and vegetables. Pomegranate juice (PJ) is a beverage rich in ACNs compounds that shows high antioxidant activity compared to other fruit juices and beverages. This study aimed to separate the ACNs as natural red pigment from PJ using LXA-10 macroporous resin in a batch system [2]. All adsorption and desorption processes on the resin have been optimized for maximum separation efficiency. The ACNs maximum adsorption condition (contact time: 40 min, pH: 2.5, a PJ to resin ratio: 30 ml/0.7 g), and ACNs maximum desorption (contact time: 8 min and a 6-bed volume solvent) were obtained as optimum operating conditions. In which the maximum of 94.0% adsorption and 93.3% desorption percentage of ACNs were achieved. The different adsorption isotherms models were tested which results concluded that Freundlich model with R2 = 0.96 fitted adequately with the experimental data. A kinetic study was carried out that showing the ACNs adsorption data correctly adjusted by an equation corresponding to a pseudo-second-order chemical reaction with R2 = 0.99. The constituents and the contents of the purified products were analysed, and the antioxidant activities were determined using FRAP test. The purified product contained five major ACNs in PJ and showed strong antioxidant activity (8.8 mmol Fe (II)/L sample) in comparison with initial PJ (1.4 mmol Fe (II)/L sample). In conclusion, purification by LXA-10 macroporous resin was a highly efficient and economical method for purification red natural pigment from PJ.

Keywords: Macroporous resin, FRAP, Anthocyanins, Batch system

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Formulation of enriched olive leaf lipid based nanocarriers and natural polymer coating by nanospray dryer

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Olive leaves have had many therapeutic applications in traditional medicine since ancient times. Scientific studies confirm the existence of therapeutic properties including cardioprotective properties, antioxidant, anti-inflammatory and antifungal properties, attributing these properties to existing compounds such as oleuropein, tyrosyl, hydroxytyrosol, luteolin-7-glucoside, apigenin-7. Glucoside. Among them, oleuropein is the most abundant compound in olive leaf extract. Due to the structural properties of oleuropein, it is unstable in acidic environment. The use of nanocarriers is a method to maintain the structure of this compound in the gastrointestinal tract and improve its stability [1]. The purpose of this project was to select a suitable method for encapsulating olive leaf extract and increase its stability and effectiveness. For this purpose, whole olive leaf extract was enriched using HP-20 macroporous resins. The enriched extract was then loaded into liposomals. For this purpose, liposomes were prepared by thin layer hydration method and converted to nano-liposomes with a size of 98 nm by sonication. Given that liposomes are essentially unstable systems, natural polymer coating method was employed to stabilize them. Chitosan was used as the coating layer on the nano-liposomes. Due to the susceptibility of natural polymers to ambient pH, they are suitable for targeted release in the gastrointestinal tract. Therefore, alginate was selected as the second polymer layer [2]. Using a nano spray dryer, the nanoparticles were coated with alginate polymer. To evaluate the effect of polymers on release rate, alginate with different concentration (0.1, 0.2, 0.5 and 1%) were used. In terms of release, the behavior of the formulations in the gastric environment was investigated at pH = 1.2 for 2 hours and in the intestinal environment at pH = 6.8 for 6 hours. Finally, one of the formulations, which had a release in the intestinal environment, was selected as the most optimized formulation.

Keywords: Olive leaf; encapsulation; nano spray dryer; Natural polymers ; polymer coatings

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Enrichment of Symphytum officinal extract by macro-porous resins and optimization of resin parameters

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The most commonly polyphenolic compound of comfrey extract is rosmarinic acid, which shows valuable biological effects, including antioxidant, anti-inflammatory and antibacterial properties.[۱] Enrichment and isolation of rosmarinic acid are leading to increase in anti-inflammatory properties. In this study, macroporous resins (DM-130, LXA-880, LSD-001, LXA-10, HP-20, LXA-17) were used for enrichment of rosmarinic acid and removal of pyrrolizidine alkaloids in comfrey. Meanwhile, LSD-001 was selected. then desorption processes were optimized to achieve maximum enrichment efficiency[2]. Accordingly, by using the LSD-001 resin, the amount of rosmarinic acid was enhanced 7 fold in desorbed extract. In addition, the selected resin has demonstrated a high capability in phenolic compounds separation with 3.26 fold increase in desorbed extract. The results of total alkaloid showed that the reduction of alkaloid was noticeable in desorbed extract by using LSD-001 resins. According to the results, LSD-001 resin was selected for enrichment of rosmarinic acid and elimination of alkaloid compounds. Isotherm studies showed that the Langmuir model with $R^{۲}$ = 0.98 highly fits with the experimental data and proves the multilayering of the adsorption process. Moreover, based on kinetic studies, the adsorption data of rosmarinic acid were correctly adjusted by the pseudo-second order kinetic model with R^2 =0.98. Rosmarinic acid-enriched by HPLC-UV was qualitatively and quantitatively analyzed according to the rosmarinic acid standard. The antioxidant activity was assessed by using the DPPH test and the total phenolic content was determined by using Folin–Ciocalteu method. The total alkaloid and adsorption content were investigated by extracting the alkaloid using chloroform solvent and using a spectrophotometer, respectively.

Keywords: Symphytum officinal, Macroporous Resins, Rosmarinic Acid, Enrichment of extract

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Chitosan-coated alginate microcapsule of Urtica dioica hydroalcoholic extract

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Diabetes is a metabolic disorder in which glucose metabolism is impaired and if left untreated can have devastating effects on the body of diabetic patients. In fact, in type2 diabetes, the body's cells couldn't properly receive glucose which leading to high blood glucose levels [1]. The inhibition of the activity of two blood sugar-boosting enzymes in intestinal system called alpha amylase and alpha glucosidase can be effective in the lowering of blood sugar which subsequently reduces the long term effects of diabetes [2]. The hydroalcoholic extract of nettle is one of the useful medicinal plant products to reduce glucose uptake because of its components which inhibit the activity of enzymes in the intestine. Nettle extract encapsulation is a suitable method for coating the extract and save bioactive compounds from destroyed effect of acidic environment of stomach [3]. In this study, chitosan-coated alginate microcapsules containing nettle extract were prepared (with different percentages) and the loading efficiency of 50% was obtained. The SEM images showed size of microcapsules between 500 and 800 micrometers. The release of microcapsules in the simulated acidic and basic environment was examined. The results showed that increasing of chitosan amounts as coating layer caused to obtain slower release for microcapsules compared with non-coated or coated with lower amounts of chitosan. The results of this research can be used in the preparation of encapsulated products of nettle hydroalcoholic extract for the reducing of glucose uptake from diet to control of type2 diabetic.

Keywords: Urtica dioica, Hydroalcoholic extract, Encapsulation, Chitosan, Sodium alginate, Type2 diabetic.

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Metabolic Profiling and Biological Activities of Terminalia chebula, Rosa canina, and Nigella sativa Extracts

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Recently, the emergence and spread of pathogenic bacterial resistance to many synthetic antibiotics have been increasing throughout the world. This phenomenon is of great concern and there is a need to find new compounds as an appropriate alternative to antibiotics. In this regard, natural antibiotics derived from medicinal plants, some of which have been used in traditional medicine for centuries and have competitive effects compared to some commercial antibiotics, can be studied as alternatives [1-2]. In this study, the antibacterial and antioxidant activities as well as total phenol and flavonoid contents were assayed in the ethanolic extracts obtained by ultrasound-assisted extraction method (UAE) from Terminalia chebula, Rosa canina, and Nigella sativa. The ethanolic extracts were screened against two gram-negative (Escherichia coli ATCC25922 and Pseudomonas aeruginosa ATCC27853) and two gram-positive (Bacillus cereus ATCC11778 and Bacillus subtilis ATCC6633) bacteria with the disk diffusion method. The highest antibacterial potentiality was exhibited by the ethanolic extract of N. sativa against E. coli (16.5 mm). The ethanolic extracts were assessed for their antioxidant activity using DPPH radical scavenging assay. According to the results, the highest antioxidant activity related to T. chebula with the percentage inhibitory of 80.66%. Also, ethanolic extract of T. chebula (140.53 mg GAE/ g plant) showed the highest phenolic content. The highest amount of total flavonoid content was observed in N. sativa extract (11.88 mg QE/g plant). So, T. chebula can be used in food, medicine, and cosmetic industries.

Keywords: Antioxidant, Antibacterial, Phenol, Flavonoid, Medicinal plant

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Chemical composition and insecticidal effects of salvia yangii leaves and flowers essential oils against Phthorimaea operculella

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Phthorimaea operculella (Zeller) is one of the most prominent pests of potatoes throughout tropical and subtropical regions [1]. Some natural and botanic compounds would be potential alternatives to synthetic chemical fumigants against P. operculella in storage [2]. In this study, fumigant toxicity and oviposition deterrent activity of volatile oil of different plant organs (leaves and flowers) of Salvia yangii were tested against P. operculella. The average essential oil content of leaves and flowers was obtained at 1.2%, and 0.99% (w/w), respectively. GC-MS phytochemical profile of this species showed the major compounds identified in S. yangii leaves were 1,8-cineol (14.67%), δ-3-carene (5.98%), and linalyl acetate (12.33%). In addition to 1,8-cineol and δ-3-carene, some compounds such as linalool format (10.72%), linalool (6.72%), and α-pinene (4.59%) were found in the flowers in higher percentages than leaves. Results of fumigant toxicity showed LC_{50} values of leaves and flowers were 13.82 and 15.77 µL/L air for one-old-day eggs, and 9.37 and 12.04 µL/L air for one-old-day adults, respectively. The essential oils also showed oviposition deterrent activity against adults of P. operculella. Results indicated the mean number of hatched eggs was 2.00 and 1.66 eggs for leaves and flowers, respectively, in comparison to the control (50.66 eggs). It can be concluded that different parts of S. yangii essential oil have the potential for development into natural insecticides for integrated storage pest management.

Keywords: Salvia yangii, essential oil, Phthorimaea operculella, Insecticidal activity, Oviposition deterrent

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Essential oil chemical composition and leaf morphology of Salvia rhytidea and Salvia yangii aerial part from Taftan region

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Salvia (Lamiaceae family) is one of the widespread genus (nearly 1000 species) displaying a remarkable diversity in growth forms, secondary compounds, floral morphology, and pollination biology [1]. Salvia subgenus Perovskia is a group of plant species, prior to 2017 were detected as the separate genus Perovskia. DNA studies have since shown that Perovskia is so closely aligned to Salvia that it is now formally changed names [2]. According to the taxonomic and morphologic literature, the sections or groups identified in Salvia are not in accordance with each other [3]. In this study, two species including Salvia yangii (previously perovskia atriplicifolia), and Salvia rhytidea were analyzed through their essential oils, together with the morphological characteristics of the leaves. The results showed that there are clear differences in the essential oil quantity (1.3 % for S. yangii and 0.33% for S. rhytidea) and quantity. The major compounds identified in S. rhytidea were α-Terpinolene (19.28%), sabinene (7.00%), trans caryophylen (7.05%), and limonene (5.5%) while 1,8 cineol (14.55%), δ-3-Carene (9.03 %) and linalyl acetate (12.48%) were the major compounds in S. yangii. The morphological differences (leaf base, margin, apex, and density glandular trichrome) are also pronounced in the leaf of species. Clear distinctions between the investigated Salvia and subgenus of perovskia species in essential oil chemical composition and leaf morphology were observed.

Keywords: Salvia species, essential oil, morphology

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Biaoactive diterpenoids of Salvia sub-genus perovskia, emphasizing Iranian species

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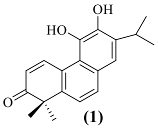
The subgenus Perovskia Kar. (Lamiaceae), comprises several species with an ethnobotanical value and medicinal potential [1]. Three species including Salvia abrotanoides Karel. Salvia yangii B.T. Drew and Salvia artemisioides Boiss. are distributed in Iran. A comprehensive survey in the electronic databases published from the past to 2022, with keywords of 'perovskia' and Salvia subgenus perovskia 'showed that more than twenty new compounds belonging to diterpenoids have been isolated and successfully characterized from different Iranian Perovskia species. The nor-abietan (1-3), seco-norabietane (4-5), isopimarane (6) and icetaxan (7-8) diterpenoids are the main construction of aerial parts and roots new diterpenoids [1-4]. As a result, a great number of the described diterpenoids such as carnosol, carnosic acid, ferruginol, miltiodiol, and crypto-tanshinone, exhibited interesting biological activities e.g antibiofilm, antiprotozoal and antiproliferative.



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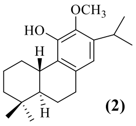

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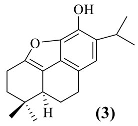

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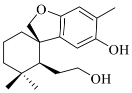

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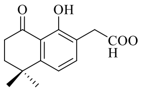

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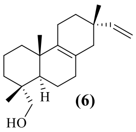

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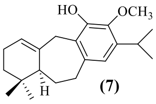

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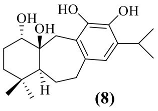

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Keywords: Salvia subgenus perovskia, Diterpenoids

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Chemical composition of Artemisia aucheri aerial part essential oils from two different Iranian bio-climatic areas

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The large genus Artemisia L., Asteracea family, comprises important medicinal plants which are currently the subject of phytochemical attention due to their bioactive compounds [1]. Climatic conditions affect qualitative and quantitative properties of plant essential oils [2]. This work was designed to study the chemical composition of Artemisia aucheri essential oil obtained from two different bio-climatic areas belonging to semi-arid, cold (Khaf in Razavi Khorasan province), and very arid, warm with windy and dust (Taftan in Sistan and Baluchestan province) regions of Iran. All samples were investigated using GC-FID, and GC-MS methods, to evaluate phytochemical constitutions. The sample yields were in 1.1% and 1.3% content for essential oil of Khaf and Taftan respectively. It was observed that A. aucheri growing at semi- arid, cold such in Khaf region had a higher quantity in camphor (63.52%), and 1,8-cineol (14.00%) while those growing at the very arid, warm with windy and dust climate had a lower camphor (9.89%) and 1,8-cineol (12.01%) quantity. According to findings, it can be concluded that quantitative and qualitative properties of Artemisia sp. essential oil are affected by bio-climatic conditions such as temperature, air humidity and wind speed.

Keywords: Artemisia aucheri, essential oil, bio-climatic factor.

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Separation of cyclotids from Viola ignobilis by Open Column Chromatography

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Cyclotides are a large family of plant peptides that have valuable biological activities such as antiviral, antibacterial and anti-cancer properties. Due to their unique cyclic structure, they have high thermal and enzymatic stability [1, 2]. Isolation of cyclotides have been performing by semi-preparative and preparative HPLC. In this research, an attempt has been made to purify and separate them by classical column chromatography methods. The Möbius group of cyclotides from Viola ignobilis were selected for isolation due to their high amount compared with the bracelet subfamily. Cyclotides were extracted with a mixture of ACN/H20/0.1%FA solvents using the electric field method. Then, they were purified by SPE cartridges as non-polar fraction. Then, the obtained 50% ethanolic fraction from desorption process was used for study on open column normal phase chromatography. Different non-polar solvent systems were selected to work and the column outputs were monitored by HPLC. The results showed that the mixture of cyclotides were separated to different fractions. In fact, the mentioned method can be considered as a kind of offline two-dimensional chromatography by switching cyclotides from C18 reverse phase to silica gel normal phase chromatography [3].

Keywords:Viola ignobilis, Open column chromatography, Two-dimensional chromatography, Column switching, Isolation

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Distribution of Cyclotids in Different Organs of the Aerial Parts of Viola Ignobilis

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In this study, distribution of cyclotides in different organs of Viola ignobilis aerial parts were investigated. After collecting the plant, different organs of its aerial parts such as flower, stem attached to the flower, petals, calyx, sepals, leaves and stems attached to the leaves were separated and then dried in the shade. Extraction from different parts of the plant was performed using ultrasonic waves with a mixture of ACN/H20/0.1%FA. After purification by SPE C18 cartridges, 50% ethanolic eluted fraction was selected for the study of Möbius cyclotides, which have high amounts in the plant, for further studies. All fractions were analyzed by HPLC and chromatograms were compared for their cyclotiodes peaks. The results showed the greatest difference between the petals and leaves in the terms of cyclotid distribution. This study showed that if the different organs of the plant can be examined separately before extraction, it will be more likely to reach the less crowded fractions which help to have simple isolation process [1,2].

Keywords: Viola Ignobilis, Cyclotids distibution, Aerial parts, Petals

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Comparison of Cyclotide Fingerprints of Viola ignobilis and a Viola Species Collected from Osku

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In this study, Cyclotide fingerprint of an unknown Viola species collected from Osku, with the highest morphology likeness to Viola ignobilis, was compared with Viola ignobilis. After collecting a Viola species from Osku region which had highest morphology similarity to the Viola ignobilis, findnig a new source for vigno cyclotides was purposed. For this, all Aerial parts of unknown plant were separated and dried alnoe. All organs were extracted with CAN/H2O/0.1%FA for obtaining of their cyclotides extracts. For the purification step, extracts were cleaned-up using SPE C18. Then 50% and 80% ethanolic eluted fractions from SPE cartridg were analyzed by HPLC. Resulted chromatograms were compared with Viola ignobilis. The obtained results showed that there were identical differenes in cyclotides contents. This fact proposed that there is opurtunity for discovering of new cyclotides from studied unknown Viola species [1-3].

Keywords: Fingerprint, Cyclotides, Viola ignobilis, Osku

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Insecticidal activity and Chemical Composition of Perovskia abrotanoids Karel essential oil against Phthorimaea operculella

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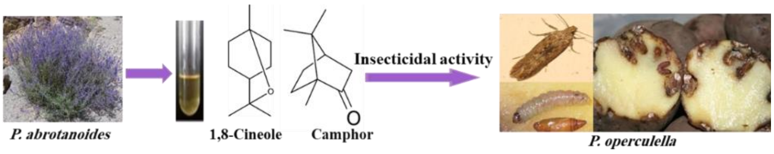
Potato tuber moth (PTM), Phthorimaea operculella Zeller is a significant insect pest of cultivated potatoes in Iran. Since the potato is one of the most valuable sources of human food, non-chemical control of potato pests is important. Plant essential oils (EOs) could be used as promising alternatives to synthetic insecticides due to their safety to non-target organisms, low-level resistance, and relatively low cost. Perovskia abrotanoides is an aromatic erect herb that is used in Iranian folk medicine, especially for the treatment of cutaneous leishmaniasis [1,2]. The composition of the isolated essential oil obtained from the flowering aerial parts of P. abrotanoides, collected from Chenaran county, was analyzed by GC and GC-MS. Altogether, 32 chemical compounds were identified in the essential oil with 1,8-Cineole (20.4%) and Camphor (25.3%) as dominant chemical metabolites. The present study was conducted to investigate the insecticidal activity of P. abrotanoides essential oil (PAEO) for the safe-efficient management of P. operculella. Fumigant toxicity of PAEO was evaluated against one-day-old eggs, adults, and penetration of first instar larvae of P. operculella into potato tubers and leaves under laboratory conditions at 26 ± 1ºC, 65 ± 5% RH, and a photoperiod of 8: 16 (L: D). Probit Fumigant toxicity analysis showed PAEO was effective against P. operculella adults and eggs that exhibited LC_{50} values equivalent to 4.33 and 7.93 µL/L air, respectively. Results demonstrated that PAEO caused 3.33 and 9.66% of neonate larval penetration, respectively. Therefore, the EO had inhibitory activity against neonate larvae of PTM. Our results suggested that PAEO could be used as a novel-effective tool for P. operculella management techniques to protect potatoes.



Keywords: Perovskia abrotanoides, Phthorimaea operculella, Insecticidal activity

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Phytochemical Investigation from aerial parts of Salvia macilenta Boiss

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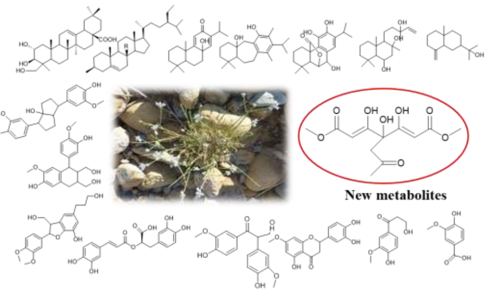
The genus *Salvia* is one of the largest members of the Lamiaceae family and nearly about 900 species spread throughout the world. This genus is comprised of 61 annual and perennial species in Iran, of which 17 are endemic [1]. *Salvia macilenta* is an aromatic subshrub and endemic species that grows in southern Iran (Kerman, Hormozgan, Baluchistan, and Yazd provinces) possesses antioxidant activity, antibacterial activity, neuroprotective effect, antiglycating activity and protects PC12 cells against H_2O_2-induced apoptosis [2]. In the present work, we have undertaken a phytochemical investigation for the first time on *n*-Hexane- Ethyl acetate extract from the aerial parts of *S. macilenta*. Investigation of the n-Hexane- Ethyl acetate extract on Silica gel column and Sephadex LH-20 chromatography, and RP-HPLC, led to the isolation and identification of 31 secondary metabolites that one of which is a new compound. chemical profiling of this species contained a wide array of natural compounds, including terpenes, flavonoids, lignans, and phenols, of which triterpenoids, abietane type diterpenoids, phenolic acids, and one sesquiterpene (*β*-eudesmol) were the predominant compounds. Their structures were elucidated by extensive spectroscopic methods, including 1D (1H NMR) and 2D-NMR (COSY, HSQC, and HMBC) as well as HRMS and ECD spectra.



Keywords: Salvia macilenta, Lamiaceae, Column chromatography, HRMS

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Comparison of isocratic and gradient elusion for separating and purifying bee venom peptide compounds using RP-HPLC

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Bee venom is an odorless and transparent liquid containing a hydrolytic mixture of proteins with acid pH (4.5 to 5.5) that bees often use as a defense tool against predators. One drop of bee venom consists of 88% of water and only 0.1μg of dry venom. The latter is an extremely complex blend of peptides including melittin, adolapin, apamin, and MCD-peptide. It also contains enzymes, most importantly PhospholipaseA2, and compounds of low molecular weight like bioactive amines (e.g., histamine and epinephrine) and minerals [1-2]. Bee venom due to chemical constituencies of several peptides and enzymes, especially melittin peptide, which makes up 50-60% of venom, has effective applications in pharmacy, medicine, and the cosmetics industry. Therefore, analysis and purification of the main compounds in bee venom require up-to-date and cost-effective techniques. In this study, the separation and purification of bee venom peptide compounds were investigated using high-performance liquid chromatography with two different elusion conditions, isocratic and gradient. For that RP column(C_{18}) was a stationary phase and acetonitrile and water were used as a mobile phase. The obtained results were shown that the optimal elusion condition for gradient strategy was 50 minutes with the ability to completely separate all the compounds, the resolution and the number of theoretical plates were 3.58 and 294113.89 respectively. In contrast, the optimal isocratic method with ACN: H_2O (38:62) as mobile phase, was 35 minutes, which was able to separate melittin as the main peptide from other compounds. In this method, the number of theoretical plates was 1729.6068. Therefore, the isocratic method with ACN: H_2O (38:62) can be used to purify melittin at a later time, with the possibility of reusing the mobile phase which reduces the cost. However, this method is not suitable for analyzing and purifying other compounds in bee venom and it is better to use the gradient method instance.

Keywords: Bee venom, Melittin, Isocratic, gradient

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Investigation of phenolic compounds in fruits of 55 Iranian Berberis spp. genotypes

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The genus Berberis belongs to the Berberidaceae family, with 15 genera and 650 species around the world. It has been used in traditional medicine since ancient time due to its diversity and pharmacological uses[1, 2]. This study was aimed at exploring the phenolics composition in fruits of 55 Iranian Berberis spp. genotypes by HPLC. The Berberis fruits were collected from the Barberry Collection Garden of Mashhad and also different natural habitats in Iran. The samples were air-dried, finely grounded, and extracted by methanol at room temperature. Three phenolic compounds including chlorogenic acid, caffeic acid, and rutin were found in fruit extracts by HPLC which the first one had the highest amount (3.01 $mg.g^{-1}$ DW of fruit). Overall, the results of HPLC proved the suitable phenolics diversity of the Iranian Berberis fruits and the importance of Iranian Berberis germplasm for the future breeding programs of this genus.

Keywords: HPLC, Phenolic compounds, Berberis

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Calicined product (Kushta) as nano-materials in Unani system of medicine

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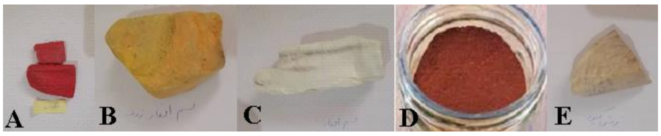
Ayurvedic and Unani/Tibb are the two most popular health care systems of traditional medicine in Pakistan, India, and Iran. Arabs and Muslim physicians such as Rhazes and Avicenna further developed Unani medicine based on their related experiences. In Unani medicine, Kushta (Calx; carbonates or oxides forms), the most prehistoric form of nano-medicine is utilized since 1000 BC to treat various ailments [1]. The very small particle size of kushta is responsible for its rapid absorption in the body leading to instant therapeutic actions. Low dose, high efficacy, and more stability are some benefits of kushtajat [2]. Due to the lack of communication among traditional healers and physicians and the unavailability of the literature in English, no efforts have been made to study this type of dosage. The purpose of this study is to collect information that some local therapists in some parts of Iran use calx for the treatment of health problems. Based on a questionnaire, and interviews with local therapists in Chabahar county, some common types of kushta are reported in this work. Khusta Shingraf (**A**; calx of Copper sulfate) is useful in general and sexual debility, improving digestion and the nervous system. Kushta Sammulfar (**B**,**C**; Arsenic trioxide), is an aphrodisiac of a high order, which increases appetite, and improves digestion. Kushta faulad (**D**; Iron dust) is useful in hepatic weakness and anemia. Kushta Raskapoor (**E**; Calomel) is used for cancer. According to the therapist, in the classical calcination process of kushta, the correct proceeding guarantees the production of Kamil (perfect), while a deviation from the method results in a Naqis (imperfect) Kushta, which is at risk to initiate unfavorable impacts [3]. Physicochemical properties of all Kushta products for the impurities detection and metal contents are examined by scanning electron microscopy, dynamic light scattering, Fourier transform infrared, and X-ray analysis. Some recommendations have also been given to provide the path to initiate research in this area of potential therapeutic value.



Keywords: Kushta, calcination, Unani medicine

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GC/MS-Based Activity Profiling of the Essential Oil of Three Endemic Iranian Helichrysum Species

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The Helichrysum genus, comprising over 600 species distributed mainly in Africa, Madagascar, Australasia, and Eurasia, has been used traditionally for the treatment of infections, digestive and hepatic disorders, colds, coughs, and wounds. From phytochemical point of view, Helichrysum species contain essential oils constituting mainly monoterpenes and sesquiterpenes. The most well-known Helichrysum species in this regard is H. italicum whose essential oil has been used for the treatment of different diseases and applications. Many products of the essential oil from H. italicum are available in the market. The most important activity reported for the essential oil of some Helichrysum spp. including H. italicum is as anti-infectious and anti-microbial agent. In Iran, 19 Helichrysum species exist of which 8 species are endemic to the country. The plants H. oocephalum, H. leucocephalum, and H. oligocephalum are three endemic Iranian species with good distribution in the country. Unfortunately, no phytochemical study reporting the essential oil composition of these species is available so far. Thus, in this study, we attempted to have a comparative methabolite profiling of their essential oils and activity. The plants were collected from different parts of Iran and their voucher specimen are deposited at the herbarium of Mashhad University of Medical Sciences. After the plants were dried, their essential oil were obtained by water distillation usind a Clevenger apparatus. Then, the essential oils were subjected to GC/MS analysis. Besides, the antimicrobial activity of the essential oil were evaluated against some bacterial and fungal strains. The GC/MS data were analysed and the chemical compostion of the essential oils were identified according to their Kovats index and fragmentation pattern. In addition, the essential oils of these species were compared using a heat map.

Keywords: Helichrysum, essential oil, sesquiterpene, antimicrobial

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The Use of Macroporous Synthetic Adsorbents in the Extraction and Purification of Anthocyanins from Iranian Saffron petal (Crocus sativus L.)

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Today, the need to use natural extractable pigments, including anthocyanin pigments, in various industries such as food and medicine, has led researchers to look for a new source of dye. The biological properties [1] of anthocyanins have doubled the importance of its study, so that among all the properties, strengthening the cardiovascular system and its function as a free radical scavenger makes anthocyanins a valuable source to control cancer, thus designing a method of increasing the percentage purity of anthocyanin pigments, like extractable sources of anthocyanin pigment in Saffron petals, called discarded part of saffron flowers, can be valuable [2]. Using synthetic adsorbents for the extraction of anthocyanin pigment compounds from saffron petals, as an acceptable source for economic efficiency and reduction of environmental pollution, will be a suitable method. Therefore, the adsorption and desorption of anthocyanin on synthetic porous adsorbent based on Di-Vinyl-Benzene, resin *LXA-860* which show a good behaviour in the adsorption and of anthocyanin compounds, was investigated by static experiments in laboratory scale. The amount of total monomeric anthocyanin equivalent to dried petals was calculated to be 0.82 g / 100g which is not high. High performance liquid chromatography analysis and also measurements based on adsorption and desorption formulas, confirm this enrichment and increase in purity percentage of anthocyanins after loading on resin. LXA-*860* resin showed good ability in the adsorption of the anthocyanin compound of delphinidin 3,5-O-diglucoside as the predominant anthocyanin in the plant according to the specific properties of the adsorbent. Because of the importance of the compound mentioned, optimization on the paraments of the initial concentration of loaded extract, kinetic of adsorption and desorption and the appropriate amount of adsorbent was optimized. Then dynamic experiments were performed on the glass column and the parameter of loading extract amount and washing volume was optimized.

Keywords: anthocyanin, adsorption, desorption, synthetic adsorbents, saffron petal

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Enrichment of Saffron’s Crocin and Picrocrocin by Macroporous resin

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Crocin as the most important carotenoid glycoside is the color agent of saffron. Due to its major role in the treatment of diseases, enrichment and purification of its metabolites are valuable. Cost-effective crocin purification is a major industry concern [1]. The use of porous resins is an efficient method for enriching and purifying compounds from natural sources and plant extracts. Polystyrene-based vinyl benzene-based polymer resins can be used to purify carotenoids [2]. In this project, we used HP20 resin and investigate the optimal concentration and loading, and desorption conditions by static systems. The results have shown that crocin has higher adsorption and desorption percentage than picrocrocin due to its non-polar chain and the similarity of its structural polarity to the resin used. Under the obtained optimal conditions, the percentage of adsorption for crocin was 81.48 ± 0.10% and for picrocrocin was 76.17 ± 0.10% and the rate of desorption for crocin and picrocrocin was 88.71 ± 0.20% and 78.13 ± 0.20%, respectively. Isotherm studies have shown that the Langmuir model is highly consistent with experimental data for crocin with R2 = 0.98 and picrocrocin with R2 = 0.96, and proves that the adsorption process is integral. Also, according to the kinetic studies, crocin and picrocrocin adsorption data were correctly adjusted by the pseudo-second-order model with R2 = 0.99.

Keywords: Chromatogaraghy; Saffron; Isotherms; Macroporous resin

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Application of solvent-antisolvent crystallization technique for excellent enrichment of Crocin from saffron

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Saffron (Crocus Sativus L.) is a medicinal plant that is obtained from the stigmas dried of the plant [1]. This plant originally cultivated in the East, Middle East and later in some Mediterranean countries. Its main components consist crocin, picrocrocin and safranal [2]. Saffron is used as the spice to give color, taste and aroma to foods and beveragesPurification of crocins as the most bioactive compounds insdie saffron is one the main concern of pharmaceutical industry. Looking for a cost effective method, in this work, solvent-antisolvent recrystallization technique was used for extraction of crocins from saffron. We used ethanol and ethylacetoacetate as solvent and antisolvent, respectively. Some important experimental parameters such as solvent:antisolvent ratio, temperature, injection rate and extract concentration were examined and optimized. Under optimized conditions, crocin 1 was enriched up to 47% while the extraction of picrocrocin was excluded. However, the extraction of crocin1and picrocrocin in crude extract was 26%, 23%, respectively

.***Keywords:*** Saffron, Crocin, Solvent-antisolvent, Recrystalization

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Antibacterial Activity of Pimpinella anisum, Carum copticum, and Heracleum persicum Extracts

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The traditional medicinal practice has been known for centuries in many parts of the world for the treatment of various human ailments. The use of antibiotics has revolutionized the treatment of various bacterial infections. However, their indiscriminate use has led to an alarming increase in antibiotic resistance among microorganisms [1], thus necessitating the need for the development of novel antimicrobials [2].On the other hand, Foodborne disease is a global issue with a significant impact on human health. With the growing consumer demand for natural preservatives to replace chemical compounds, plant antimicrobial compounds must be thoroughly investigated for their potential to serve as biopreservatives [3]. Therefore, this study focused on the search for antibacterial agents among natural products. The ethanolic extracts of 3 plant species of the Apiaceae family, including Pimpinella anisum, Carum copticum, and Heracleum persicum were evaluated for antibacterial activity using the agar disk diffusion method against two gram-positive (Bacillus cereus ATCC11778 and Bacillus subtilis ATCC6633) and two gram-negative (Escherichia coli ATCC25922 and Pseudomonas aeruginosa ATCC27853) bacteria. The extracts were extracted from dry seeds of the used plants by ultrasound-assisted extraction method (UAE). All the extracts had an inhibitory effect against studied bacteria. The most sensitive strain was E. coli, while the most resistant strain was B. cereus. The highest inhibitory zone was shown by the extract of C. copticum against E. coli (22.5 mm). Also, the extract of C. copticum was found to be better effective compared to positive control. Laboratory screening of plant extracts showed encouraging results indicating their potential uses in the control of selected pathogenic bacteria. According to the results, C. copticum has the highest antibacterial potential and can be used by the pharmaceutical, food, and cosmetic industries.

Keywords: Antibacterial, Apiaceae, Ethanolic extract, Medicinal Plant

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A Comprehensive HPTLC Metabolite Profiling of Iranian Safflower Genotypes

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Safflower (Carthamus tincturius) is one of the world's oldest crops. Safflower petals contains two pigments red (0.83 w/w %) and yellow (30 w/w%) [1]. The structures of safflower red and yellow pigments are reported as C-glucosyl quinochalcone moieties that present only in C. tinctorius . The yellow pigment include Hydroxy safflower A and hydroxy safflower B. Precarthamin is the minor yellow pigment [2]. Traditionally, safflower was grown for its seeds and coloring, and flavoring food, as medicines and for making red and yellow dyes [3]. Safflower pigments are safe for food and have curative effects on diseases such as lack of oxygen coronary heart diseases , myocardial infarction , cerebral thrombosis and renal thrombosis etc [4]. The purpose of this research is to purify the pigmentation of safflower on an industrial scale as well as to investigate the different species collected from this plant. the silica gel column followed by HPLC semi-Prep used as purify the yellow and red color of the plant and then to measure the three main safflower metabolites from different species , HPTLC technique was developed , which is a fast and inexpensive system . solvent for extraction was optimized as water : acetone (1:1) for quantification of safflower yellow and red. silica TLC plates were used with the solvent system containing n-buthanol, acetic acid , water, methanol. analysis of color was performed at the absorbance mode of 400 nm for yellow and 520 nm for red. The highest amount of Hydroxy safflower yellow A , hydroxy safflower B and carthamin was 32.87%±0.1 (Padideh) 13.78%±0.2 (Padideh) , 9 % (TN79604) and the lowest amount of hydroxy safflower A ,hydroxy safflower B and carthamin was 4.72%±0.13% (TN79815) , 4.07±0.01% (TN79815) , 0.02% (S-541) respectability. HPTLC method is a user friendly method that can be successfully used for the qualitative and quantitative analysis of herbal materials with different species of safflower.

Keywords: High-performance thin-layer chromatography (HPTLC) ، Carthamidine ،Carthamin ، Safflower

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Interaction of Levodopa with boron nitride nanotubes as a drug delivery carrier

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The overall goal of utilizing nanotubes in drug delivery is to treat a disease effectively with minimum side effects. With common methods of taking the drug, such as orally and intravenously, the drug is distributed throughout the body and the whole body is affected by the drug and adverse effects of the drug occur. As nanotubes can release drugs into the tissue cells without damaging the healthy cells, it is necessary to determine the structural properties of Drug-Boron nitride nanotubes(BNNTs) complexes which may have led to the development of optimal BNNTs as new effective drug transporters [1]. In the present work, the adsorption behavior of levodopa and boron nitride nanotube (BNNT) has been investigated using B3LYP density functional at the 6-31G (d) level [2]. It was observed that the levodopa molecule prefers to adsorb on BNNT with adsorption energy of about –19.13 kcal/mol. Studies, including Natural Bond Orbital (NBO) analysis [3], Atoms in Molecules (AIM) [4], Density of state (DOS), Homo and Lumo orbits, and thermodynamic properties were performed [5]. The results of adsorption energy, charge transfer, electronical and structural parameters imply that Levodopa molecule strongly prefers to be adsorbed on BNNTs. Our results suggest that the BNNTs can be an effective adsorbent respect to the Levodopa molecule in drug delivery.

Keywords: Boron nitride nanotube, Density functional theory, Levodopa, Adsorption energy.

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Long-term proliferation and delayed senescence of bone marrow derived human mesenchymal stem cells on metformin co-embedded HA/Gel electrospun compositenanofibers

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The Current study was aimed to evaluate the efficacy of hyaluronic acid/Gelatin (HA/GEL) encapsulated with metformin-loaded mesoporous silica nanoparticles (MET@MSNs) on the prolonged in vitro proliferation of bone marrow derived human mesenchymal stem cells (BMhMSCs) without prompting aging [1]. For this propose, composite scaffolds consisting of MET and MET@MSNs in combination with HA were fabricated by electrospinning technique [2]. The morphology and biochemical configuration of fabricated scaffolds were characterized using FESEM, TEM, TGA, and FTIR. The enhanced proliferation rate and metabolic activity of the BMhMSCs seeded on MET@MSNs incorporated into HA/Gel scaffolds (MET@MSNs HA/Gel NFs) were confirmed via PicoGreen and MTT test assay, respectively, over 21 days of culture. The obtained data from MTT and PicoGreen assays also revealed improved metabolic activity and expansion rate for BMhMSCs grown on the MET@MSNs-NFs compared to other types of NFs after 14 and 21 days of incubation These results confirmed the capability of MET@MSNs HA/Gel NFs for persistent and controlled discharge of MET in the design of a novel platform for neutralizing cellular aging and attaining adequate quantities of fresh BM-hMSCs for tissue engineering applications.text.

Keywords: Bone marrow derived human mesenchymal, Metformin, Mesoporous silica nanoparticles, Tissue engineering.

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Synthesis of a novel benzene sulphonamide using functionalized lysin amino acid as a new antibacterial drug

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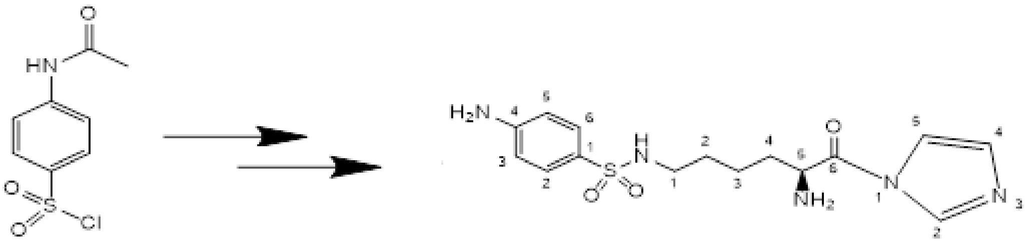
An attempt was made to synthesize a new compound of benzenesulfonamide derivatives as a class of powerful antibacterial drugs based on amine heterocycles in a molecular framework[1, 2].To extract this compound, a multi-step, efficient approach was developed. Adding an imidazole ring to the end of the lysine amino acid chain is a key step in the designed reaction. This paper reported the synthesis of a new derivative in a multi-step method in a one-pot reaction with high efficiency. The final product of synthesis is brown powder. The biological studies of new drugs are in process, and it is expected the new compound as an antibacterial agent will bring good results. The structure of the synthesized compounds was confirmed by FTIR and NMR spectroscopy.



Keywords: Benzene sulfonamide, Amino acid, Lysine, imidazole, antibacterial, NMR.

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Synthesis of a new benzenesulfonamide derivative based on amino acids as a new antibacterial drug

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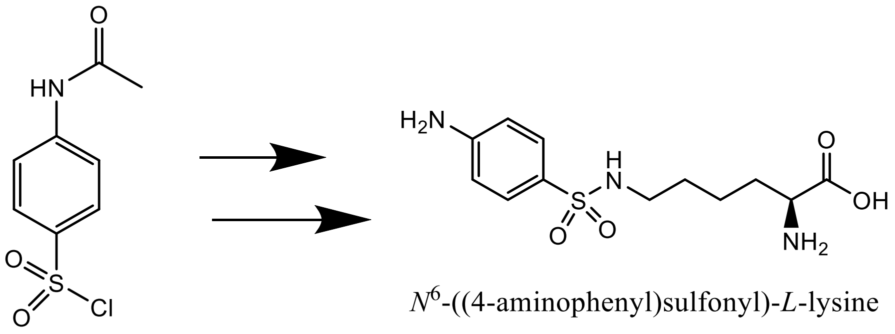
In the development of new antibiotics, amino acids have been considered a new generation of antibiotics. Infection is caused by bacterial, fungal, parasitic, and viral agents, and in addition to inhibiting the growth inhibitory effect, it kills them[1, 2]. This project aimed to synthesize a new combination of benzenesulfonamide derivatives based on the lysine amino acid as a class of antibacterial drugs which was developed to obtain this efficient compound in a multi-step reaction. The final product was observed as a dark powder. Biological studies of the synthesized drug are underway, and we expect to have acceptable results from the new compound as an antibacterial agent. FT-IR, ^{1}HNMR, and ^{13}CNMR analyses were approved chemical structures of the product.



N^{6}-((4-aminophenyl)sulfonyl)-*L*-lysine

Keywords: Antibiotics, Amino acid, Benzenesulfonamides, Lysine, NMR

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Neuroprotective effects of modified graphene oxide on spinal cord injury

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Nervous system lesions are generally entangling and crucial problems worldwide. Renovation and recovery of nervous system damages have been challenging compared with other tissues because of their function and anatomy. Spinal cord injury (SCI) is a portion of the central nervous system (CNS); almost two million people worldwide suffer from it. Different researchers have investigated recent treatment and regeneration of damaged tissue, sensory recovery, and motor function globally [1,2]. Graphene oxide (GO)-based nanomaterials as considerable materials with wonderful and precious properties propose numerous chances for designing pioneer scaffolds in neural tissue engineering to cure the central and peripheral nervous system injuries by neuron-regenerative therapies [3,4]. In this study, GO was synthesized by the modified Hummer method and functionalized with different polyethylene glycol content (1, 2, and 4 wt.%) at 45°C for 12 hours to improve functionality and biocompatibility properties. Follow-up chemical analysis; Preliminary in vitro studies on mesenchymal stem cells (MSCs) have shown that the prepared nanocomposites are nontoxic and increase cell proliferation.

Keywords: Graphene oxide derivatives, Central nervous system (CNS), Spinal cord injury (SCI), Poly ethylene glycol (PEG).

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Development of collagen-chitosan scaffold with graphene oxide for application in nerve tissue regeneration

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Spinal cord injury (SCI), as a complex and unsolved disease, causes patients suffering (personal, social and financial) all over the world. Due to the complications of the physiological structure of the nervous system, there is no practical method for renovation and clinical treatment of damaged nerve tissue [1,2]. Recently, hydrogels have been attractive as excellent biomaterials due to their great potential to fill wound places and carry out minimally invasive post-transplant strategies for tissue engineering, drug delivery, and cell therapy in the lesion microenvironments [3]. In this research, graphene oxide (GO) nanosheets were synthesized using the modified Hummers method. Type I collagen was extracted from the Wistar rat tail. Collagen-Chitosan-GO (Col-Chi-GO) hydrogel-based scaffolds were prepared in Col: Chi, 1:1, and GO, with 30%, 50%, and 70% weight ratios. Characteristic analyses were performed. We investigate the preliminary in vitro studies on mesenchymal stem cells (MSCs).

Keywords: Hydrogel, Chitosan, Collagen, Graphenic nanomaterials, Neural regrowth

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All-Trans Retinoic Acid-Grafted-Poly (Beta-Amino Ester)-Poly (Ethylene Glycol) Methyl Ether Micelles Loaded with docetaxel: A Dual Drug Delivery System for Cancer Treatment

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Combination chemotherapy has been intensively regarded as an alternative strategy in order to overcome the limitations of monotherapy including the inadequate drug-mitigating response, serious side effects, and poor therapeutic efficacy [1, 2]. The rationale for combination chemotherapy is to use drugs with different mechanisms of treatment and deliver multiple drugs at their maximum tolerated doses [3, 4]. In this study, All-Trans-Retinoic Acid-Grafted-Poly (Beta-Amino Ester)-Poly (Ethylene Glycol) Methyl Ether (ATRA-PBAE-MPEG) copolymer was synthesized, and the micelles were formed from the copolymer to encapsulate docetaxel (DTX). ATRA and DTX were respectively formulated by chemical and physical encapsulation into a single nanomicelle-system to obtain a novel cytotoxic drug delivery system that can release these drugs simultaneously with different release kinetics. Design-Expert software was performed to optimize the size of micelles. CMC, zeta potential, morphology, drug release, and blood-compatibility were evaluated. In vitro cytotoxic activity of micelles was investigated for breast cancer cell line and human umbilical cord vascular endothelial cells in comparison with pure DTX and ATRA. Furthermore, the anti-angiogenic effects of compounds were examined in vitro. No significant hemolysis was observed from the nanomicelles, they showed higher cytotoxicity and anti-angiogenic activity than that of free ATRA and DTX. In conclusion, ATRA-PBAE-MPEG micelles could be considered as a promising ATRA and DTX dual drug delivery system in cancer chemotherapy to improve therapeutic effect and minimize adverse effects.

Keywords: All-trans retinoic acid, Dual drug delivery, Docetaxel, Poly (beta-amino ester)-poly (ethylene glycol) methyl ether, Polymeric micelle

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Study the Antipyretic Activity of Bioactive Compounds of Ginger (Zingiber Officinale) Using Molecular Docking

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Ginger (*Zingiber officinale*) is a well-known herb used in ethnomedicine [1]. It is used in traditional medicine for many human disorders, including fever, gastrointestinal complications, arthritis, rheumatism, hypertension, and various infectious diseases due to its anti-inflammatory, antioxidant, antimicrobial, and antiemetic properties [2]. 6-gingerol and 6-shogaol, with phenolic nature, are the significant constituents of ginger. Both gingerols and shogaols exhibit a host of biological activities. There is convincing evidence indicating that these phenolic compounds could serve as essential lead molecules for developing therapeutic agents to treat various life-threatening human diseases, particularly cancer [3]. This study investigates the antipyretic potential of two bioactive compounds of ginger, 6-gingerol and 6-shogaol. An in-silico molecular docking approach is carried out to evaluate the probable effect. Prostaglandin E2 (PGE2) is the critical component in the fever mechanism. So the isoforms of the cyclooxygenase enzyme, COX-1, and COX-2, which are reported to inhibit PGE2, are selected as receptors. 6-gingerol and 6-shogaol are docked to the target proteins, and the best binding modes are analyzed. 6-shogaol showed better binding affinity against the receptors COX-1 and COX-2, with a docking score of -6.23 and -6.00 kcal/mol, respectively. Therefore, 6-shogaol might be used as a therapeutic agent for treating fever.

Keywords: Antipyretic, Ginger, 6-Gingerol, 6-Shogaol, Molecular docking

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Molecular Docking Study on the Antiitch Potential of Alpha-linolenic acid against Human G-Protein Coupled Receptor

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Alpha-linolenic acid (ALA) is an omega-3 fatty acid found in plants. It is found in flaxseed oil and canola, soy, perilla, and walnut oils [1]. It has been reported to inhibit prostaglandin synthesis, reducing inflammation and preventing certain chronic diseases. A 2021 review found that ALA intake is associated with a reduced risk of mortality from all causes, cardiovascular disease, and coronary heart disease but a slightly higher risk of cancer mortality [2]. Chronic pain and itch are common hypersensitivity syndromes affected by endogenous mediators. Current treatments often provide only partial or transient relief and have substantial side effects [3]. Various agents have been proposed as anti-itch products with poorly understood mechanisms, and they are effective with variable success. Medicinal plants, which are recognized as a possible source of therapeutic aids, are playing a crucial role for humans and provide potential health care content in every part of the world in health systems. This study used a molecular docking technique to investigate the probable anti-itch activity of alpha-linolenic acid. The results of the in-silico docking studies were compared with the anti-itch-approved drug, Gabapentin. It revealed that alpha-linolenic acid shows better anti-itch efficacy than Gabapentin. Alpha-linolenic acid showed good binding affinity toward the target protein, the human G-protein coupled receptor, with a docking score of -7.61 kcal/mol and inhibition constant of 2.65 µM.

Keywords: Alpha-linolenic acid, Anti-itch, G-Protein receptor, Molecular docking

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QSTR models for toxicity predicting of DMIs (Demethylation inhibitors) antifungal agents using Genetic algorithm multiply linear regression (GA-MLR)

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DMIs (Demethylation inhibitors) are a widespread group of antifungal agents targeting sterol biosynthesis in pathogenic fungi [1]. However, the global use of these chemicals in agriculture and medicine may cause potential toxic effects on non-target organisms [2]. Herein, we developed quantitative structure–toxicity relationship (QSTR) models for toxicity prediction of DMIs based on the LD_{50} values against rats [3]. The genetic algorithm combined with multiple linear regression (GA-MLR) was used to generate QSTR models based on all molecular descriptors and another based on the three-dimensional ones. The cross-validated leave-one-out Q^2_{LOO} metric of both models (0.7524 and 0.7145, respectively) revealed their optimistic predictive quality. The models exhibited the importance of 3D-molecular descriptors (3D-MoRSE, WHIM, and RDF descriptors) in the toxicity prediction of this type of chemical. From a risk assessment perspective, both models in this manuscript can be used as a checkpoint to evaluate the probable hazards of proposed DMIs in the future.

Keywords: DMIs, QSAR, SBIs fungicides, Genetic algorithm, MLR

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Design and optimization of a metformin nanoparticle-impregnated buccoadhesive film

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Metformin, an oral antihyperglycemic drug, is typically the first-line oral treatment for type II diabetes [1]. Conventional oral dose forms of metformin (regular and extended-release formulations) result in substantial changes in plasma drug concentration and offer no control over drug administration [2]. Metformin's key drawbacks are its relatively low bioavailability (about 50–60 percent) and short half-life [3]. This study aimed to develop a buccoadhesive film containing metformin nanoparticles (NPs) for increased medication bioavailability. Metformin nanoparticles were produced via nanoprecipitation and subsequently cast into an HPMC-Chi mix film. The essential formulation variables were evaluated using a three-factor Box–Behnken design with three stages. The penetration of the medication was also studied using buccal mucosa from sheep. The results confirmed the creation of spherical nanoparticles with an average size of 177.8 6.42 nm and entrapment effectiveness of 78.03 0.1%. The nanofilms possessed satisfactory physicochemical properties and drug concentration. Additionally, the ex vivo study revealed that the buccal mucosa has a high drug permeability. The optimal conditions for nanofilms were anticipated to be 700 mg of hydroxypropyl methylcellulose, 50 mg of glycerol, and 0.15 percent by weight of chitosan. The nanofilm demonstrated a high drug penetration within 6 hours and provided an exceptional opportunity for buccal medication administration.

Keywords: Buccal, Buccoadhesive, Metformin, Nanofilm, Nanoparticles

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Investigation of Novel Formulation of Dry Powder Inhaler Capsules: Effect of different plasticizers on the morphology, puncturing size, and surface properties

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Today, the principle of research and development is pulmonary drug delivery due to the potential for maximizing therapeutic effects for patients by direct drug targeting the pathology site in the lungs [1]. Amongst the convenient delivery alternatives, the Dry Powder Inhaler (DPI) is the favored device to remedy a variety of diseases [2]. In this regard, the fabrication and development of a novel formulation for DPI capsules have been investigated. We studied the effects of various parameters, such as percentages of polyethylene glycol (PEG), propylene glycol (PG), glycerol (Gly), brittleness, test conditions, and particle release of manufactured DPI capsules.The results illustrated that the lower molecular weight of PEGs presented the better plasticizing capability of gelatin. Owing to the hygroscopicity of the utilized plasticizer, PEG400 increased the capsule flexibility for a longer time and its stability under environmental conditions in gelatin capsule formulation, likewise, no particle release was observed in the gelatin/PEG capsule. The prepared gelatin/PEG400 capsules were compared with pure gelatin and HPMC capsules. The capsules were evaluated in terms of loss on drying (LOD), surface morphology, roughness, and puncture type. Besides, gelatin/PEG capsules have no particles due to the smooth surface after the punching process. The as-produced capsules are not blocked again after punching, allowing the patient to take the drug completely. In fact, the present research provided substantial insight regarding the development of DPI formulation in capsule investigations on an industrial scale.

Keywords: Gelatin; Hard capsule; Dry powder inhaler; Plasticizer; Poly ethylene glycol.

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Antimicrobial effect of loaded smoked plant extracts on silica nanoparticles

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Medicinal plants because of their antibacterial and antifungal traits have been used for treating various diseases for a long time ago and they can be substituted for the synthesized drugs they are important because of their higher medical influence and economic points. Nowadays nanoparticles are used for drug delivery, especially for herbal active ingredients. Silica nanoparticles are one of the suitable Nano-carriers because of their important traits which are physical stability, nontoxicity, and their ability to get bonded with different molecules and polymers. Silica nanoparticles have the uniform porous texture in size of 2-10 nanometers. In this research smoke extracts of *Peganum harmala* and *Boswellia* were prepared and these extracts were loaded into nanocomposite with the matrix of silver grafted silica nanostructure. The antimicrobial activity of this nanocomposite was investigated against *Escherichia coli* and *Staphylococcus aureus* bacteria. To identify the nanocomposites structure the FTIR, XRD, and SEM tests were taken.

Keywords: Antibactrial, Smoked plants, Peganum harmala, Boswellia, Silica nanoparticles

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Developing Novel Anticancer Palladium(II) Agents to Integrate Chemotherapy and Overcoming Drug Resistance

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Palladacycles are versatile organometallic compounds that show potential for therapeutic use. The first mono- and binuclear Pd(II) complexes bearing benzoxazoles directives have been synthesized and characterized by ^{1}H and ^{13}C NMR spectroscopy, IR, and mass spectrometry. These palladocycle complexes are potent antiproliferative agents against different cancer lines (for the most part, IC_{50} values fall in the range 0.02–0.5 μm). By choosing 1,3,5-triaza-7-phosphaadamantane (PTA) as co-ligand, we can improve the selectivity toward tumor cells, all the complexes exhibit an optimal balance of hydrophilicity/lipophilicity. Also, all of these complexes are quite stable in physiological conditions and interact well with DNA and the transport protein HSA. The cytotoxic effects of these complexes were examined on HeLa, MCF7, and A549 human cancer cell lines as well as Hek293 as a representative of normal cells. The main structure–activity relationships and the most promising palladocycles were outlined. These complexes are more cytotoxic than cisplatin against the cancer cells screened, can quickly penetrate into A549 cells and mainly localized in mitochondria [1,2].

Keywords: Palladocycle, Benzoxazoles, Antiproliferative, Mitochondria,DNA/HSA

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Synthesis of a Temperature-Responsive Injectable Hydrogel for the Controlled Delivery of BAMLET Anticancer Drug

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The severe side effects of systemic high doses of chemotherapy, as well as the development of drug resistance, make anticancer therapy less safe and effective. Pain, cardiotoxicity, hepatotoxicity, and renal toxicity are all adverse effects of traditional chemotherapy [1,2]. As a result, novel strategies for improving anticancer medication therapeutic index by targeted administration to tumor locations are constantly being researched and developed. Among a variety of options, hydrogels are a potential option because they can be made up of smart materials that respond to environmental influences and change their characteristics appropriately, allowing for targeted drug delivery [3]. Injectable thermosensitive hydrogels for drug delivery have been extensively studied [4]. Thermosensitive hydrogels are a type of drug delivery system that is liquid at the moment of administration. This paper reports on a the synthesis of a temperature-responsive hydrogel for the controlled release of BAMLET, a complex of bovine alpha-lactalbumin and oleic acid, as a model anticancer drug. BAMLET was originally isolated from bovine milk as a potent anticancer agent. It kills a wide range of cancerous cells of various origins while leaving healthy cells largely unaffected both in vitro and in vivo. Poly(N-isopropylacrylamide) polymer as a thermoresponsive hydrogel was synthesized via the free-radical polymerization method. The formulation of the BAMLET-Hydrogel was optimized and the following values were used as the optimum: 10% w/w polymer, 50 µL of the drug, and phosphate buffer of pH 7. Under the optimized conditions the cloud point, lower critical solution temperature, and the swelling ratio of the formulation were 26˚C, 30˚C, and 2.6 (at 37˚C), respectively. In vitro release experiments showed that BAMLET was slowly released from the formulation. Therefore, BAMLET-loaded thermosensitive hydrogel based on poly(N-isopropylacrylamide) polymer is a promising sustainable delivery system for cancer therapy.

Keywords: Temperature-responsive hydrogel, Controlled release, Anticancer drugs, BAMLET, Injectable hydrogels.

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The combinatorial use of quantum mechanics (QM) along with molecular dynamic simulation (MD) to design novel inhibitors of MTH1

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According to many studies, there exists a direct association between cancer and the loss of balanced redox homeostasis. Moreover, when the level of the cellular production of the oxidants such as reactive oxygen species (ROS) rockets, the damage to the cell will be inevitable. The ROS are essential in oxidizing the nucleobases in the free deoxynucleotide triphosphate (dNTP) pool. One of the leading products of ROS is 8-Oxo-2'-deoxyguanosine. The insertion of 8-Oxo-2'-deoxyguanosine into the DNA structure can prevent tumor growth [1]. On the other hand, MTH1, also known as human NUDIX hydrolase, sanitizes the nucleotide pool of 8-oxo guanine triphosphates by hydrolyzing the oxidized purine nucleoside triphosphates to their monophosphates and pyrophosphates forms. In the first stage, 8-oxo-dGTP is converted to 8-oxo-dGMP by the intervention of MTH1. 8-oxo-dGMP is further converted to its corresponding nucleoside 8-oxo-dG [2]. 8-oxo-dG cannot be incorporated into DNA structure. It should be noted that exposure to high oxidative stress levels is typical in cancer cells, leading to high levels of the accumulations of the oxidized bases and nucleotides in their nucleotide pools, such as 8-oxo-dGTP. One of the strategies of the cancer cells to escape from apoptosis is the overexpression of MTH1 to eliminate 8-oxo-dGTP [3]. Thus, MTH1 can be a potent target for anticancer drug design. Studies have revealed that crizotinib can inhibit the activity of MTH1 (crizotinib is also in clinical usage and is considered a tyrosine kinase inhibitor) [4]. Many side effects such as persistent unilateral non-inflammatory conjunctival chemosis for crizotinib have been reported [5]. As a result, in this study, we designed novel and non-toxic inhibitors of MTH1, which are based on natural products. The combinatorial use of quantum mechanics (QM) and molecular dynamic simulation (MD) has been used in this study to exactly signify the inhibition of MTH1 by the novel designed drugs and compare them with the known inhibitors.

Keywords: MTH1, Reactive oxygen species, Non-toxic inhibitors, Molecular dynamic simulation

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A Pseudohomogeneous Nanocarrier Based on Carbon Quantum Dots as an Efficient Gene Delivery Vehicle

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A pseudo homogeneous carrier as an emerging term refers to subnanometric carbon-based vehicle with a high ability to interact with genetic materials to form stable carboplex and successfully transfer them into the cell which will result in inhibiting or expressing of therapeutic genes. Chitosan is a non-toxic polyaminosaccharide [1,2] used as a precursor in the presence of citric acid to produce carbon quantum dots (CQDs), which decorated with arginine as a surface passivation agent with high amine density in hydrothermal methodology. In this regard, the carboplex are formed by electrostatic conjugating of Arginine-CQDs with DNA to protect it from enzymatic degradation. Moreover, the carboplex, like the chitosan precursor, has not shown toxicity against AGS cell line. Interestingly, the Arginine-CQDs have exhibited an excellent ability to overcome cell barriers to deliver into cells compared to chitosan at the same weight ratio. The Arginine-CQDs/pEGFP (W/W) nanocomplex, not only lead to transfection with a relatively higher efficiency than PEI polymer, which is the "golden standard", but carboplex also demonstrates no significant toxicity. Indeed, the EGFP expression level has reached to 2.4 ± 0.2 via Arginine-CQDs carboplex at W/W 50 weight ratio. To the best of our knowledge, this is the first report includes chitosan-based CQDs functionalized by arginine which is applied to serve as a pseudo homogeneous vehicle for gene transfection.

Keywords: Nanocarrier, Carbon quantum dots, Chitosan, Gene delivery vehicle.

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Synthesis and Characterization of Arginine-Decorated polymer dots for loading and protection of DNA from enzymatic degradation

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Chitosan is a non-toxic polyaminosaccharide [1,2] used as a precursor in the presence of citric acid to produce polymer dots (PDs), which decorated with arginine as a surface passivation agent with high amine density in hydrothermal methodology. The Arginine-PDs are comprehensively characterized by Fourier-transform infrared spectroscopy (FT-IR), Ultraviolet–visible spectroscopy (UV–vis), Atomic force microscopy (AFM), field emission scanning electron microscope (FE-SEM), Energy-dispersive X-ray (EDX) mapping, fluorescence, High-resolution transmission electron microscopy (HR-TEM), zeta potential and X-ray powder diffraction (XRD). In this regard, for the first time, carboplex are formed by electrostatic conjugating of Arginine-PDs with DNA. In addition, the PDs show high ability for loading DNA and protect it from enzymatic degradation. This emerging 0-Ds particle open new avenue for DNA storage and treating genetic disorder.

Keywords: Polymer dots, Chitosan, DNA protection , Enzymatic degradation.

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Effect of Gd_2O_3/ZSM-5 nanocomposite on water protons relaxation rate

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Zeolites are crystalline microporous materials consisting of SiO_4 and AlO_4 with a wide range of applications in environmental protection, industry, and medicine. The porous structure of zeolites provides the possibility of their use as support for iron oxide nanoparticles in magnetic resonance imaging (MRI) [1-3]. The present study aimed to evaluate the effect of Gd_2O_3/ZSM-5 nanocomposite on water protons relaxation rate. Gd_2O_3/ZSM-5 nanocomposite was synthesized by hydrothermal method [4]. The XRD, SEM, and VSM tests were carried out to determine the structure, morphology and size, and magnetic property of the nanocomposite, respectively. Besides, an MTT assay was used to consider the effect of the nanocomposite on the cell viability, and MRI was performed to investigate the relationship between the 1/T1 relaxation rate and Gd^{3+} concentration of the nanocomposite. The nanocomposite showed a spherical shape, paramagnetic property, cytocompatibility, and linear changes of the water protons relaxation rate with Gd^{3+} concentration. The change of water protons relaxation rate using Gd_2O_3/ZSM-5 nanocomposite suggests the effective role of ZSM-5 support in contrast enhancement of the MRI images.

Keywords: Gd_2O_3, ZSM-5, MRI, Relaxation rate

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Development of Antimicrobial Bioactive Composite Containing Silver and Zinc Oxide Nanoparticles

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Self-cure composite resin is widely used in orthodontic treatment. However, tooth discoloration around the bonded areas in the form of white spot lesions are susceptible to bacterial adhesion and colonization [1]. Recently, synthesis of bioactive composite resins containing silver/zinc oxide (Ag/ZnO) nanoparticles and the effects on mechanical, cytotoxic, biocompatibility, and antimicrobial properties were reported [2]. The aim of this study was to investigate the antibacterial properties of a composite containing Ag and ZnO nanoparticles, separately. Ag and ZnO nanoparticles were prepared and characterized by X-ray Diffraction (XRD), Field Emission Scanning Electron Microscopy (FE-SEM), Energy Dispersive X-ray (EDX). The as-synthesized nanoparticles were mixed with composite and disc-shaped specimens were prepared and floated in separate culture media containing Streptococcus mutans, Lactobacillus, and Candida albicans. Addition of 1 and 3 wt% of nanoparticles caused colony reduction in all types of tested microorganisms about 94% and 100%, respectively. Antibacterial properties can help reduce the unfavorable odor of the mouth, decalcification and carious lesions.

Keywords: Ag, ZnO, Nanoparticles, Composite, Antibacterial properties

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Self-healing polymeric hydrogels based on PVA/cellulose/ Metal Organic framework and investigation of their pharmaceutical applications in wound dressings

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Wound dressings are coatings that are placed on the surface of the wound to protect wound cells from environmental factors and by preparing an environment similar to the body environment, provide the basis for the growth of fibroblasts and skin repair cells. Make it possible in a shorter time Skin repair. Natural and synthetic polymers are the most import ant materials used in the production of wound dressings these biomaterials can be used in various forms. Hydrogel dressings are one of the most important forms of this biomaterial. Hydrogels are three-dimensional structures with hydrophilic functional groups that are able to absorb large amounts of water without dissolving them. Hydrogels have been used as wound dressing, due to their high biocompatibility, high water content, low surface tension, and similar mechanical properties to the body. The cavities in the structure of these compounds have made the drug better placed inside them and therefore have received a lot of attention as a drug delivery system. But in addition to these benefits, direct loading of the drug into the hydrogel results in rapid drug release, and there is also the potential for drug degradation. Therefore, to reduce this limitation can be used nanocarriers such as organic-metallic frameworks (MOFs) [1-2]. The main goal of this project is to prepare a self-healing hydrogel wound dressing containing an organic-metal framework. To increase wound dressing biocompatibility, have been used cellulose as a natural polysaccharide with antibacterial properties and a suitable substrate for fabricating the metal-organic framework consisting of Fe and Ag core by solvothermal method. Then self-healing hydrogel was prepared by blending nanocomposite cellulose/MOF, poly(vinyl alcohol) (PVA), and borax. Also, curcumin was used to increase the antibacterial properties of the wound dressing. The stractures of this compounds were identified with Infrared Fourier transform (FT-IR), X-ray diffraction (XRD), thermal analysis (TGA) and SEM analysis.

Keywords: Hydrogel, Wound dressings, Metal organic frameworks curcumin

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Synthesis, characterization and cytotoxicity investigation of juglone palladium complex; Theoretical and biological properties of juglone as an employed ligand

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Metal-based chemotherapeutics, especially platinum complexes, are widely used in the treatment of various types of cancer. Recent studies have shown that palladium compounds have similar or even greater cytotoxic properties than platinum complexes. Juglone (5-hydroxy-1, 4 naphthoquinone), as a natural compound, has anti-tumor properties on various cancer cell lines. In this study, complex of palladium (II) with juglon and phenanthroline was synthesized and its cytotoxicity property on MCF-7 (human breast cancer cell line) were evaluated. The fluorescence images have been presented to detect the antiproliferative effect. The [Pd(Jug)(phen)]Cl complex was found to have more cytotoxic properties (IC_{50}: 5.2 μM) on MCF-7 cell line than juglone (IC_{50}: 12 μM). Furthermore, the interaction of the complex [Pd(Jug)(phen)]Cl with HSA, DNA and 2JVU has been investigated using molecular docking method. This compound is considered with potential of anti-tumor activity and can be a good candidate for the next stages of in vitro and in vivo screening

Keywords: Palladium complex, Juglone, Cytotoxicity, Molecular docking

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Microencapsulation of Saffron extract using spray drying technique and cellulose-based derivatives as wall materials

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Encapsulation technology has been widely applied to protect active compounds from environmental conditions. Saffron as the world's most expensive spice is very sensitive to the harsh conditions [1]. In this work, microencapsulation of saffron extract by various cellulose-based polymers such as ethyl cellulose (EC) and hydroxypropyl methylcellulose phthalate (HPMCP) was studied as an effective way to improve stability of its active compounds [2]. Emulsions with a constant ratio of saffron extract/wall material of 1:8, were prepared using a homogenization and then spray dried. Powders were characterized in terms of encapsulation yield, efficiency, and stability. The amount of picrocrocin, safranal and crocin after spray drying was analyzed by UV analysis at 250, 308 and 440 nm, respectively and confirmed by HPLC. The stability and release of loaded crocin, safranal, and picrocrocin in multiple emulsions were investigated over time and different storage conditions. The result showed the emulsion also provided a high protection of crocin, safranal, and picrocrocin in the gastric condition. In conclusion by using of this technique the stability of saffron extract has been improved [3].

Keywords: Microencapsulation, Saffron, Spray drying, Ethyl cellulose, Hydroxypropyl methylcellulose phthalate

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Discovery of natural selective inhibitors of the CYP11B1 enzyme for the treatment of Cushing's disease

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Cortisol is responsible for the inflammatory response of the immune system, the overproduction of which causes Cushing's disease, and its biosynthetic pathway is stimulated by glucocorticoid receptors and the activity of the enzyme cortisol synthase (CYP11B1)[1]. Cortisol synthase (CYP11B11) is structurally like aldosterone synthase (CYP11B2), which regulates blood pressure in the human body[2]. The use of selective cortisol synthase inhibitors, which have more negligible effect on aldosterone synthase, is a more selective treatment for Cushing's disease and causes fewer side effects for hypertension-related diseases[3]. Based on selective pharmacophores screening of around 10000 natural compounds obtained from the Zinc15 database. Over 10,000 natural compounds obtained from the Zinc15 database were selected for selective pharmacophore screening. Screening of these compounds based on selective pharmacophores showed 387 compounds that had a fitness score of ≥ 1.5 compared to the selected pharmacophore pattern and were selected to investigating their grid docking score. The Glide docking application with the extra precision protocol (XP) conducted the molecular docking with CYP11B1 receptor showed that more than half of the compounds revealed good scores ranging from -9.10 to -5.80 Kcal/mol. Ten ligands with the highest docking scores were selected for Induced Fit Docking (IFD) and molecular mechanics with generalized Born and surface area solvation (MM/GBSA) analysis. IFD docking results showed that selected compounds inhibit the CYP11B1 receptor well, but only 4 of these 10 ligands were able to selectively inhibit the CYP11B1 receptor and showed little interest in the CYP11B2 receptor. NP-5 (Zinc ID= 65057928) had the highest IFD score with CYP11B1 receptor and the lowest IFD score with CYP11B2 receptor. ADME and QSAR studies were also performed, and the result was that NP-5, as the superior ligand, could selectively inhibit CYP11B1 receptor.

Keywords: Cortisol synthase (CYP11B1); Aldosterone synthase (CYP11B2); Molecular docking; Pharmacophore

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Ultrasound and microwave assisted synthesis of bimetallic cellulose/Fe-Ag MOF as a nanocarrier

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Ultrasound and microwave assisted synthesis of material is a newly developed, rapid, economic and environmental friendly. The main advantage of this technique is in terms of simplicity, reduced reaction times and energy efficiency, high pressure and temperature in reaction. also metal-organic frameworks (MOFs) have received a lot of attention due to their unique properties such as permanent porosity and high surface area and abundant functionalities. in addition, biopolymers and composites have been widely used in designing controlled release systems due to their adjustable chemical composition, low cytotoxicity, and good biological recognition. Among different biopolymers, cellulose has been widely used in this area as the most renewable and abundant biopolymers in the world. the main purpose of this work is to use ultrasonic and microwave assistance to prepare bimetallic MOF / cationic cellulose nanocomposite by combining cationic cellulose and iron and silver salts and terephthalic acid as a cross-linker through a single-pot, efficient and simple method. This strategy leads to the production of drug carriers with suitable properties.The structure of the nanocomposite was confirmed by the FT-IR، XRD and SEM techniques.

Keywords: Metal-organic frameworks (MOFs), Cationic cellulose, Bimetallic MOF

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Self-healing polymeric hydrogels based on PVA/cellulose/ Metal Organic framework and investigation of their pharmaceutical applications in wound dressings

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Wound dressings are coatings that are placed on the surface of the wound to protect wound cells from environmental factors and by preparing an environment similar to the body environment, provide the basis for the growth of fibroblasts and skin repair cells. Make it possible in a shorter time skin repair. Natural and synthetic polymers are the most important materials used in the production of wound dressings these biomaterials can be used in various forms. Hydrogel dressings are one of the most important forms of this biomaterial. Hydrogels are three-dimensional structures with hydrophilic functional groups that are able to absorb large amounts of water without dissolving them. Hydrogels have been used as wound dressing, due to their high biocompatibility, high water content, low surface tension, and similar mechanical properties to the body. The cavities in the structure of these compounds have made the drug better placed inside them and therefore have received a lot of attention as a drug delivery system. But in addition to these benefits, direct loading of the drug into the hydrogel results in rapid drug release, and there is also the potential for drug degradation. Therefore, to reduce this limitation can be used nanocarriers such as organic-metallic frameworks (MOFs) [1-2]. The main goal of this project is to prepare a self-healing hydrogel wound dressing containing an organic-metal framework. To increase wound dressing biocompatibility, have been used cellulose as a natural polysaccharide Drug carrier and effective in dynamic rheology of hydrogels properties and a suitable substrate for fabricating the metal-organic framework consisting of Fe and Ag core by solvothermal method. Then self-healing hydrogel was prepared by blending nanocomposite cellulose/MOF, poly(vinyl alcohol) (PVA), and borax. Also, curcumin was used to increase the Anti-inflammatory and antioxidant properties of the wound dressing. The stractures of this compounds were identified with Infrared Fourier transform (FT-IR), X-ray diffraction (XRD), thermal analysis (TGA) and SEM analysis.

Keywords: Hydrogel, Wound dressings, metal organic frameworks curcumin

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Synthesis of drug carrier of pioglitazone-loaded polyethylene glycolated nanoliposome and evaluation of its in vitro release

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One of the main and common problems of people in terms of health related problems is type 2 diabetes mellitus. Type 2 diabetes mellitus consists of an association of disorders characterized by hyperglycemia and created from the combination of resistance to insulin action, shoartage of insulin secretion, and excessive or improper glucagon secretion [1]. Pioglitazone is a an insulin sensitising thiazolidinedione agent that has been used for the treatment of type 2 diabetes mellitus [2]. Besides this, there are some adverse effects of pioglitazone such as heart failure, peripheral edema, weight gain and immediate release that created some problems for the people when it comes to use this drug. To overome these obstacles, drug nanocarriers are used. Among different species of nanocarriers, nanoliposomes are one of the the great nanocarriers beacuase of their simple synthesis procedure, biocompatibility, lack of toxicity and non-immunogenicity. Besides, nanoliposomes have an amphiphatic properties which mean that they can be used for encapsulation of both hydrophilic and hydrophobic drugs [3]. However, conventional nanoliposome have some limitations to use, but the limitaions can be avoided through surface functionaliztion of nanoliposomes via polyethylene glycol. In this project, pioglitazone is loaded into polyethylene glycolated liposomal nanocarrier by reverse-phase evaporation method to enhance bioavailibility and decrease adverse effect of this drug. Physicochemical and morphological properties were evaluted such as TEM, SEM and DLS to inform the integrity of compound and in vitro release of that compound was estimated through dialysis bag technique to show the controlled release of compound.

Keywords: Diabetes mellitus, Pioglitazone, Polyethylene glycol

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Construction and optimization of chitosan nanoparticles containing the anti-cancer compound curcumin

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Cancer is one of the leading causes of death in the world. Cancer is caused by the uncontrolled growth of cells. Breast cancer is the third most common cancer in the world. Chemotherapy, radiation therapy, surgery, etc. are common methods for treating cancer. In these methods, in addition to cancer cells, healthy cells are also damaged. For this reason, they are looking for methods that purposefully transfer anticancer agents to cancer cells. For this reason, the targeted drug delivery in nano scale for treatment of cancer is examined [1,2]. In this study, chitosan nanoparticles were synthesized by ionic gelation method. To improve the synthesis and effective entrapment of curcumin (anti-cancer compound), the role of several factors including chitosan concentration, chitosan to TPP linker ratio and drug concentration were investigated [3]. Using spectrophotometric technique, FTIR analysis and electron microscopy (SEM), the fabrication of nanoparticles and the entrapment of curcumin in nanoparticles were confirmed. The results also showed that the highest rate of curcumin trapping occurs in the chitosan bed with one percent. The effect of using detergents such as Tween 80 had an adverse effects on the entrapment of curcumin in the nanoparticle, so that in the absence of Tween 80, maximum entrapment was observed, which is probably due to the severe hydrophobic properties of curcumin. Among the different ratios of chitosan to TPP, a ratio of 2 to 1 was the best for making nanoparticles and trapping curcumin. Also, chitosan nanoparticles showed better release of curcumin at pH and physiological temperatures in this ratio. At high and low concentrations of the TPP linker, the nanoparticle structure probably does not have the desired cross-linking to curcumin entrapment and its release [4].

Keywords: Cancer, Drug delivery, Chitosan, Curcumin

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Cyanoacetohydrazide linked to 1,2,3-triazole derivatives: a new class of α-glucosidase inhibitors

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Diabetes Mellitus (DM) is one of the most common diseases affecting million people worldwide. There are three main diabetes types, among which type 2 diabetes (T2DM) with over 85% of diabetics is known as the major type of DM. α-Glucosidase is an exocyclic enzyme hydrolyses the 1,4-α-glycosidic linkages of oligosaccharides and disaccharides to form monosaccharides. α-Glucosidase inhibitors slow down the digestion and absorption of simple carbohydrates in the intestine. 1,2,3-triazole based compounds were recently introduced as potent α-glucosidase inhibitor. In this respect, a novel series of hybrid 1,2,3-triazoles were designed and synthesized as α-glucosidase inhibitors[1]. Desired compounds were synthesized through a three-step synthetic pathway: (*I*) initially, reaction of 4-(prop-2-yn-1-yloxy)benzaldehyde derivative and freshly prepared azides derivative in H_2O/*tert*-BuOH at room temperature through click reaction[2]. (*II*) later compound obtained by the reaction of excess amount of hydrazine hydrate 6 and ethyl 2-cyanoacetate at room temperature. (*III*) The target compounds were synthesized by the reaction of compounds from the first step and 2-cyanoacetohydrazide in methanol in the presence of a few drops of acetic acid (HOAc) under microwave irradiation at 700 W for 10–12 min. In this work, we synthesized 14 novel compounds. All compounds were easily purified and characterized by IR as well as ^{1}HNMR and ^{13}CNMR. These compounds demonstrated considerable inhibitory activity against α-glucosidase compared to acarbose.

Keywords: 1,2,3-triazole, Diabetes, Hydrazides, Synthesis, α-glucosidase

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Predicting blood-brain barrier permeability via natural language processing

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To identify possible molecules that can be promising to be a new CNS drug, it is crucial to identify and predict the permeability of chemicals through the blood-brain barrier[1]. To predict the different properties of these molecules, fast and accurate models and tools are necessary due to rapid improvements and the development of new drug-like molecules through deep learning. There have been numerous models published to date to predict the permeability of molecules across the BBB. Nevertheless, most of them use the same approach. Therefore, we decided to implement natural language processing models in this case. For this purpose, we came up with two distinct approaches and four NLP models. Our first approach used SMILES strings of chemical molecules as input. As input, the second approach uses the IUPAC of those molecules. Each of these two methods contains two NLP models. For the IUPAC string, two different models were created. One is a Bert-based pre-trained model on a large IUPAC that we fine-tuned to our data. The other method is Bidirectional LSTM layers. For SMILES string, we also developed two different models. The first is a Roberta-based pre-trained model developed by deepchem[2]. we fine-tuned our data on it. Moreover, the other approach is Bidirectional LSTM layers similar to the IUPAC model. For implementing Bilstm models, we used the TensorFlow package. The SMILES and IUPAC strings were tokenized and fed to the NLP models using a chemical dataset containing 7807 chemicals (4956 BBB+ and 2851 BBB-). For the SMILES strings approach, the best performance was by the fine-tuned Roberta model, which achieved an overall accuracy of 85%, ROC-AUC score of 93%, sensitivity of 82%, and specificity of 88% on the test dataset. For the IUPAC string method, the best results were by the fine-tuned Bert model, which achieved an overall accuracy of 85%, ROC-AUC score of 92%, sensitivity of 77%, and specificity of 90% on the test dataset. All the code, models, and data are available at this GitHub. For using all the models easily, please use this colab notebook.

Keywords: Blood-brain barrier, Natural language processing, Deep learning, Drug design

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Design and synthesis of 2-(arylthio)-3-(*o*-tolyl)quinazolin-4(3H)-ones as anticancer agents

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Cancer is becoming one of the main causes of death worldwide. Anticancer agents have many side effects. Therefore, finding compounds with fewer side effects and greater efficacy has always been one of the challenges for researchers. Thioquinazolinone derivatives have various biological activities such as antimicrobial, anticancer, and anti-HIV.[1] In the present study, a group of thioquinazolinone derivatives was synthesized as anticancer agents. A mixture of anthranilic acid and 2-methylphenyl isothiocyanate in the presence of triethylamine was refluxed in ethanol at 80 ˚C for 4-5 h. After cooling at room temperature, the resulting product was filtered. The final compounds were synthesized by the reaction of thioquinazolinone derivatives with benzyl chloride derivatives in the presence of sodium hydroxide in methanol at room temperature.[2] A group of thioquinazolinone derivatives was synthesized in good yields and the structure of the compounds was confirmed by 1H-NMR, and ESI-MS. The anticancer activity of these compounds is under investigation.

Keywords: Thioquinazolinone, Anti-cancer, Synthesis.

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Drug-Drug interaction prediction using deep learning

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Prediction Drug-Drug interactions play an essential role in finding the side effects that can cause by taking multiple drugs simultaneously. These interactions can cause different side effects and reduce the effectiveness of those drugs. Predicting the drug-drug interaction before the prescribed plays a vital role in preventing hospitalization and any problems that can happen by those interactions. Using machine learning approaches is essential as the wet lab experiments can be insufficient and slow. We design a deep learning model based on Natural language processing(NLP) that can detect 86 drug-drug interactions with an outperformed accuracy. There have been similar approaches to solving this problem[1]. In this research, we use the Drugbank dataset provided by Therapeutics Data Commons[2]. The dataset contains 191,808 drug-drug interactions paired with 1,706 drugs. For this task, we develop a deep neural network based on the SMILES string of the input drugs. Each pair contains two drugs. Each SMILES string will first be tokenized and fed to a Roberta-based pre-trained model designed and trained by deepchem[3]. This model will have two Roberta encoders, each for one SMILES string as input. Next, the two outputs of those Roberta encoders will concatenate and be fed to three Dense layers. The last layer is for classification and has a shape of 86, equal to the number of classes for this multi-label classification task. To our knowledge, this neural architecture has never been tried by any other researchers. We train this model on a single P100 GPU on the Kaggle website. As a result, this model achieved an overall accuracy of 95% on the classification tasks that outperformed different methods for solving this problem. All the codes and models are available free of charge at this GitHub repository.

Keywords: Drug-Drug interaction, Natural language processing, Deep learning, Drug design, DDI

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Easy-to-understand study and training for energy storage in batteries, especially lithium-ion batteries

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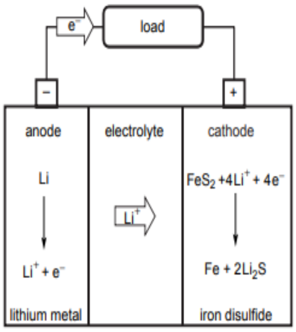
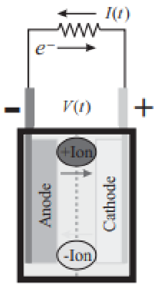
Cameras, laptops, cell phones, and cars have one thing in common - they all require batteries. Energy storage is vitally important to many applications, ranging from small-scale portable electronics to large-scale renewable energy sources. During charging, the negative electrode material dissolves in the electrolyte solution to form a positive ion and an electron in what is called an oxidation reaction. The positive electrode consumes electrons by depositing positive ions from the electrolyte in what is called a reduction reaction. The reactions are reversible in secondary (or rechargeable) batteries so that discharging the batteries returns the electrodes to their pre-charged states. The ions move through the electrolyte under diffusion and migration Li-ion batteries are commanding a greater market share owing to their high energy density, which makes them attractive for applications where weight or volume are important.They have a long cycle life and low self-discharge rate. Although a complete battery does not exist and may never exist, electrochemical engineers continue to invent new types with it. Step-by-step training with a conceptual understanding of electronic and ionic transitions in oxidation and reduction processes and then charge and discharge mode to store energy in batteries, especially lithium-ion batteries has been considered in this research.





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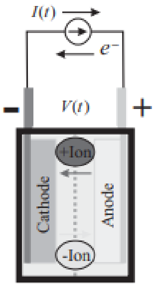
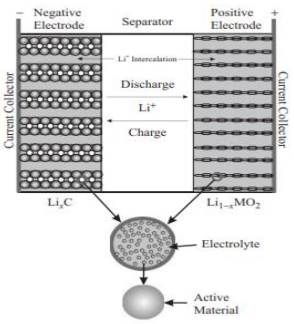


Charge



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Keywords: transfer, energy, Li-ion batteries, charging

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Organizing the learning of chemistry lessons in students using the mind map method

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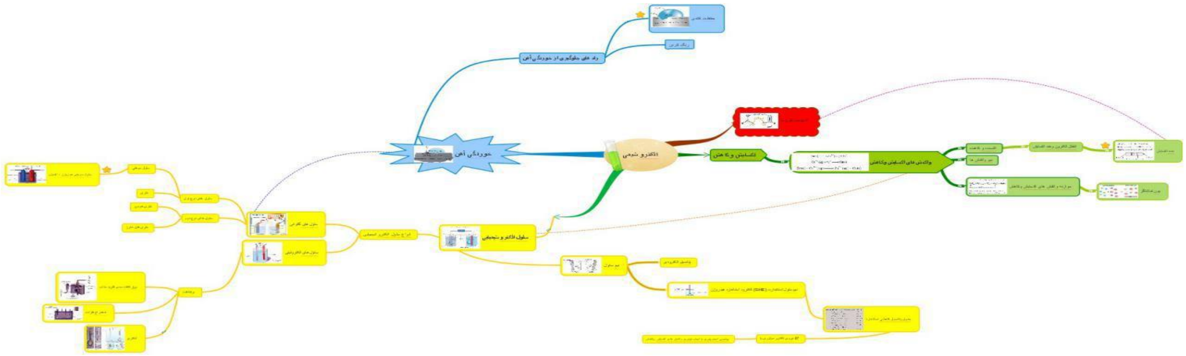
The best way to learn complex content is to organize the content**.** Learning content that is organized and relevant to what has already been learned is faster.They are scattered and unrelated and are easier to remember. Information stays in short-term memory better when categorized, As a result, the power of mental focus increases. Concept map template. The best type of mind map (animated concept map) is an example of a complex way of organizing content, which makesIt becomes more meaningful, strengthens the thinking and retains the content in the learners' memory.

A concept map is a set of concepts whose main purpose is to show a subject and facilitate its absorption. [1]. A concept map is a type of graphic organizer that is used.It helps students organize and demonstrate knowledge on a particular topic. Concept maps of an idea or The general concept of the beginning and then subdivided to show how an idea can be broken down into specific titles[2]. A mind map is a tree diagram used to express words, ideas, activities, or other things. Mind map design is very easy. It is enough to use one draw a circle or oval in the middle of the page and write the title of the subject in it. Then by adding branches different connected to the center, side threads are added. To draw a mind map various software are available including full software application can be mindmup, Xmind, iMind Map, Concept draw. , Microsoft office Visio pointed out in this Mind map research created for chemistry lessons by iMind Map software is. Sample mind map designed by the researcher with iMind Map software for electrochemical lessons:



Keywords: Mental organization, Concept map, Mind map, Meaningful learning

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The relationship between play and chemistry education

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The purpose of this study is to investigate chemistry education using games. In this article, the findings of researchers in recent years are reviewed to analyze them to make a general conclusion in this regard. This article was conducted by searching the English keywords of education, games, chemistry and organic chemistry in scientific databases and new articles were used for this study. The data of the articles were used to write the findings of this article and the findings of the research include 5 games about teaching different topics of chemistry and organic chemistry, each of which is briefly described. The results show that it is difficult to understand the topics of chemistry due to their abstraction, but it is possible to make this lesson sweet and enjoyable for students by implementing educational games along with teaching. These games also increase the collaborative work between students and increase their motivation to learn. In other lessons, educational games should be used so that students can learn the concepts with more interest and motivation.

Keywords: Chemistry Education, Games, Chemistry Teaching, Organic Chemistry

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Determine the density of liquids with a pycnometer and Hydrometer

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A- Determining the density with a pycnometer is a very accurate and simple method. They use liquids of known density, such as water. In this research, we use distilled and fluid water with a certain density for calibration, through which temperature-dependent density values are placed in a glass flask with a glass lid with a hair hole. This small hole fills the pycnometer and releases excess fluid from the top of the pycnometer. By knowing the weight of an empty and full pycnometer and the ratio of the mass difference to the volume of a pycnometer, it can be used in direct instruction to students in understanding density in this study.

B- Hydrometer, a device for measuring some properties of a liquid, such as its density (weight per unit volume) or specific gravity (weight per unit volume relative to water). The device consists essentially of a weighted, sealed, long-necked glass bubble that is immersed in the liquid being measured. Floating depth indicates the density of the liquid, and the neck can be calibrated to read density, specific gravity, or some other related characteristic.

Keywords: pycnometer, hydrometer, Density determination of liquids

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An inquiry of the upheavals carried out by universities and chemical institutes in the course of the corona virus pandemic

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Since, the onset of the corona epidemic education procedures were transferred to virtual platforms. To nurture public health and preserve the principle of social distance this conclusion came to being. Hence, universities and chemical establishments throughout the world were required to provide education in various forms. These techniques should guarantee dynamic learning, maintaining student`s participation in education procedure, providing absolute course content, fabricating practical and laboratory capabilities, and finally students' analytical skills during this category of training. Arrangements based on such conditions made teachers and the students to face serious and new provocations. Teachers had to submit the content of the lessons with the help of online and virtual teaching implements on the Internet, while maintaining their best correlation with the student, creating interest in the session and maintaining their participation during the teaching process; On the other hand, the students to learn well in this new context, they have to be vigorous and disciplined in order to follow the lessons [1]. Virtual education in the pandemic time has led to the flourishing of virtual methods using the benefits and capabilities in the field of chemistry education [2]. In this paper, we intend to examine the different methods of virtual education and their impact on student`s comprehension of chemistry. Our focal point in this article is to look at the successes and challenges that have arisen in the virtual chemistry education path and the obstacles to the realization of this form of tuition, especially in laboratory lessons. In addition, this study can provide informators with superior and more utter course materials and helps executives of universities and educational establishments planning more sufficiently during such times [3].

Keywords: Corona Virus, Chemical Education, Virtual Reality

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The effect of using educational software on and memorizing the chemistry course of the second year of high school

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According to the document of fundamental change, by producing and using electronic content in accordance with the needs of students and schools and making it electronic Update the content of textbooks for teaching methods to improve faster learning and retention of information. In a study entitled the effect of the use of educational software (educational multimedia) on learning and memorization of elementary school mathematics.The results showed that the method of using educational software has a positive effect on learning and memorizing mathematics compared to the traditional method [1]. In another study, the use of teaching aids in increasing students' learning compared to the traditional method is significantly different [2].

The purpose of this study was to evaluate the effect of using educational software on students' learning and memory in the subject of electrochemistry in the course of chemistry in comparison with the traditional method. This research is applied in terms of purpose and in terms of quasi-experimental method and its sampling method was simple random. This research was conducted in the fifth district of Tabriz and in a girls' high school. The number of samples was 60, of which 30 were in the experimental group and 30 in the control group. The method of using researcher-made educational software was used for the experimental group and the traditional teaching method was used for the control group

In this research, researcher-made pre-test and post-test tools have been used. Pre-test was performed on students before the performance and the analysis of the results using the test showed that the two groups were not significantly different. At the end of the performance, both groups underwent a post-test under the same conditions. Analysis of the results using dependent t-test and analysis of covariance showed that the two groups were significantly different. After one month, a retention test was taken from them, which showed that the group trained with the software were significantly different from the control group. Therefore, the results showed that the method of using educational software has a positive effect on learning and memorizing chemistry lessons compared to the traditional method.

Keywords: Educational software, Training, Learning, Memorization

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Analysis of Students' Misconceptions about Chemical Bond Concepts: A Meta-Synthesis Study

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Misconception is defined as a different idea, concept and subjects' thought that is different with scientific conception [1]. The literature called misconception as misunderstandings, naıve conceptions, and alternative conceptions [2]. Unfortunately, chemical bonding is an abstract concept for learners to grasp and this can lead to misconceptions. The concept of chemical bonding also related with another concept such as thermochemistry, chemical equilibrium, and others. The lack of concept in chemical bonding will influence the next topics related each other. Therefore, the need for a correct understanding of abstract scientific concepts of chemistry by learners caused the present study. The aim of this study is to investigate the students' understanding about some aspects of the chemical bond and to determine their related misconceptions. The research methodology is a meta-synthesis approach. This qualitative meta-synthesis employed systematic review of literature data bases according to Sandelowski and Barroso's seven steps [3]. This study synthesizes 22 years (2000-2022) of research on chemical bonding misconceptions. After careful examination of the literature, several factors have been found to be responsible for the students' chemical bonding misconceptions.

Keywords: Chemical bonding, Misconception, Meta-synthesis

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Science education through debates: case-study in Azerbaijan

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The competence-based high school education demanded modification of content, goals and technologies of process. So, modern interactive technologies in science education form satisfied conditions for implementation of competency orientated programs [1].

As known, the innovative educational models applied on activation of mental functions, generation of learning and academic speech [2].

The innovative educational models applied on activation of mental functions, generation of learning and academic speech. Debates have also been used as an educational tool in various scientific disciplines. In the manuscript [3] author points out: “I have been pleased by how much students enjoy and report learning benefits from using student mini-debates. Retrospectively, this shouldn’t be surprising as one of the pillars of how students learn is metacognition-thinking about thinking. Student mini-debates provide an important opportunity for students to scrutinize their thinking about scientific concepts and practice “talking science.” Despite the above, studies dedicated to science debates are not that many.

Presented research was carried out among 2nd year education bachelors of chemistry faculty on speciality “Chemistry teacher” of Baku State University. For the formation via chemistry education of the basic educational competences, debate interactive technology applied. The control and experimental groups were established. The questionary and observation were used for control the experimental results.

The research showed the high effectiveness of debate educational technology for formation various important skills must gained by bachelors. There have been several positive developments over the period of lessons: critical thinking skills and the ability to express thinking, capacity to find contradictions in topics, build a defense against attacks, formulate own arguments, look for and find imbalances, listen to counterarguments etc.

It also be concluded that the greatest possibilities of the debate methodology are covered using them as an element of the lesson: in the process of updating knowledge, systematizing and consolidating the material, providing "feedback" or organizing students' independent work. The use of debate as a form of lesson requires a lot of advance preparation and the inclusion of all students during the lesson.

Keywords: chemistry, education, debates, interactive, technologies

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Study and development of research tools in chemistry education

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In the field of educational research, more researchers are using many tools to answer a wider range of questions in chemistry education. This study provides an overview of issues and tools related to chemistry education research projects. The goal is to highlight existing information that may be useful to people involved in chemistry education research projects. For convenience, the content is organized into four sections[1]. Qualitative research strategies. Quantitative analysis of research data; Cognition-based tools for chemistry in education research. Applied topics for planning, conducting and publishing chemistry education research have been used in this research and Important areas that are rarely addressed in other projects are practical issues with how to plan, conduct, and disseminate chemistry education research. While the importance of careful design and planning for data collection and analysis is emphasized in this study, this is generally done in terms of ensuring data quality[2].

Keywords*:* tools in chemistry, Cognition-based, chemistry education

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Nanoscience Education for High School Students; Insight Into the Strengths and Weaknesses of the High School Chemistry Curriculum

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Nanotechnology is a relatively new interdisciplinary STEM field that integrates concepts from chemistry, engineering, physics, biology, or more and is foundational for all sector of the economy. Job opportunities are expected to be created in the near future that require familiarity with nanotechnology, therefore students' familiarity with nanotechnology should be started from school, so that even those who do not enter the university can be beneficial in these jobs [1]. Because at the high school curriculum, chemistry is most relevant to nanoscience, we investigated the connection dots between high school chemistry and nanoscience, in chemistry books of the ministry of education of Iran, to identify the strengths and weaknesses.

To teach nanoscience, two basic concepts must be introduced; 1) size and scale, 2) surface area-to-volume ratio (SA/V) [2]. In the case of first concept, In Chemistry 1 book, the student is first introduced to the structure of atom and discret energy levels, the student learns to compare the continuous energy content with the discret energy levels that leds to the linear emission spectrum. The properties of nanomaterials can be expressed between bulk material and atoms, so that as the dimensions of the material become smaller, their behavior tends to that of atoms, and the discrete energy levels appears in nanomaterials too. The crystalline structure of materials is discussed in Chemistry 3 book, by adding a small portion, nanomaterials can be defined there. In the case of SA/V, the related topics are discussed in chemistry 2 book, with titles such as calculating the surface-to-volume ratio, comparing the burning of iron powder with the red glowing of bulk iron, and some ther examples. Some other topics related to nanoscience include semipermeable membranes, macromolecules, colour of gold colloid, lithium ion batteries, graphene, pigments, finer ceramic mesh sizes in car's exhaust catalysts, or even subjects such as light and light interactions with materials that can be used to characterization of materials, are mentioned in high school chemistry curriculum. But unfortunately, nanomaterial is not mentioned in any of the cases, and even nanomaterial word is not mentioned in high school chemistry . Considering the potential of high school core courses and existing experiences [3], we suggest a nanoscience education booklet that covers the topics of high school chemistry, physics and biology be prepared and included in the curriculum. Better results are achieved when the 5E learning cycle is followed. For this purpose, the Ministry of Education and schools must provide the necessary facilities.

Keywords: High school, Nanoscience, Chemistry Curriculum

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Conceptual Mapping Approach and Learning of Atomic Orbitals

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One of the key aspects of learning is the acquiring and integrating the old and new sciences which entails acquiring process and new learning skills [1]. There has been a continuous focus on exploring new teaching strategies to improve the understanding of concepts. Several studies investigated the effectiveness of composite use of concept maps and traditional method on student achievement in selected topics in chemistry [2].

A concept map is a two dimensional diagramming that emphasises the relationship between concepts. According to many researches, concept mapping is one of the best instructional tool that can be used by teachers to generate a meaningful learning. The potentials of concept mapping motivated the researcher to study the effectiveness of it as a tool for teaching chemistry [3].

This study investigates the effects of concept mapping on learning Atomic Orbitals. The research was conducted with a total of 40 students enrolled in inorganic chemistry course at Farhangian University. In this research, a questionnaire about atomic orbital concepts were used as data collection tools [4]. It was established that concept map has positive effect on the students' learning. Therefore, chemistry educators will have a creative field to use the various concept map and facilities the educational environment in chemistry classes.

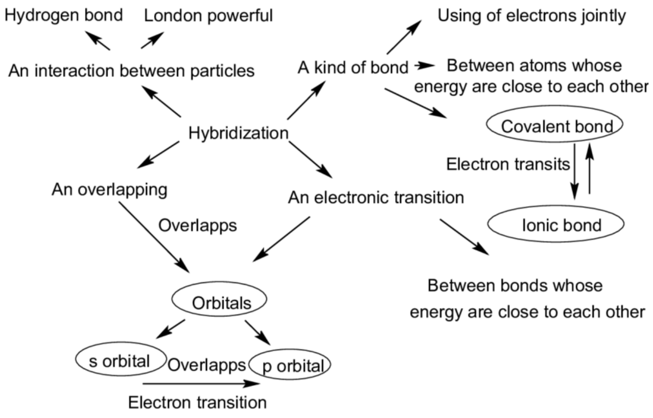

Fig 1. Students' description map of hybridization [5]

Keywords: Concept mapping, Atomic orbitals, Learning

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Teaching Chemistry using POGIL Activity: A Systematic Review

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Traditional teaching methods have not been successful in making beneficial changes in learners' perceptions. Although traditional teaching methods may be successful in transferring the facts, laws, processes, and models of a field, they are ineffective in helping learners construct their own beliefs about scientific concepts [1]. According to Johnstone, in order that learners can learn the abstract concepts of chemistry, chemistry teachers must macroscopy the learning process, resulting in reduced load of working memory [2]. POGIL (Processes Oriented Guided Inquiry Learning) model is a guided method in which the content and process of learning are in a path where learner's success is not blocked with alternative concepts. Due to a need to advance chemistry teaching in bachelor level of education, the POGIL pedagogy was developed with the investment of the National Foundation Science [3]. POGIL was first developed for bachelor chemistry courses in 1990 [4] and was extended to high school chemistry and biology classes. POGIL philosophy is based on a learner-based research and the kind of pedagogy of science in which students are guided in small groups on an exploratory path with the help of carefully designed activities to construct knowledge of chemistry [5].

The aim of this study was to investigate the effect of POGIL method in reducing students' misconception about chemistry concepts. The research approach is systematic review and the statistical population includes all related research from 2000 to 2020, which is systematically searched from the databases of Persian publications. The statistical population included all findings showed that POGIL pedagogy, has positive effect on correcting students' misconception of chemistry concepts. Based on the results and due to the effectiveness of POGIL teaching on correcting students' misconceptions, educators can use this method in chemistry classes according to the subject and the characteristics of the audience.

Keywords: Misconception, Chemical concept, Active learning, POGIL

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Processes Oriented Guided Inquiry Learning and Chemistry Perception in Virtual Classes

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According to Johnstone, in order that learners can learn the abstract concepts of chemistry, chemistry teachers must macroscopy the learning process, resulting in reduced load of working memory [1]. Processes Oriented Guided Inquiry Learning model is a guided method in which the content and process of learning are in a path where learner's success is not blocked with alternative concepts. Due to a need to advance chemistry teaching in bachelor level of education, this pedagogy was developed with the investment of the National Foundation Science [2]. Processes Oriented Guided Inquiry Learning philosophy is based on a learner-based research and the kind of pedagogy of science in which students are guided in small groups on an exploratory path with the help of carefully designed activities to construct knowledge of chemistry [3]. This pedagogy could be improve students' learning in virtual classes (Fig. 1). The aim of this study was to investigate the effect of Processes Oriented Guided Inquiry Learning method in improving students' perception about chemistry concepts in virtual classes.

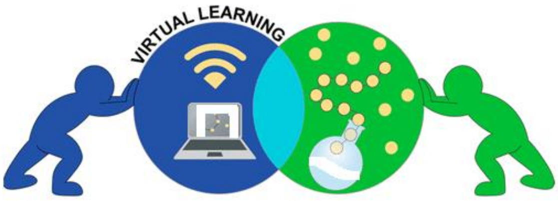

Fig 1. Learner-based education in virtual classes

In this descriptive-cross-sectional study, the success rate of the Processes Oriented Guided Inquiry method was extracted based on the chemistry concept type and class form. The data were extracted from the national and international documents between 2019 and 2022. Data were analyzed using descriptive statistics. Based on the results and due to the effectiveness of Processes Oriented Guided Inquiry Learning teaching on correcting students' misconceptions, educators can use this method in chemistry classes according to the subject and the characteristics of the audience.

Keywords: Chemical concept, Learner-based approach, Virtual classes

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A novel and highly-sensitive electrochemical-based genosensor applying perovskite-graphene oxide nanocomposite for determination of miRNA-21 as a significant biomarker for rapid diagnosis of gastric cancer

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MiRNAs are important regulatory micromolecules in gene expression that regulate gene expression by interfering with intracellular messenger RNA (mRNA). MiRNAs can be used as diagnostic biomarkers in the diseases, especially cancer detection. There are many clinical techniques for detecting miRNAs. The most important of them are microarrays and qRT-PCR that the limited linear quantification range, imperfect sensitivity for long sequence homogeneity, and the inability to detect new miRNAs and to determine the abundance of miRNAs are the disadvantages of the miRNA microarray detection techniques and for qRT-PCR its high cost and the need for a computing infrastructure to analyze and interpret data.[1] Therefor, due to the disadvantages of these clinical methods, attentions has been gained on developing biosensing assay. Electrochemical biosensors are fast, sensitive, selective, and low-cost analytical instruments that allow the evaluation of very low levels of sample in the bloodstream with the minimum requirement for sampling volume and are compatible with the multiplex capabilities of a diagnostic test.[2] In this study, an electrochemical oligonucleotide genosensor was developed to detect and measure miRNA-21. To achieve this goal, perovskite and graphene oxide multilayer nanocomposites were produced. The obtained nanocomposite was immobilized on the surface of the working electrode. The single-stranded RNA probe was then immobilized on the electrode. The interaction of the RNA probe with the target miRNA affects the electrode or the interphase function. Electrochemically active reporter changes in electrode properties due to miRNA hybridization to signal. As a result, it is possible to identify and detect miRNA in the sample. Using this technology, we were able to detect miRNA-21 sensitively with a low limit of detection, with a linear range of 1 fM to 1 nM and limit of detection 0.13 fM. The results were also confirmed by examining real samples. In addition, the designed biosensor had a special selectivity against the mismatches.

Keywords: Genosensor, MiRNA-21,Electrochemical, Perovskite

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Simple and Precise Protocol to Assess Trypsin Activity in Biological Samples

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Trypsin is a digestive enzyme that assists in the digestion of food. The small intestine contains trypsin. Fungus, plants, and bacteria may all be used to produce it. However, it is mainly manufactured for commercial uses from livestock pancreas. Serum trypsin determination seems to be a specific diagnostic for acute pancreatitis. In clinical diagnostics and drug research, it's critical to develop innovative detection techniques for trypsin activity assays.

A simple spectrophotometric procedure for trypsin, a protease generated in the pancreas, was developed in this study. Trypsin could preferentially cleave cytochrome c, a fundamental component of trypsin, into heme–peptide fragment. The resulting peroxidase-like activity catalyzes the oxidation of 3,3′,5,5′-tetramethylbenzidine (TMB) in the presence of hydrogen peroxide. This produces a blue-colored product with a maximum absorption wavelength of 620-525 nm. We used the Box-Behnken design (BBD) with response surface methodology (RSM) as an index of assay precision to optimize the synthesis of a blue colored product. In matched samples, this new method was compared to a Bland-Altman plot study of trypsin activity using the standard method.

With a detection limit of 0.5 IU/L, the procedure was able to measure trypsin in the range of 2–250 IU/L. For the assessment of 100 IU/L trypsin solution, the protocol exhibited improved accuracy, with a relative standard deviation of 1.4 percent. This protocol was used to investigate the inhibitor of trypsin, and the IC50 values for benzamidine hydrochloride were determined to be 2.2 g/mL, suggesting its potential use in drug development and disease treatment. Our research showed a simple, simple, low-cost, sensitive, and selective protocol for assessing trypsin enzyme that may be utilized to investigate its clinical value and pharmacological interference.

Keywords: Box-Behnken design, Trypsin activity, Response surface methodology, Spectrophotometry, Tetramethylbenzidine

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An Optimized Method to Estimate the Glutaminase Activity in Biological Samples

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Background: Spectrophotometric methods have been used to estimate glutaminase activity, using diverse reagents to form colored complexes that absorb light within the visible spectrum. The current study describes a simple, precise, and accurate protocol for measuring the activity of glutaminase, is an important enzyme in the glutamine hydrolysis and is also responsible for the modification of glutamine metabolism.

Methods: The current protocol assesses glutaminase activity by incubating glutaminase samples at 37°C for 30 min with suitable concentrations of glutamine dissolved in a buffer (pH 8.6). The enzymatic reaction contains suitable activity of glutamate oxidase, which acts to convert glutamate to hydrogen peroxide and 2-oxoglutarate. After the incubation period, a working solution that contained vanadate (V) and pyridine-2,6-dicarboxylic acid was added to stop the enzymatic reaction.

Results: The reaction between undissociated hydrogen peroxide and the added reagent forms a stable orange-colored chelate complex known as oxo-peroxo-pyridine-2,6-dicarboxylato-vanadate (OPDV) that demonstrates maximum absorbance at 435nm. To optimize the formation of the method (the OPDV-Glutaminase assay), we applied the Box-Behnken design (BBD) by utilizing the response surface methodology (RSM) as an index of precision of the assay. This novel method was validated against a Bland-Altman plot analysis of catalase activity using the Nessler method in matched samples.

Conclusion: The comparison between the two methods resulted in a correlation coefficient equal to 0.99, demonstrating that the new method is just as effective as the reference method.

Keywords: Box-Behnken design, Glutaminase activity, Pyridine-2,6-dicarboxylic acid, Response surface methodology, Spectrophotometry,vanadate (V).

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The enzymatic and Non-Enzymatic Effects of Secretion Phospholipase A2 and Relationship with Some Anti- Oxidant and Vitamin D3 in Asthma Patients.

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Phospholipases A2 (PLA2s: 3.1.1.4) are an important enzyme which lead to asthma, through two pathways, which includes; enzymatic mechanism which release arachidonic acid from phospholipid. Arachidonic acid (AA) aids in the synthesis inflammatory compounds including leukotrienes, thromboxane, and prostaglandins. While, the second mechanism is not related to enzymatic activity, through which it is linked of enzyme (sPLA2) to the M-type receptors, located on the cell membrane. This spur the inflammatory cells to excretion two types of cytokines, interleukin-6 (IL-6) and tumor necrosis factor-α (TNF-α). IL-6 stimulates interleukin-13(IL-13) which increases the secretion of mucus. While, TNF-α stimulates of epithelial cells to produce inducible nitric oxide synthase (iNOS) which act on liberation nitric oxide NO which plays an important role in the onset of symptoms of asthma. This study involved 80 participants, with 40 of these patients suffering from asthma, 40 healthy individuals were also involved from different age groups. A variety of tests were performed using ELISA and Spectrophotometry, included (total IgE, TNF-α, IL-6, sPLA2-X, sPLA2-llA, Superoxide dismutase (SOD), iNOS, Catalase (CAT), Malondialdehyde (MDA), calcium, and vitamin D3) By the SPSS statistics program.The observed data indicated a positive relationship between the level of IgE and the level of sPLA2-X (r = 0.535). There is also a positive correlation between IgE and TNF-α (r = 0.255), while, an inverse relationship between IgE and vitamin D (r = -0.5). The study also showed a positive relationship between the level of IgE and the level of (iNOS, and CAT) (r = 0.542, r=0.46,) respectively. The data also showed a positive correlation between the level of sPLA2-X and the level of cytokines (TNF-α, IL-6) (r = 0.235 , r = 0.565) respectively. While, the study indicated an inverse relationship between sPLA2-X and vitamin D (r = -0.49). There is also a positive correlation between the level of sPLA2-X and the level of the iNOS, and CAT (r=0.416,r=0.392)respectively.

Keywords: Asthma, sPLA2-X, sPLA2IIA, iNOS, D3, SOD, CAT, MDA, Calcium.

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Design of a developed optical system to estimate the activity of the enzyme superoxide dismutase (SOD) by optical reaction

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Superoxide dismutase (SOD) enzymes are mineral proteins found in all cells whose metabolism is dependent on oxygen metabolizing cells. (SOD) has various types of isoenzymes related to organ location and organism type, such as Mn-SOD, which was found in the cytosol and mitochondria, and Cu-Zn SOD, which was also found in the cytosol of advanced cells. Instead of the traditional method, a new design of radiation source was utilized in this study: an aluminum box with dimensions of 75x50x20 cm, equipped with two Led lights as the source of light emitted with 20 watt each.At a temperature of 25°C, the intensity of light for a 10-minute illumination is 5596x10-9 Einstein * sec-1 *L-1. (When compared to prior techniques that used gamma rays as a source of radiation, the new design technique yielded more results.) The nitro blue tetrazolium competed with SOD on O2•-, and the activity of SOD was determined based on the half-inhibition, which was 37 percent. SOD enzyme activity was found in serum at pH 7.8 of phosphate buffer. The less sample volume of serum was used to estimate of SOD activity is 150μl.

Keyword: Super oxide dismutase activity, Photoreaction of SOD. Riboflavin, NBT.

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Syntheses, antimicrobial activity and spectroscopic studies on the interaction of calf thymus DNA of cupper(II) and nickel(II) complexes

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Two proton-transfer metal–organic compounds that formulated as, [Cu(pydc)2].3H2o (1) [Ni(pydc)2].3H2o (2) synthesized and characterized by elemental analysis single-crystal diffraction, infrared spectroscopy, TGA/DTA and antimicrobial studies, where pydc is pridine-2,6-dicarboxylic. Microbiological activity of complexes were studied against some bacteria and fungus. It is to be noticed that both complexes exhibit the best antimicrobial activity with a large spectrum and the lowest MIC values for all bacterial as well as the fungal tested strains. These complexes under investigation is shown some antibacterial behavior, which is more pronounced against S. marcescens than other five organisms for both complexes in antibacterial activity and is more active against S. cerevisiae in antifungal activity for complex (1) .The action of the complexes on Gram- positive is better than Gram-negative bacteria.Therefore Ni (II) compound is more toxic against bacteria with MIC of 16 µg/ml, IZD of 18mm and Cu(II) compound is more toxic against fungi with MIC of 32 µg/ml, IZD of 16mm. .The interaction of native calf thymus DNA with this complexes has been investigated by absorption, emission, circular dichroism, melting temperature (Tm) curves and viscosity studies. Spectrophotometric studies of the interaction of this complexes with DNA have shown that it can binds to CT-DNA and the DNA binding constant (Kb = (4.9 ± 0.1) × 103 M-1) for complexe (1) and (Kb = (4.8 ± 0.2) × 103 M-1) for complex (2), is comparable to groove binding drugs. Competitive fluorimetric studies with hoechst 33258 have shown that two complexes exhibit the ability to displace the DNA-bound hoechst 33258 indicating that it binds to DNA in strong competition with hoechst 33258 for the groove binding.

Keywords: Proton-transfer, Microbiological activity, Groove binding, DNA interaction

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Relationship of the serum Electrolytes Level with Echocardiographic parameters and risk factors in Patients with Acute Coronary syndrome

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Acute coronary syndrome (ACS), a common complication of coronary heart disease. Serum electrolytes changes in ACS have not been studied extensively and there is paucity of information in the literature in this regard, electrolyte imbalance is one of the probable causes of ventricular tachycardia in patients with ACS.Materials and Methods: 143 people were included in study divided to 93 patients and 50 as control groups. Study group comprised confirmed diagnosis of recent onset of ACS. The blood samples of both groups were analyzed for Serum electrolytes (Na+, K+) by flame-photometry (Bio-Lab Diagnostic kit). Serum levels of glucose and lipid profile were obtained by calorimetry. Results: There was statistically significant increase in serum sodium and potassium levels in study group compared to control group. The mean□SD value of serum sodium and potassium concentrations was found non-significantly higher in Female group than Male group, (P-value=0.3). t- test revealed there was non significant difference in the mean ±SD levels of serum sodium and potassium in the presence or absence of diabetes mellitus, Dyslipidemia, Hypertension, Smoking, and obesity, there were non-significant difference in mean ±SD values of serum Na and K levels among stages of diastolic dysfunction. The mean □ SD values of serum sodium and potassium concentrations were increased with increase MR severity.The study showed that there was non-significant positive correlation between age values and serum k levels (r = 0.2) (P= 0.1), while there was non-significant negative correlation between age values and serum Na levels (r = - 0.04), (P = 0.8). Non-significant inverse relationship was noted between serum Na, K concentrations and left ventricular ejection Fraction (LVEF). Conclusion: Early assessment of serum electrolyte concentration is needed in order to implement proper supplementation and serve as important aid in diagnosis of ACS. The value of serum sodium and potassium concentrations increased with increased MR severity. The value of serum sodium and potassium concentrations was found non-significantly difference in the presence of risk factors.

Keywords: Echocardiographic parameters, ACS

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Association of ATP1A2, rs373796693 Gene Variant with Preeclamptic Patients in Placental Tissue

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Preeclamptic is a human pregnancy-specific disorder defined by the appearance of proteinuria-related hypertension after the twenty weeks of gestation in a previously normotensive woman and entirely cured by the sixth postpartum week. It is the main cause of morbidity and mortality during pregnancy. It is a multisystem sickness, but its etiology is unknown. Preeclamptic has been associated with system anomalies, such as ion transport deficits in neonatal, maternal, and placental cell lines.

This is the first study in Iraq, the objective is to evaluate the relation of rs373796693 variant with preeclamptic and study the sequence of gene alpha 2 to obtain genotyping, by conducting a case-control association study. This study was consisting of 90 cases that were divided into two groups, 50 normal pregnancies (control), and 40 preeclamptic (patients). For genotyping, we designed and optimized a ‘polymerase chain reaction- single strand conformation polymorphism (PCR-SSCP) method with the presence of internal splicing. While the sequence employed by sending the PCR products of ATP1A2 gene to macrogen company in Korea for performed DNA sequencing. The results were analyzed using the statistical package for social sciences (SPSS®) software version 28.0. A p-value of ≤ 0.05 was considered significant.

The results of the genetic test showed that there was no significant allelic or genotypic association recorded between patient and control groups for the gene studied. While the sequence data for gene ATP1A2 (rs373796693) showed TCCT deletion in the investigated samples.

Keywords: Preeclamptic, ATP1A2, Rs373796693, Sequence, PCR-SSCP.

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Ultra-fast colorimetric detection of Glutathione by CeO2 nanozyme

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In this study, we presented a colorimetric sensor based on CeO2 nanostructures to detect glutathione (GSH), an important biological thiol in cells involved in many physiological processes in the organism and regulates the pathological processes of cells [1]. Several analytical methods are currently available for GSH measurement, including high-performance liquid chromatography, capillary electrophoresis, mass spectrometry, fluorescence spectroscopy, and absorbance spectroscopy. Among these methods, absorbance spectroscopy offers significant advantages due to its high sensitivity, selectivity, and simplicity [2]. The mixed-valence of cerium ion (Ce3+/Ce4+) suggests the possibility of reversible switching from Ce3+ to Ce4+. Whereas Ce3+/Ce4+ can confer a mimic enzyme property to Ce compounds (e.g., cerium dioxide). The Ce-based nanomaterials have been employed as target sensors [3]. Therefore, the nanostructures of CeO2 were synthesized using a hydrothermal method. The synthesized nanostructures showed good peroxidase-like activity, which was confirmed by the oxidation of 3,3,5,5 -tetramethylbenzidine (TMB) in the presence of hydrogen peroxide (H2O2) in a few seconds with a change an of color from colorless to blue. The presence of GSH can inhibit the peroxidase-like activity of CeO2 and lead to the disappearance of the blue color of TMBox. Thus, the adsorption of GSH on the surface of nanostructures leads to a decrease in the absorbance of the UV–vis spectra. The possible catalytic mechanism of TMBox conversion to TMB by GSH was proposed and based on the GSH concentration can be estimated by this method, which is known as the turn-off sensor. All of the experimental data were obtained using scanning electron microscopy (SEM), X-ray diffraction (XRD), and UV–vis absorption spectroscopy. The detection limit of GSH was in the micromolar range. Moreover, the proposed colorimetric method is feasible, simple, and inexpensive, and will have promising applications in the analysis of biological samples.

Keywords: CeO2, Glutathione, Sensor, TMB, Hydrothermal method

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Effect of Caffeine and Chlorogenic acid on α–galactosidase Enzyme

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α - galactosidase is a glycoside hydrolase enzyme (EC 3.2.1.22) that hydrolysis the terminal alpha-galactosyl moieties from glycolipids and glycoproteins α –galactosidase producing bacteria is isolated from Erysipelothrix rhusiopathia. α -Galactosidase released from the cells, then purification steps include precipitation by ammonium-sulfate 40% then resuspended & dialyzed by dialyze tube cut off number (10-14 KD) overnight against the phosphate buffer (pH=7) and further purified with DEAE- cellulose column chromatography with a (33.4) folds[1,2] .The enzyme showed maximum activity at (45 °C) and optimum pH at (6.5). The molecular weight of enzyme was determined by using SDS- PAGE analysis and found to be (55 KD). Km and Vmax for this enzyme was determined by (p-nitrophenyl- α -D-galactopyranoside) as substrate, to be (6.6 mM), and (833.3) µmol/min of protein, respectively. The purified enzyme was treated with caffeine and chlorogenic acid and experiments with caffeine suggest that the inhibitor has an equal affinity for the enzyme as the substrate pNPG. Measurements of the reaction rates at different concentrations of substrate and inhibitor observed a non-competitive inhibition and was shown the Km value was ineffective (6.66) mM and decrease in Vmax values (555.5) µmol/min. While when we treated chlorogenic acid with α -galactosidase that is purified from Erysipelothrix rhusiopathiae this substrate acts as uncompetitive inhibition with substrate pNPG as the catalytic site that reflected the enzyme has single active that results from the change of Km and Vmax (3.22 mM) and (400 µmol/min) respectively.

Keywords: Coffee, Caffeine, Chlorogenic acid, α–galactosidase, Erysipelothrix rhusiopathiae

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Mechanism of Amyloid Inhibition Using Aromatic Compounds

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A number of human diseases, including Alzheimer's and Parkinson's, are associated with protein misfolding. Under such condition, a protein or polypeptide undergoes misfolding and converts to an aggregation known as amyloid [1],[2] . In this study, a series of novel aromatic compounds were investigated as amyloid inhibitors. Our strategy has been using computational chemistry to identify compounds that bind and inhibit amyloid formation. Initially, molecular docking was employed to identify compounds that bind to the amylogenic region of lysozyme as a model protein. Subsequently, experimental approaches were used to measure the degree of inhibition of amyloid. Gel electrophoresis and Thioflavin-T binding assay were conducted to detect the aggregation intermediates. Furthermore, in order to study the influence of aromatic compounds on amyloid formation in terms of the size of the aggregations and conformational changes, AFM and FTIR respectively were applied. The initial results demonstrated that some aromatic compounds were showed amyloid inhibitory activities.

Keywords: Amyloid inhibition, Aromatic compounds, Protein misfolding

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Physicochemical stability of diluted solutions of the monoclonal antibody rituximab under freeze-thaw stress

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Rituximab (RTX) is a chimeric monoclonal antibody (mAb) approved for the treatment of non-Hodgkin lymphoma, rheumatoid polyarthritis, and chronic lymphoid leukaemia [1,2]. Its anti-CD20 activity results in the elimination of CD20-positive cells. Due to its proteic composition, RTX is susceptible to undergo a range of chemical and physical degradation processes under different stress situations [3,4]. This research aimed to examine the stability of diluted RTX at 1 mg/mL and 4 mg/ml under various freeze-thaw cycles using orthogonal techniques including cation-exchange chromatography, size exclusion chromatography, attenuated total reflectance-Fourier infrared spectroscopy, and dynamic light scattering. The results indicated that diluted rituximab stored in polyolefine bags was stable following three freeze-thaw cycles. No evidence of physical or chemical instability was found. The hydrodynamic diameter of RTX was observed to be unchanged. The charge heterogeneity profile of stressed samples was unaffected by freeze-thaw cycles compared to the profile of the control sample. Through cation exchange chromatography, neither a new peak nor a decrease in the area under the curve was detected. There were no modifications to the secondary structures of the protein. However, to assure the biological stability of mAbs in addition to their physicochemical stability, additional study is necessary to test the bioactivity of the stressed sample using an appropriate bioassay method.

Keywords: Physicochemical stability, Monoclonal antibody, Rituximab, Freeze-thaw, Stress

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Investigation of the folding behaviour in a protein tertiary fold: A computational study

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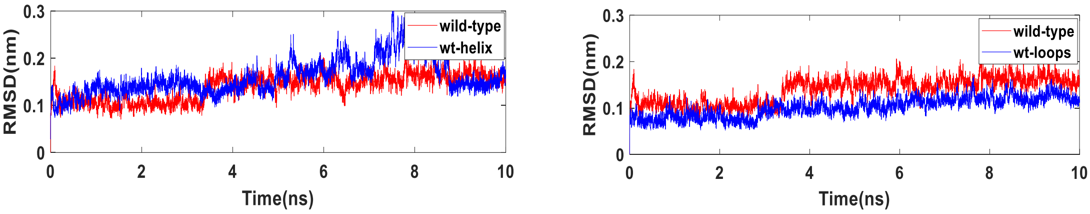
Due to the importance of proteins in biological systems, many efforts have been made to effectively mimic the structure and function of proteins by artificial factors, with different sizes and complexities.[1] Numerous studies have been conducted over the last two decades to overcome the problems associated with peptides and proteins as drug targets, and various strategies have been developed to modify the backbone of natural proteins.[2-4] In this study, the tertiary folding of the B1 domain of Streptococcal protein G (GB1), which contains all common elements of the secondary structure in a single chain, was selected for the design of artificial synthetic oligomers. To this end, molecular dynamics simulation was performed on GB1 protein and its five analogues for 10 ns at the temperature of 300 K to assess the folding stability of mutant structures under real conditions. In the design of the analogues, two groups of artificial backbone units in the GB1 protein, including the β^3-residues and N-methyl α-residues were used. All MD simulations were performed using the GROMACS package. The OPLS/AA force field was used with TIP3P water model. The stability of the elements of the second structure was calculated by examining the changes in the secondary structural elements and hydrogen bonding, etc., and to investigate the third folding of the protein, the distribution of RMSD analysis in the mutant proteins (Schem. 1) was calculated. We found that by replacing natural α residues with artificial building blocks in the protein backbone, the secondary structure of proteins is preserved, and although the stability of some analogues is altered, their third structure is preserved.



Schem. 1. The time evolution of RMSD for the backbone are provided for the wild-type structure and two analogues.

Keywords: GB1, tertiary fold, Molecular dynamics

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The chemistry of Alzheimer's disease

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Alzheimer's disease (AD) is a multifactorial neurodegenerative disorder, characterized by the formation, aggregation, and accumulation of amyloid-beta, metal dyshomeostasis, and metal-induced oxidative stress [1]. Analysis of autopsy of AD brain has demonstrated the presence of abnormally high levels of some metal ions, mainly Zn^{2+} (69 μg/g, ~1055 μM), Cu^{2+} (25μg/g, ~393 μM) and Fe^{3+}, (52μg/g, ~980 μM) in the senile plaques. The Zn^{2+} metal ion is closely associated with glutamatergic neurotransmission under which it controls the overall excitability of the brain as well as affects synaptic plasticity. It is well established that Zn^{2+} binds Aβ promoting its aggregation to form neurotoxic species. On the other hand, the redox-active metals Cu and Fe, which regulate various essential processes of the central nervous system (CNS), like neurotransmitter synthesis, oxygen transportation, myelin production, and synaptic signaling, are a source of reactive oxygen species (ROS) [2]. In addition, the implication of metal ions in AD, their interaction with the Aβ peptide, and redox properties leading to ROS production are discussed, along with both in vitro and in vivo oxidation of the Aβ peptide, at the molecular level. It has demonstrated that Cu and Zn levels can reach up to three times the normal levels observed in healthy brains [3]. Copper bound Aβ peptides involved in the pathology of AD. Spectroscopic evidence reveals that two intermediates, Cu_2O_2-bis-m-oxo and Cu(II)–OOH, are formed in the reaction of Cu– Aβ and H_2O_2. Reduced Cu– Aβ can react with O_2, where the Cu gets oxidized and H_2O_2 is generated via disproportionation of the O_2^- produced. The H_2O_2 generated from dissolved oxygen in blood can trigger the oxidation of serotonin. This is exactly the same case as indicated by the gradual appearance of the bands corresponding to the oxidized products of serotonin when incubated with a solution of Cu– Aβ reduced with ascorbic acid in aerated buffer solutions albeit the extent of oxidized serotonin produced is much less under these stoichiometric conditions. Oxidative degradation of neurotransmitters like serotonin generating neurotoxins like tryptamine-4,5-dione is a hallmark of AD, which can lead to impaired neuronal signaling. The formation of a Cu(II)–OOH species was confirmed by the combination of EPR and resonance Raman spectroscopy [4].

Keywords: Metal ions, Amyloid β, Alzheimer's disease

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Optimization of carbon quantum dot synthesis based on amino acid and study of it's interaction with acetylcholinesterase

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Carbon quantum dots (CQDs) are zero dimensional carbon-based nanostructures with a diameter of less than 10 nanometers. These nanostructures are semiconductors that due to their uniqe optical, photoluminesence and electrochemical properties have many applications in different fields [1]. These nanoparticles can be absorbed by the body and interact with body proteins during the production or application process[2]. The interaction of these nanoparticles with the neuronal enzyme acetylcholinesterase has been investigated in this study. For this purpose, Using amino acids such as lysine, histidine, arginine and methionine as the main sources of synthesis of CQDs and by hydrothermal method, a variety of CQDs were synthesized. In order to study the interaction of synthesized nanoparticles and acetylcholinesterase, experiments were performed by examining two quantitative factors of nanoparticle to enzyme ratio and duration of interaction and a qualitative factor of nanoparticle type using Central Composite Design method at five levels. analyzes such as dynamic light scattering, ultraviolet-visible absorption pattern, circular dichroism spectrum pattern and gel electrophoresis were performed to investigate the properties of CQDs before and after corona complex formation. we synthesized CQDs based amino acids with sizes between 1 and 3 nm that emit blue light when exposed to a wavelength of 360 nm UV light. The results showed that the best enzymatic activity and the highest fluorescence emission were obtained in the interaction of histidine CQDs with the enzyme at CQD-to-enzyme ratio of 25% after 20 minutes incubation. This ratio was 17.5% for CQDs based on the lysine, methionine and arginine after 10 minutes incubation. The CQDs based on the histidine are most affected and also has the greatest effect on this enzyme. The enzyme had the least effect on the CQDs synthesized from the arginine source and CQDs based on the lysine had the least effect on the enzyme.

Keywords: Carbon quantum dot, Acetylcholinesterase, CQD enzyne intraction, Fluorescence

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Construction of chitosan-polyethylene glycol nanohydrogels containing curcumin for use in diabetic wounds healing

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Nanohydrogels are cross-linked networks of macromolecules that swell in water or biological fluids. They are swollen, a good system for controlling drug delivery, wound healing and the transfer of biologically active macromolecules [1]. The reason for focusing on nanohydrogels is their behavior in response to minor environmental changes such as pH, temperature, ionic strength and soluble compounds that cause controlled changes in their volume [2]. A wide range of materials, such as natural and synthetic polymers, are used as effective drug carriers. Chitosan, a natural polymer, stands out as a first choice material for hydrogels elaboration in biomedical, cosmetic, and health related applications, owing to its interesting properties as biocompatibility, biodegradability, antimicrobial capacity, and mucoadhesive [3]. Also, chitosan has been found to promote cell proliferation, stimulate tissue reorganization, promote collagen deposition and enhance increased production of hyaluronic acid at the wound site and also acts as hemostatic agent, thus helps in wound healing with minimal scar formation [4]. Polyethylene glycol is also a synthetic polymer, which can be used in the preparation of hybrid nanohydrogels. Curcumin, a natural product of the rhizomes of *Curcuma longa,* has been widely used as coloring agent and spice in food. But studies have shown that curcumin could significantly accelerate the healing of wounds and enhance wound repair in diabetic impaired healing [5]. In this study, first, chitosan nanohydrogels (CSNH) and chitosan-polyethylene glycol nanohydrogels (CS-PEGNH) were made by ionic gelation method. During the production of nanohydrogels, curcumin was trapped in nanohydrogels. Then, spectrophotometric and SEM analysis were used to confirm the production of nanohydrogels and entrapment of curcumin. According to the results of SEM images, the average diameter of CSNH were below 50 nm and the average diameter of CS-PEGNH were approximately 50 nm. Also, the results showed that the entrapment of curcumin in CSNH with 97.25 %, is more than the amount of curcumin entrapment in the CS-PEGNH with 95.62 %. Finally, the release of curcumin from nanohydrogels at pH and physiological temperature (pH=7.4 and $T=37^{\circ C}$) were investigated. The results also showed that the curcumin release, in the first hours, in CS-PEGNH was more than CSNH. This is probably due to the presence of polyethylene glycol in the structure of the nanohydrogels, which, due to its thermoplastics, allows better release of curcumin.

Keywords: Nanohydrogel, Chitosan, Polyethylene glycol, Curcumin, Diabetic wounds

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Structural crosstalk between proteins and diseases

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The proper folding of a protein is necessary for its biological activity. The three-dimensional structure of a protein arises due to different types of interactions (hydrophobic, covalent, and weak forces) between its amino acid sequences. It is well established that partially folded or misfolded proteins are highly prone to aggregation, especially at high concentrations as compared to their native protein. The proteins with high β-sheet contents are more prone to form amyloids as they exhibit a high propensity for self-aggregation [1]. More than 20 polypeptides have been identified to undergo misfolding transition associated with diverse human disorders including Alzheimer’s (AD) and Parkinson’s diseases (PD), amyloidosis, type 2 diabetes, and prion diseases. Misfolded proteins include β -amyloid (Aβ) peptides, α-synuclein, and tau associated with various age-related neurodegenerative diseases. Intracellular inclusions containing misfolded α -synuclein aggregates are a hallmark of several neurodegenerative diseases such as PD. Several studies suggest that AD and PD pathologies are significantly overlapped presumably due to synergistic interactions between misfolded tau and α -synuclein. Tauopathy is the hallmark of a wide range of neurodegenerative diseases such as AD and frontotemporal dementia [2]. The α-Synuclein is present in various conformations within the cell, from its physiological conformation of soluble monomers to pathological oligomers and fibrils formed by aggregation processes. When misfolded into fibrils, α -syn adopts a crossed β-sheet conformation, whose properties confer on it the classification of an amyloidogenic protein. Amyloid formation in α -syn involves PD [3]. Islet amyloid polypeptide (IAPP) or amylin is the most characteristic morphological islet feature of type 2 diabetes, to some degree present in more than 90% of type 2 diabetes pancreata [4]. While protein aggregation may conceivably lead to protein inactivation via sequestration, the aggregates themselves can exert toxicity by interfering with intracellular functions or cell- to-cell signaling. Post-translational modifications can alter the folding and structure of proteins and thus modify their biochemical activity. It is, therefore, possible that post-translational modifications can lead to the dysfunction of proteins and contribute to unfolding or misfolding. On the other hand, protein misfolding itself can lead to altered post-translational modification, especially when crucial enzymes are involved [5].

Keywords: Misfolded protein, Amyloidosis, Protein aggregation

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Carbon fiber cloth supported CoP/g-C_3N_4 as excellent electrocatalyst for oxygen evolution reaction

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Rising energy demands and environment problems have promoted extensive research on the development of alternative energy resources and storage devices with high efficiency and environmental friendliness. Among them, water splitting is a promising strategy for the formation of clean energy resource and storage but the main challenge of this renewable-energy technology is to enhance the kinetics of oxygen evolution reaction (OER). Therefore, developing efficient electrocatalysts with high catalytic activities and stability is of great importance for high-performance water splitting. Recently, a considerable amount of research has been devoted to the development of new OER electrocatalysts with low-cost, highly efficient, and excellent stability properties [1]. Transition metal phosphides (TMPs) and their composite-based catalysts are extensively used for replacing previously used noble metals such as Pt, Au, and Ag due to scarcity, instability, and high price. Predominantly, nickel and cobalt phosphides based materials among all TMPs have proven to be excellent catalysts for water splitting [2], because these catalysts have shown some of advantages, such as high conductivity, earth abundance reserves, and good physicochemical properties. In this research, carbon fiber cloth (CFC) supported with high mass loading of cobalt phosphide and graphitic carbon nitride (g-C_3N_4) was synthesised through a three-step process consisting of cobalt electrodeposition at -10 V for 3 s, followed by CVD growth of g-C_3N_4 at 950 °C by using melamine as precursor and finally phosphorization treatment in inert atmosphere. This CoP/g-C_3N_4@CFC electrocatalyst demonstrated a superior electrocatalytic performance for OER activity, and excellent durability in alkaline media under 1000 sweeps at a high scan rate 100 mV s^{-1}. Remarkably, the CoP/g-C_3N_4@CFC exhibited a low overpotential of 270 mV to deliver 10 mA cm^{-2} current density. Moreover, the synthesized electrocatalysts were charecterized by several techniques such as X-ray diffraction (XRD), scanning electron microscopy (SEM) and map element analysis to confirm the formation of CoP and g-C_3N_4 with special morphology on the surface of CFC.

Keywords:metalphosphide, OER, graphitic carbon nitride, carbon fiber cloth.

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The role of Halloysite in the design of electrochemical biosensors for measuring diazinon in environmental and biological monitoring

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Diazinon is one of the most widely used organophosphate pesticides, which is widely used in agriculture. Due to the high consumption of pesticides and their destructive effects on humans and the environment, the choice of a sensitive, simple and rapid method for measuring these compounds is very important. Reproducibility and sensitivity are high. Can be used to measure organophosphate compounds. In this study, an electrochemical biosensor was designed to measure diazinon based on the modification of a gold electrode with the enzyme esterase (extracted and purified from bacteria (*Bacillus sp.HP 96*) and halloysite (natural nanotubes made of mineral clay). The performance of the electrochemical biosensors such as the electrochemical behavior of diazinon and pH were investigated and the proposed electrochemical biosensors were successfully used to measure diazinon in environmental and biological samples.

Keywords: Diazinon; Electrochemical biosensors,Halloysite, Organophosphate compounds

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Experimental and Theoretical Study of Human Serum Albumin (HSA) Binding of Fibroblast Activation Protein inhibitor (FAPi)

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Fibroblast activation protein (FAP) is a cell-surface serine protease that acts on various hormones and extracellular matrix components. FAP is highly upregulated in a wide variety of cancers, and is often used as a marker for pro-tumorigenic stroma. FAP is difficult to detect in non-diseased adult tissue, but it is generally expressed at sites of tissue remodeling [1-2]. Several potential FAP-targeted approaches consisting of vaccines, antibodies, prodrugs, and inhibitors have been exploited in preclinical studies [3]. Among them, a class of FAP inhibitors (FAPi) with a N-(4-quinolinoyl)-Gly-(2-cyanopyrrolidine) scaffold displayed nanomolar affinity and high selectivity against other interfering dipeptidyl peptidases and prolyl oligopeptidase [4]. In this study, FAPi-46, as well-known FAP inhibitor, were selected and prepared. Quantum chemical calculations of these compounds have been carried out by DFT at the B3LYP/6–311++G(d,p) level. An analysis of the calculated vibrational frequencies was performed by theoretical method and significant bands were specified. Furthermore, the binding affinity between the above-mentioned inhibitor and human serum albumin (HSA) was studied under simulated physiological conditions (using molecular docking (MD)) and experimental analyses (using fluorescence and CD spectroscopies). The obtained results revealed that the formation of a complex between HSA and FAPi-46 was responsible for quenching the native fluorescence of protein at 343 nm and can be illustrated by the static mechanism. The binding constant (K_a= 2.65 mM^{-1}) and number of binding sites were considered and proposed that the combination of hydrophobic and electrostatic forces were the principal intermolecular forces stabilizing the complex. Also, theoretical results show that the FAPi-46 compound has high affinity for binding to HSA.

Keywords: FAP; DFT; Molecular Docking; CAFs; HSA.

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Spectroscopic analysis and molecular modeling on the interaction of Naphthalene-based Schiff base with human serum albumin (HSA)

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Studies on supramolecular interactions of drugs or organic compounds with biological macromolecules have significantly contributed to the understanding of the structures and functions of bio-macromolecules and some biophysical processes [1]. By binding to human serum albumin (HSA), most drugs circulate in plasma and reach the target tissues and their distribution is mainly controlled by HSA [2]. Hence, drug binding to proteins has becomes an important determinant of pharmacokinetics, e.g. prolonging in vivo half-life, restricting the unbound concentration and affecting distribution and elimination of the drug. HSA is the most abundant protein in human blood plasma and has high affinity to many endogenous and exogenous compounds, serving as a solubilizer and transporter for drugs and other organic molecules to their targets [3]. In this study, new Schiff-base {N,N′-Bis(2-hydroxy-3-methoxy-benzylidene)-naphthalene-1,5-diamine (NSL), has been synthesized by the reaction of 1,5-naphthalenediamine (p-ND) with the 2-hydroxy-3-methoxybenzaldehyde and characterized by UV–Vis, FT-IR, ^{1}H-NMR, and mass spectroscopy. Interaction between Naphthalene-based Schiff base (NSL) with HSA was studied by means of UV/Vis and fluorescence spectroscopy. The intrinsic fluorescence of HSA was quenched by NSL, which was rationalized in terms of the static quenching mechanism. The results show that NSL compound can obviously bind to HSA molecules. According to fluorescence quenching calculations, the bimolecular quenching constant (K_q), apparent quenching constant (K_{SV}) at 27 °C was obtained. The binding constants, K, is 23.5 L.mol^{-1} and the number of binding sites (n) is 1. Also, molecular docking results suggested that the binding site of NSL was site IA of HSA.

Keywords: HSA; DFT; Molecular Docking; Schiff base; UV/Vis.

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DNA interaction and Molecular Docking Studies of Adenine- Based Carboxamide Ligand

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The interaction of drugs with DNA is among the most important aspects of biological studies in drug discovery and pharmaceutical development processes[1]. many studies demonstrate that DNA is the primary intracellular target of antitumor drugs, because the interaction between small molecules and DNA can cause DNA damage, blocking DNA synthesis in cancer cells. Therefore, under physiological conditions, many compounds which can efficiently bind and cleave DNA are considered as potential candidates for use as therapeutic agents in medicinal applications and for genomic research [2-3]. Herein, a carboxamide ligand has been synthesised by the reaction of adenine with picolinic acid (HL_1) in the presence of tetrabutylammonium bromide (TBAB) and characterised by different spectroscopic techniques. The optimized structure of HL_1 has been investigated using the DFT/B3LYP method with the 6–311++G(d,p) basis set. For the investigation of the anticancer activity the interaction of this ligand with calf thymus DNA was studied by isothermal titration method in tris buffer which was contained sodium chloride (10 mM) and pH= 7.4 at 27 and 37 °C and thermodynamic parameters were obtained. Also, the modes of binding of the ligand to ct-DNA was investigated by fluorescence spectroscopy and circular dichroism. Data indicate that this ligand interacted probability of groove binding with DNA via noncovalent mechanism.

Keywords: DNA; DFT; Molecular Docking; Carboxamide; UV/Vis.

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Construction, characterization and application of Fe3O4-Guanidine/GO-Guanidine as an efficient and recycle magnetic nanocatalyst for fabrication of Hantzsch 1,4-dihydropyridine derivatives

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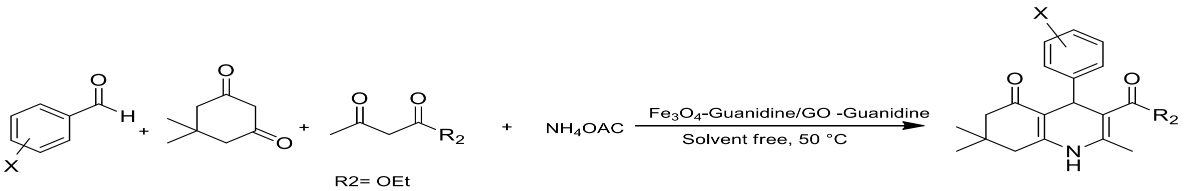
Hantzsch 1,4-dihydropyridines (1,4-DHPs) and their other derivatives are considered as one of the most significant type of bioactive molecules which are extensively applied in the field of drugs and pharmaceuticals [1]. Nano-based catalysts have brilliant properties which make them excellent materials for utilization in different fields [2].

Between different type of carbon materials, graphene oxide (GO) has amazing properties like porous structure, high surface area, high adsorption capacity, easily modification, low toxicity, excellent biocompatibility and high physical, chemical and thermal stability [3, 4].

The purpose of this work was fabrication and investigation of Fe3O4@Guanidine/Go-Guanidine as a novel, efficient and reusable nanocatalyst for synthesis of Hantzsch 1,4-dihydropyridine derivatives. To achieve the optimum conditions and high yield, the effect of different factors like amount of nanocatalyst, temperature and type of various solvents was assessed.



Schem. 1. Synthesis of 1,4-dihydropyridine derivatives at optimum conditions using nanocatalyst

Keywords: Magnetic nanocatalyst; Guanidine based catalysts; Hantzsch 1,4-dihydropyridine derivatives; recycle catalyst.

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In silico investigation of CaO nanocluster in lithium and sodium atom/ion batteries

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Although Li-ion batteries have some disadvantages such as cost, lifetime, low-temperature performance and safety, they are very practical in many portable power and electronics devices and light vehicles [1]. Regardless of their eminent efficiency in comparison to different kinds of rechargeable batteries [2], wide availability, low cost, and nontoxicity of sodium make Na-ion batteries a good replacement for Li-ion batteries [3].

Additionally, among all $X_{12}Y_{12}$ nanoclusters, the metal oxide clusters, such as $Be_{12}O_{12}$, $Mg_{12}O_{12}$, and $Ca_{12}O_{12}$, have metal-oxide bonds with a substantial ionic character in result in some noticeable attributes. So many researches were done using these nanoclusters [4]. Between them, because of its extensive availability and accessibility in natural minerals and substantially higher ionic character along with its lower cost, the CaO metal oxide has an outstanding position in fundamental research. Relatively high basic sites, nontoxicity character with low solubility in methanol to produce it from inexpensive resources like lime stone and calcium hydroxide makes the CaO as the one of the most favorable heterogeneous base catalysts which is highly recommended for scientists and other industrial purposes.

DFT calculations at the B3LYP-D3/6-31G (d) level of theory was employed to study the possibility of the $Ca_{12}O_{12}$ nanocluster in Li and Na atom/ion batteries using Gaussian. For this reason, the interaction of $Ca_{12}O_{12}$ nanocluster with Li/Na atoms and Li+/Na+ cations was calculated. Based on results the adsorption energies for two Li+/Na+ cations are considerably higher than their corresponding atomic species. Eg value of $Ca_{12}O_{12}$ nanocluster slightly increases in adsorption of Li/Na atomic forms while it was narrowed as consequence of the cationic forms adsorption. The values obtained for the cell voltage of Li/$Ca_{12}O_{12}$ and Na/$Ca_{12}O_{12}$ were 1.82 and 2.49 V respectively which show that $Ca_{12}O_{12}$ may be appropriate for application in both lithium and sodium ion-batteries. Moreover, the cell voltage of Na@$Ca_{12}O_{12}$ is considerably high which shows that this nanocluster is highly beneficial for storage performance ion batteries.

Keywords: $Ca_{12}O_{12}$ nanocluster; Lithium; Sodium; Battery; DFT.

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Electrodeposition of nickel-cobalt-selenide and lanthanum-selenide on nanocone substrate for high performance hybrid supercapacitors

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Supercapacitors have received considerable attentions owing to their advantages such as high power density, fast charging- discharging, long life and environmentally friendly [1-3]. Transition-metal selenides have recently attracted increasing interest in supercapacitors (SCs) owning to their fascinating electrochemical properties such as a lower optical band gap and much higher conductivity than their corresponding metal oxide analogs [4]. Here, we proposed a desirable strategy for the electrodeposition of nickel-cobalt-selenide and lanthanum-selenide (positive electrode) on Ni-Co nanocone as a substrates on the nickle foam. Based on SEM image analysis, it is clear that lanthanum-selenide nanoworms which has grown on nickel-cobalt-selenide cauliflower. The positive electrode represents a substantial specific capacitance of 2075 F g^{-1} at 2 A g^{-1}, considerable rate performance and excellent durability (11 % loss after 5000 cycles). A hybrid supercapacitor was fabricated with the sujested on Ni-Co NNC substrate and AC (activated carbon) materials as the cathode and anode electrodes, respectively, in KOH electrolyte (3 M). This flexible device exhibits the good specific capacitance, the significant energ y density of 44.95 Wh kg^{-1} , power density of 662 W $kg^{-1}$and excellent flexibility.In the last few years, focus on alternative energy sources is tremendously increased due to the curtailment of non-renewable

Keywords: Nanocone, Selenide, Lanthanum, Electrodeposition.

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Design, synthesis and *in vitro* studies of novel 1,2,3-triazole-benzohydrazide hybrids as potent α-glucosidase inhibitors

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α-Glucosidase is an intestinal enzyme which catalyzes the breakage of the 1,4-α glycosidic bonds of polysaccharides and some disaccharides converting them into the absorbable glucose [1] and this enzyme is involved in various carbohydrate-related diseases such as diabetes. Currently prescribed α-glucosidase inhibitors such as acarbose, voglibose, and miglitol have depicted different side effects including bloating, diarrhea, flatulence, pain, and abdominal discomfort [2]. Hence, discovery and development of new α-glucosidase inhibitors possessing high efficacy and low side effects are still in high demand as an attractive target for medicinal chemists. 1,2,3-Triazole derivatives are undeniably important scaffold in medicinal chemistry and several 1,2,3-triazole derivatives with high α-glucosidase inhibitory activity have been reported [3]. Benzohydrazides also have been reported to possess a wide variety of biological activities like antiglycation [4]. In an effort to design and synthesize a new class of α-glucosidase inhibitor, a novel series of 1,2,3-triazole-benzohydrazide hybrids are reported as *in vitro* α-glucosidase inhibitors.

Keywords: α-glucosidase inhibitors, 1,2,3-triazole, Benzohydrazide.

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Preparation of a new solid-phase microextraction fiber based on molecularly imprinted polymers for monitoring of phenobarbital in urine samples

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In the present study, a novel solid-phase microextraction molecularly imprinted polymers (SPME-MIP) fiber based on sol-gel technology was developed. Coupling of SPME with selective MIP coating notably increased the extraction yield. The sol-gel procedure for the preparation of SPME fibers provides several advantages: it could occur under mild conditions, the coating's porous silica is homogeneous and pure, it has a high surfaces area, and the shape and size of pores are easily controllable [1]. In this work, the fiber was prepared via inserting the modified stainless steel wires in the reaction solution of (3-Aminopropyl) triethoxysilane (APTES) and tetraethylorthosilicate (TEOS) with an acidic catalyst (acetic acid). The SPME-MIP fiber used for selective extraction of phenobarbital in urine samples using high performance liquid chromatography with ultraviolet detection (HPLC-UV). Phenobarbital, as the derivatives of barbituric acid, belong to anticonvulsant drugs and have sedative and hypnotic properties [2].

The synthesized MIPs were characterized by several techniques such as field emission scanning electron microscopy (FESEM), Fourier-transform infrared spectroscopy (FTIR), and thermal gravimetric analysis (TGA). The effects of various influencing parameters on the extraction efficiency of phenobarbital were investigated and optimized. Results showed that the maximum extraction efficiency was obtained under the following conditions: pH of 5, 25 min extraction time, 500 rpm stirring rate, 15 min desorption time, and by using methanol as elution solvent. Furthermore, Langmuir and Freundlich's plot was employed to assess the isotherm study. The binding affinity of the SPME-MIP fiber properly fits with the Langmuir equation with correlation coefficient values 0.9995. The proposed method had linear characteristics in the concentration range of 0.02 to 100 µg mL^{-1} with a suitable coefficient of determination (0.9983). The limit of detection (LOD) and quantification (LOQ) were 9.88 and 32.9 ng mL^{-1}, respectively. The repeatability and reproducibility of the prepared fibers were 4.6 and 6.5%, respectively.

Keywords: Phenobarbital, Molecularly imprinted polymer, Solid-phase microextraction, HPLC-UV

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Preparation of molecular imprinted polymer based on chitosan as the selective sorbent for solid phase microextraction of phenobarbital

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Solid-phase microextraction (SPME) has been used as a suitable and efficient sample preparation techniques for determination of various analytes from complex matrices [1]. Combination of molecularly imprinted polymer (MIP) with SPME enhances the efficiency of the extraction process. Natural biopolymers have gained increased attention in recent years as a substitute for synthetic materials. Unique properties of natural biopolymers such as easy processing method, low cost, availability, nontoxicity, ecofriendly and sorption capacity of prompted the use these compounds. In this study, construction of a novel (SPME-MIP) fiber based on chitosan and glutaraldehyde as coating material composites combined with high-performance liquid chromatography with ultraviolet detector (HPLC-UV) were studied. Phenobarbital, a barbiturate derivative, is one of the most commonly prescribed epilepsy medications which was measured by the proposed method [2]. In this technique, the chitosan biopolymer, as a new coating fiber, was produced on the modified stainless-steel wire, using chitosan, glutaraldehyde and phenobarbital as functional monomer, cross-linker and template, respectively. For comparison, a non-imprinted polymer was created using the same procedure to evaluate fiber selectivity.

The SPME-MIP fiber coating was characterized by field emission scanning electron microscopy (FESEM), Fourier-transform infrared spectroscopy (FTIR), and thermal gravimetric analysis (TGA). The efficiency of fiber was then improved by adjusting the impact of numerous factors such as; pH, extraction time, desorption time, desorption solvent, and stirring rate. Results showed that the proposed fiber has a linear range 0.01-4 µg mL^{-1}, and detection limit of 7.5 ng mL^{-1}. The average recoveries in the four concentration levels for the spiked river and well water samples were 95.7 and 95.3%, with relative standard deviations of 3.8 and 5.9% for single fiber and between fibers, respectively.

Keywords: Chitosan, Molecularly imprinted polymer, Solid-phase microextraction, HPLC-UV, Phenobarbital

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A novel molecularly imprinted polymer based on tragacanth gum onto stainless steel wire for selective solid-phase microextraction of chrysophanol

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Molecular imprinting is a technique that creates recognition sites by polymerization of functional monomers and cross linkers in the presence of the template molecule. Molecularly imprinted polymer (MIP) employed as solid-phase microextraction (SPME) coating for effective and selective separation of template [1]. Natural compounds, like tragacanth gum (TG), due to unique physical, chemical and biological properties such as non-toxicity, biocompatibility, eco-friendliness and stability over wide pH ranges, have been find a lot of application in recent years [2]. In this study the TG molecule, due to presence of plenty hydroxyl and carboxylic acid groups was employed as crosslinking agent to create a novel MIP-SPME fiber for extraction of chrysophanol. To improve fiber stability and lifespan, a surface modified stainless steel wire (SSW), was used as supporting material. Polydopamine was used to covalently functionalize SSW, then the MIP was prepared by radical polymerization using chrysophanol as a template, vinyl imidazole (VI) as a functional monomer and TG as a crosslinking agent. The fiber was characterized by scanning electron microscopy (SEM) and Fourier transform-infrared spectroscopy (FT-IR). Additional properties of fiber were also studied by complementary tests such as adsorption and extraction capacity experiments. Also, the extraction conditions, including pH, extraction time, desorption time, and desorption solvent were optimized. Finally, the efficiency of the fiber was evaluated with high-performance liquid chromatography with ultraviolet detector (HPLC-UV) for determination of chrysophanol in a urine sample. It was found that the mechanism of adsorption follows the Langmuir model, with the maximum capacity of 178.57 ng. In comparison to non-imprinted polymer coating, the MIP-SPME coating exhibited significantly higher extraction amounts and excellent selectivity to the chrysophanol. The limit of quantification was 8.95 ng mL^{-1}. The recovery for the spiked sample ranged from 94.01% to 96.20%, with the relative standard deviation (RSD) of 4.30% to 5.06% for single fiber and between fibers, respectively.

Keywords: Tragacanth gum, Molecularly imprinted polymer, Solid-phase microextraction, HPLC-UV

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A simple and clean procedure for three-component synthesis of spirooxindoles using vanadatesulfuric acid nanoparticles in aqueous medium

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Spirooxoindoles as an important class of heterocyclic compounds represent a wide range of pharmacological and biological activities. Architecture of spiro compounds because of their steric strain has been a rival for organic chemists and in recent years many efforts have also been done for preparation of spirooxindoles using various catalysts. Though all reports have their own worthiness, continuing researches to find simple and versatile methods seem necessary.

Advantages of multi-component reactions are wide including simplified purification, low-cost reactants, reduced pollution and high yield. Therefore, such environmentally benign protocols are very powerful and well desired

In many cases, volatile organic solvents that are used daily in large quantities for many various applications contribute to the major source of environmental pollution. Therefore, development a chemical reaction in water as a useful alternative solvent with respect to the unique properties of water in promoting reactions and excellent selectivity has been attracted interest. In the recent years, much attention has also been focused from both economical and environmental point on the application of solid acid catalysts for synthesis of organic compounds. In addition to, reactions with these catalysts are commonly clean and selective and give high efficiency of products[1].

Based on the above observations and in continuation of our interest on application of nanocatalyst in preparation of heterocyclic compounds[2-5], we have explored the aqueous-phase synthesis of spirooxindoles by the three-component reaction of isatin, malononitrile and 1,3-dicarbonyl compounds using vanadatesulfuric acid (VSA NPs) as a recyclable and eco-benign nanocatalyst.

Keywords: Spirooxoindoles, Aqueouse-phase, Vanadatesulfuric acid nanoparticles, Reusabe catalyst.

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Fabrication of silica based nanofibers via electrospinning method for the removal of Ni^{2+} from polluted waters

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Nanofibers woven via electrospinning due to their special properties such as high surface-to-volume ratio, flexibility in surface properties, and excellent mechanical performance are capable of absorbing large amounts of contaminants and are also used in the removal of heavy metals [1]. In this work, a polyvinyl pyrrolidone/silica (PVP/SiO_2) nanocomposite was prepared and converted into a nanofiber membrane using a simple electrospining process. The prepared membrane was characterized by SEM and EDX analyses. Toxic and highly disturbing heavy metals in wastewater treatment tend to accumulate in living organisms and many of these ions are toxic and carcinogenic[2] .The nanocomposite fibers were studied for the removal of heavy metals from aqueous solutions with obtaining superior results for nickel. Various parameters for the removal of Ni^{2+} ions such as solution pH, sample volume and adsorption time under constant conditions of 0.1 g fiber and 5 mg L^{-1} Ni^{2+} were studied. For optimization of the three studied parameters a response surface method with the central composite design (CCD) was used. After performing 20 designed experiments the optimal conditions were obtained by the Minitab software. Under the optimal conditions the adsorption capacity of the nanofiber membrane was 90 mg g^{-1}. The nano adsorbent was applied to the removal of Ni^{2+} from natural and polluted water samples and satisfactory results were obtained for the samples with low ionic strength.

Keywords: Nickel, Nano composite, electrospining, Nano fiber

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Synthesis and fabrication of an agarose based magnetic nano-adsorbent for application in drug delivery of metformin

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Iron oxide magnetic nanoparticles are the materials widely used in drug release systems, due to their special properties such as small size, low toxicity and high specific surface area and magnetic properties [1] . In this work, iron oxide magnetite nanoparticles were prepared using a simple coprecipitation technique and they were coated for more stability and biocompatibility with silica/agarose to obtain the Fe_3O_4@SiO_2@Agarose nano carrier. In every stage of the synthesis, the nanoparticles were characterized by Fourier transform infrared spectroscopy (FT-IR), dynamic light scattering (DLS), scanning electron microscopy (SEM) and energy dispersive x-ray spectroscopy (EDX). The nano particles were successfully used as a carrier for metformin. Metformin is a medicine that reduces blood glucose concentration and unlike some other anti-diabetic drugs does not cause clear hypoglycemia [2] .Effects of parameters such as pH, adsorption time and temperature on the adsorption of metformin as well as its desorption conditions were investigated. In the optimal conditions (pH = 9, time = 5 min, temperature = 20 °C, 5 ml adsorbent) a high loading capacity of 41.4 mg g^{-1} was obtained for a 1000 mg L^{-1} solution of metformin. The short time of the adsorption indicates the fast uptake of the drug on the nano carrier. Up to 52% of the drug was loaded on the carrier under the optimal conditions. Relatively slow release of the drug from the nanoparticles at pH 1.6 (the gastric acid pH) was observed that makes it appropriate for drug delivery applications.

Keywords: Fe_3O_4@SiO_2@Agarose adsorbent, Drug delivery, Metformin, nano fiber

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Salen-Cu stabilized on the periodic mesoporous organosilica an efficient nanocatalyst for one-pot synthesis of 2-amino-4,6-diphenylnicotinonitrile.

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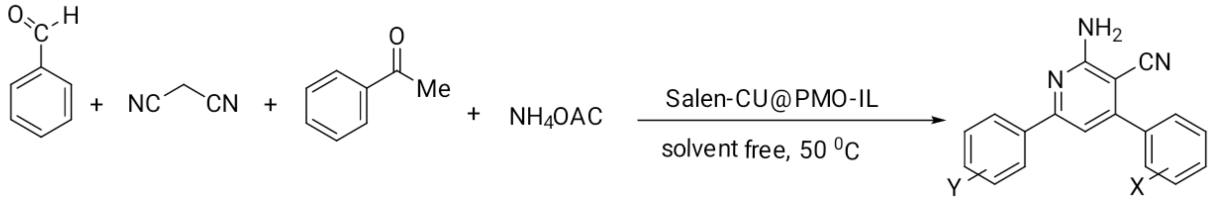
Nano porous materials have porous in the nanoscale and are very diverse, regular structure with a high ratio, selectivity of shape and size are the most important properties of these materials, which has resulted in the application of a lot of catalytic, purification, absorbent materials for separation and highlighting their role in nanotechnology[1]. Periodic mesoporous organosilicas(PMOs) is one of the most advanced organic and inorganic hybrid materials that has attracted the attention of many researchers today[2]. Assembling several molecules into the product in one reaction step is as a result of the convergent character of multi-component reactions (MCRs) which often give excellent chemo and regioselective products[3]. Increasing the importance of heterocyclic compounds in the field of pharmaceuticals and industrial chemicals has increased the development of simple, elegant and facile methodologies for their synthesis[4]. In this study, we synthesized metal salon complexes on a periodic mesoporous organosilica. As an efficiency catalyst and the study of its catalytic application in a one-pot and multi-component reaction, including condensation of benzaldehyde derivatives with malononitrile, phenyl acetylene and ammonium acetate, were used to preparation of diphenylnicotinonitrile derivates

Keywords: Copper salon complex, Periodic mesoporous organosilicas, diphenylnicotinonitrile derivate.



Schem. 1. Synthesis of 2-amino-4,6-diphenylnicotinonitrile

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Synthesis of 6-amino-1-(2,4-dinitrophenyl)-3-methyl-4-phenyl-1,4-dihydropyrano[2,3-c] pyrazole-5-carbonitrile salen-Cu stabilized on the periodic mesoporous organosilica

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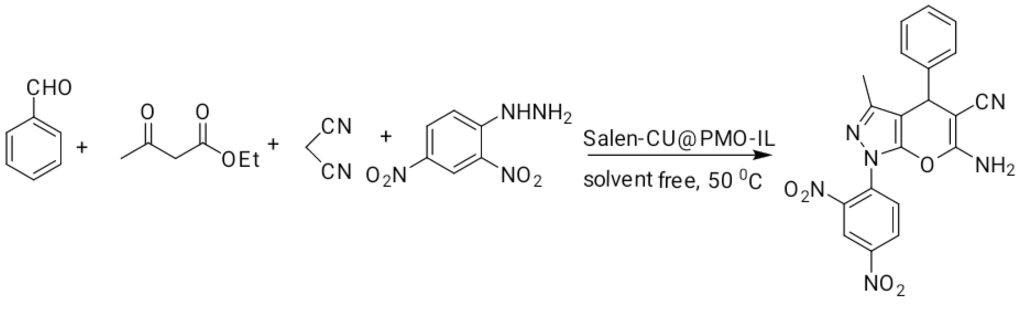
Over the past decades, the synthesis of complex biologically active scaffolds via the one-pot multicomponent reactions (MCRs) has attracted considerable attention[1]. The synthetic utility of such protocols can be improved significantly by using green solvents and an efficient heterogeneous catalyst. Pyrano[2,3-c] pyrazole derivatives are one of the biologically important scaffolds because of their wide application in pharmaceuticals2,3 and in organic synthesis as essential intermediates[2, 3]. Periodic mesoporous organosilicas is one of the most advanced organic and inorganic hybrid materials. In fact, this valuable hybrid nanoporous due to the presence of organic groups within its walls, in order to promote the use of hybrid mesoporous in various fields such as chemical adsorbents, chromatography, catalytic processes, chemical sensors, stabilization of active metal species, etc., were introduced. In recent years, much progress has been made in controlling the synthesis of periodic mesoporous organosilicas and because of the special uses of this material[4]. In this work, we synthesized a catalyst of the metal salon complexes containing a copper(I) on a periodic mesoporous organosilica. And the study of its catalytic application in a one-pot and multi-component reaction, including condensation of benzaldehyde derivatives with malononitrile, ethylacetoacetate and hydrazine hydrate, were used to prepare dihydropyrano[2,3-c] pyrazole derivatives

Keywords: copper salon complex, periodic mesoporous organosilicas, Multicomponent reactions.



Schem. 1 Synthesis of 6-amino-1-(2,4-dinitrophenyl)-3-methyl-4-phenyl-1,4-dihydropyrano[2,3-c] pyrazole-5-carbonitrile

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Design and fabrication of chitosan-based wound dressings containing reduced graphene oxide

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Types of burn wounds, diabetic wounds, bedsores are examples of painful wounds with low healing ability and are very common. In these type of wounds, various factors are involved in wound healing, the most important of which are inflammation and lack of bacterial infection [1]. Inflammation is essential for clearing bacteria and creating a conducive environment for wound healing, but chronic inflammation prevents tissue regeneration and even tissue destruction [2]. Chitosan and reduced graphene oxide are good candidate for use in wound dressings, due to the anti-inflammatory, antibacterial, antioxidant and tissue repairing properties [3, 4]. In this study, CS/rGO nanoparticles were synthesized using ion-gel method and the physical and chemical properties of the nanoparticles were investigated. FTIR results showed that our nanoparticles were prepared. The results showed that nanoparticles have good porosity. Analysis of the obtained data showed that CS/rGO nanoparticles have more antioxidant properties than chitosan nanoparticles. MTT cell test showed that the nanoparticles have good compatibility and this compatibility increases with the presence of rGO.

Keywords: Wound Healing, Chitosan Nanoparticle, reduced Graphene Oxide

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Preparation of chitosan-based nanocomposite and evaluation of its properties for adsorption of chromium ions from aqueous solution

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Many heavy metals that are highly toxic for animals and human beings are discharged into the environment as industrial wastes, causing serious soil and water pollution [1, 2]. One of the most important and widely used heavy metals, chromium, is considered as a toxic and carcinogenic environmental pollutant. Among different methods, adsorption is one of the most economically favorable and technically feasible method to remove Cr (VI) from the solution [3]. In this study, batch adsorption system using a novel nanocomposite, chitosan/montmorillonite/polyaniline (CS/MMT/ PANI) nanocomposite, was investigated to adsorption of Cr (VI) from aqueous solutions. The CS/MMT/PANI nanocomposite was synthesized by chemical oxidative polymerization of aniline in the presence of chitosan-montmorillonite dispersion. The structure and morphology of the prepared nanocomposite was characterized utilizing Fourier transform infrared spectroscopy (FTIR), X-ray diffraction (XRD), scanning electron microscopy (SEM) and transmission electron microscopy (TEM). From the results the successful preparation of nanocomposite with intercalated structure was examined. Then, the removal of Cr (VI) ions from aqueous solution using the prepared adsorbent in a batch adsorption process was investigated. Based on the adsorption studies, the nanocomposite by high adsorption capacity can be used as an industrially viable, economical and successful product to removal of Cr (VI) ions from solutions.

Keywords: Chromium, Chitosan, Nanocomposite, Adsorption

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Nanoporous organosilica–titania with IL framework as a powerful catalyst for the synthesis of tetrahydrobenzo[*b*]pyrans

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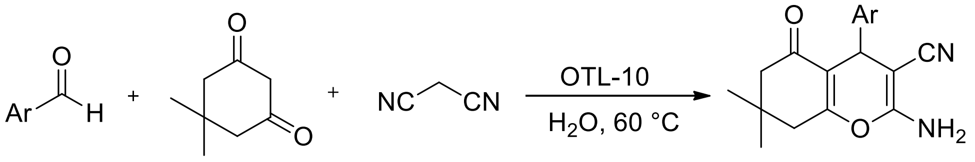
In 1983, the discovery of titanium silicate (TS-1) created a huge revolution in the catalytic industry due to Ti-containing silicates have high catalytic activities. Ti-containing mesoporous silica is an important category of this type of catalysts that used in various processes such as decomposition of dyes, reduction of CO_2 and oxidation of alcohols. In recent years, many studies have been conducted to increase the reaction conversion in the presence of these catalysts [1, 2]. In continuous of these studies, herein, a novel nanoporous organosilica–titania with ionic liquid (IL) framework is synthesized, characterized by using IR, XRD and SEM techniques and its catalytic application is investigated in the synthesis of tetrahydrobenzo[*b*]pyrans (see Fig. 1). The presence of ionic liquid groups leads to an increase in surface hydrophobicity which increases the accumulation of substrate around the catalytic active site. This catalyst was recovered and reused several times without significant decrease in its efficiency.



Schem. 1 .Synthesis of tetrahydrobenzo[*b*]pyrans using Ti-containing IL-based nanoorganosilica

Keywords: Titanium silicate, Ordered mesoporous organosilica–titania, Ionic liquid, tetrahydrobenzo[b]pyrans derivatives.

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$Fe_3O_4@SiO_2$ supported ionic liquid/manganese complex (Fe3O4@SiO2@IL/Mn): Preparation, characterization and catalytic application

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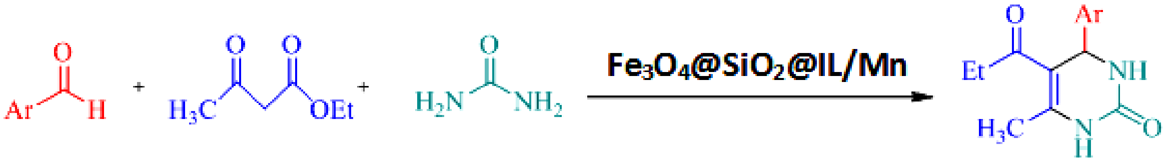
Magnetic nanoparticles are in the center of attention due to their unique chemical and physical properties such as high surface area, easy preparation and functionalization with suitable organic and inorganic moieties. These have potential applications in areas of drug delivery, MRIs, catalysis and adsorption [1]. Especially, the core-shell structured magnetic NPs are more interested due to their high stability in acidic and basic media [2]. The $Fe_3O_4@SiO_2$ NPs are a type of magnetic core-shells with magnetite core and silica shell that are widely applied as support for immobilization of homogeneous catalysts. Some or recently reported catalysts are $Fe_3O_4@SiO_2@MCM/WO_4$, $Fe_3O_4@SiO_2@MCM/IL-Pd$, and $Fe_3O_4@SiO_2@PrNH_2$ [3]. In continuous of these studies, herein, a novel $Fe_3O_4@SiO_2$ material supported ionic liquid/manganese complex ($Fe_3O_4@SiO_2@IL/Mn$) is prepared and characterized using IR, SEM, TG and analyses. The $Fe_3O_4@SiO_2@IL/Mn$ has been applied as an effective, recoverable and highly stable nanocatalyst in the Biginelli reaction (Scheme 1).



Scheme 1. The Biginelli reaction using $Fe_3O_4@SiO_2@IL/Mn$ catalyst

Keywords: Magnetic organosilica, Core-shell nanostructure, Supported ionic liquid, Biginelli reaction

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Ionic liquid/Mo_6O_{19} complex immobilized on magnetic silica nanomaterial: A robust and highly stable catalyst

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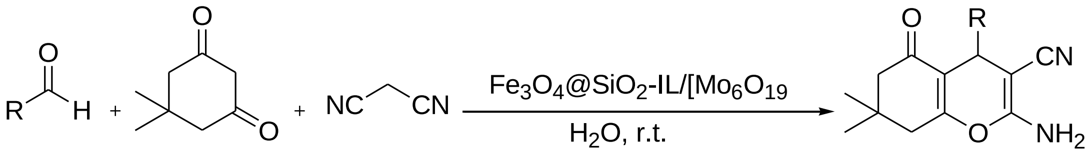
In the last decade, magnetic iron oxide NPs (MNPs) have attracted much interests and are especially employed in biomedical fields, including thermal therapy, magnetic resonance imaging (MRI), and drug delivery [1, 2]. However, MNPs are unstable in the presence of air and acidic/basic media, due to their high surface area and magnetic nature. To overcome these limitations, they are typically coated with a shell of organic and inorganic materials. Among different shells, silica is the most commonly used material to cover MNPs, due to their biocompatibility, availability, high surface area, and easy surface functionalization [3]. Accordingly, herein, a core-shell structured magnetite silica supported ionic liquid/Mo6O19 complex which denoted as Fe3O4@SiO2-IL/[Mo6O19], is prepared and characterized by using IR, XRD, VSM analyses. The Fe3O4@SiO2-IL/[Mo6O19] was employed as an effective and robust nanocatalyst in the preparation of tetrahydrobenzo[b]pyran and delivered corresponding products in high to excellent yields at room temperature (see Fig. 1). The recovery and leaching tests were also performed under applied conditions.



Schem. 1. Preparation of tetrahydrobenzo[b]pyran in the presence of Fe_3O_4@SiO_2-IL/[Mo_6O_{19}]

Keywords: Magnetic nanoparticles, Core-shell, Silica coating, Tetrahydropenzo[b]pyranes

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Synthesis of some new antimicrobial active mercury Schiff base complexes

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Schiff base compounds are an important class of ligands in the coordination chemistry. Recently various Schiff base complexes of XII metal ions have been synthesized and then their biological properties such as antibacterial, antifungal, antibiotic, antioxidant and some other activities have tested.[1-3] Though, metallic mercury is toxic but sometimes, its mercury(II) complexes are of interest in biological research fields.

In continuation of many others, herein synthesis and characterization of a new series of novel mercury(II) complexes with a tridentate Schiff base ligand using spectral, physical and analytical data such as 1H NMR, UV-Vis and FT/IR spectroscopies,melting point, elemental analysis and molar conductivity measurements is described. After that thermal behavior of the compound were studied from room temperature to 800 °C. Moreover, the in vitro antimicrobial activity of the compounds was assayed against two gram-positive, two gram-negative bacteria and two fungal strains by well diffusion method. The results showed that all compounds have antimicrobial properties. Also, the minimum inhibitory concentration and minimum bactericidal concentration of each compound were determined. Finally theoretical optimization on the complex structures were performed to suggest geometiric framework and some information about coordination sphere around the mercury ion.

Keywords: Schiff base, Complex, Symmetric, Tridentate, In vitro antibacterial activity, Minimum inhibitory concentration, Minimum bactericidal concentration

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Schiff-base/cupper complex immobilized on magnetic silica nanomaterial: A durable and efficient catalyst for Ullmann coupling reaction

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Magnetic iron oxide NPs have attracted much attention and are especially interesting in biomedical applications such as thermal therapy, magnetic resonance imaging (MRI), and drug delivery [1, 2]. However, due to their high surface area, they are chemically very active and quickly oxidize in the presence of oxygen source. Also are unstable under acidic and basic media. To overcome these problems, they are typically coated with special materials or a layer of organic and inorganic material. Among different coatings, silica is the most commonly used material to cover magnetic nanoparticles due to their low toxicity, availability, high surface area, and thermal stability [3]. Accordingly, herein, a magnetite silica core-shell supported Schiff-base/Cu complex which denoted as Fe_3O_4@SB/Cu, is prepared and characterized by using IR, XRD, VSM analyses. The Fe_3O_4@SB/Cu has been applied as an effective and highly stable nanocatalyst in the Ullmann reaction and delivered corresponding biaryl derivatives in high yield at 120 ºC (see Fig. 1). This catalyst was recovered and reused several times with keeping its efficiency under applied conditions. The hot filtration test also showed no leaching of active copper species during reaction process.

$$\text{Ar-I + Aryl Amine} \xrightarrow[K_2CO_3,\ 120\ ^\circ C]{Fe_3O_4@SB/Cu} \text{Ar-N-Ar}$$

Schem. 1. Ullmann coupling reaction catalyzed by Fe_3O_4@SB/Cu

Keywords: Magnetic nanoparticles, Core-shell, Silica coating, Ullman reaction

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[1] R. Mirbagheri, D. Elhamifar, *J. Alloys Compd*., **2019**, 790, 783
[2] S. P. Schwaminger, R. Surya, S. Filser, A. Wimmer, F. Weigl, P. Fraga-García, S. Berensmeier, *Sci. Rep.*, **2017**, 7, 12609
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$PrSO_3H$ containing IL-based nanoporous organosilica as an efficient and highly stable nanocatalyst

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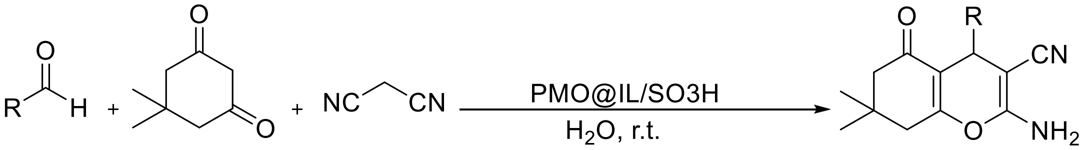
In the last decade, porous nanomaterials (PNMs) have attracted a lot of interest, due to their widespread applications in various fields, including catalysis, chemical separations, and tissue engineering [1]. Based on their pore size, PNMs can be classified into three groups of microporous, mesoporous and macroporous which mesoporous materials are the most important category owing to their high surface area and tunable pore size for entering and exiting various organic and inorganic materials [2]. Among the different kinds of mesoporous materials, periodic mesoporous organosilica (PMOs) have attracted considerable attention because of their high thermal and mechanical stability and also the uniform distribution of organic functional groups in their frameworks [3]. Accordingly, herein, a sulfonic acid containing ionic liquid-based NMs which denoted as PMO@IL/SO_3H is prepared and characterized by using IR and SEM analyses. This PMO@IL/SO_3H has been employed as a robust and highly stable nanocatalyst for the preparation of tetrahydrobenzo[b]pyrans and delivered corresponding products in high yield to excellent yield (see Schem. 1).



Schem. 1. preapartion of tetrahydrobenzo[b]pyranes catalyzed by PMO@IL/SO_3H

Keywords: Magnetic nanoparticles, Core-shell, Silica coating, Tetrahydrobenzo[b]pyranes

References

[1] R. Mirbagheri, D. Elhamifar, *J. Alloys Compd*., **2019**, 790, 783
[2] S. P. Schwaminger, R. Surya, S. Filser, A. Wimmer, F. Weigl, P. Fraga-García, S. Berensmeier, *Sci. Rep*., **2017**, 7, 12609
[3] W. Wu, Z. Wu, T. Yu, C. Jiang, W.-S. Kim, *Sci. Technol. Adv. Mater*., **2015**, 16, 023501

Synthesis, characterization, and investigation of antimicrobial activities of some novel mercury Schiff base complexes

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Nowadays, chemical compounds with biological and medical activity have great importance in chemistry. Schiff bases are organic compounds that widely use and show a broad range of applications. They also present biological activities via the azomethine or imine group in their structures [1, 2]. Schiff base compounds structure can change by changing in the organic part of Schiff base or by alteration in central metal ions [3].
Accordingly, herein, a novel tetradentate Schiff base ligand and some its mercury (II) halide/pesudohalid complexes were synthesized and characterized by multifarious physicochemical techniques such as FT-IR, ^{1}HNMR, ^{13}C-NMR and UV-Visible spectroscopies. Furthermore, thermal behavior of the synthesized compounds was assayed from room temperature to 900 °C. The synthesized compounds were tested for in vitro antibacterial activity against two types of Gram-negative bacteria, Escherichia coli and Pseudomonas aeruginosa and two types of Gram-positive bacteria, Staphylococcus aureus and Bacillus subtillis and also antifungal activities of the compounds were assessed against two fungal strains, Candida albicans and Aspergillus oryaze. The antibacterial activity of the complexes was quantified by measuring the inhibition-zone diameters in millimeters by well diffusion method.

Keywords: Schiff base, Tetradentate, Complex, In vitro antimicrobial activity

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Facile green synthesis of $Ni_{0.5}Mg_{0.5}AlFeO_4$ magnetic nanoparticles and their use as an efficient catalyst for the synthesis of 2H-indazolo [1,2-b]-phthalazine-triones under solvent free and microwave irradiation conditions

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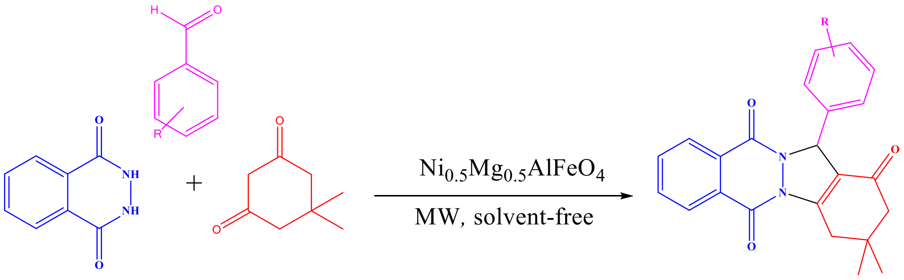
Phthalazine derivatives have attracted considerable interest over the past decade due to their excellent and wide variety of pharmacological and biological activities[1], such as anticonvulsant, cardiotonic, and vasorelaxant activities[2]. Moreover, fused phthalazines have multiple biological activities such as anti-cancer, anti-fungal, anti-microbial, and anti-inflammatory activities[3]. Therefore, the introduction of new methods for the efficient synthesis of fused phthalazines can be useful. In the present study, $Ni_{0.5}Mg_{0.5}AlFeO_4$ magnetic nanoparticles were synthesized using natural gel by the sol-gel method. $Ni_{0.5}Mg_{0.5}AlFeO_4$ MNPs were investigated using powder X-ray diffraction (XRD), Fourier transform infrared spectroscopy (FTIR), Field emission scanning electron microscopy (FESEM), energy dispersive X-ray analysis (EDX) vibrating sample magnetometer (VSM) and Transmission electron microscopy (TEM). The magnetic nanoparticles were used as a highly effective and reusable catalyst for the production of 2H-indazolo[2,1-b]phthalazine-triones by the multi-component reaction of dimedone, arylaldehydes and phthalhydrazide without solvent under microwave irradiation (scheme 1). This new procedure has notable advantages such as operational simplicity, excellent yields, short reaction time, mild reaction condition and easy work up. Also, the catalyst can be easily recovered by a magnetic field and reused for five consecutive reaction cycles without significant loss of activity.



Scheme 1. synthesis of 2H-indazolo[1,2-b]phthalazine-triones

Keywords: Indazolo[2,1-*b*]phthalazine-trione, Multicomponent reaction, Magnetic spinel nanoparticles.

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An efficient one pot multicomponent synthesis of 2, 4, 5-triarylimidazole derivatives using $Cu_{0.5}Zn_{0.5}Fe_2O_4$@ZnO magnetic nanoparticles

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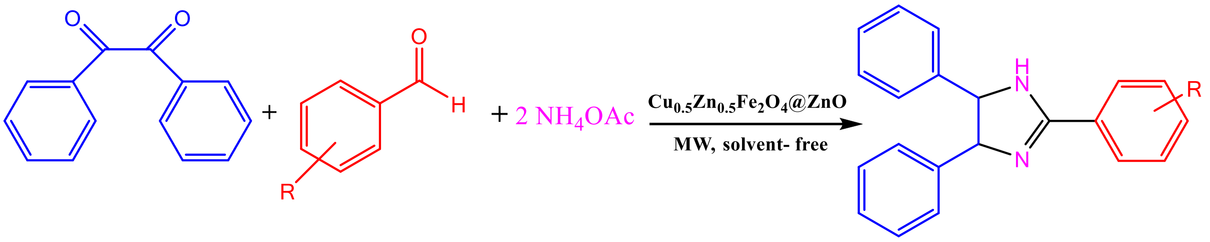
Triarylimidazole compounds have gained remarkable importance due to their widespread biological activities and their use in synthetic chemistry. Imidazole ring system is one of the most important substructures found in a large number of natural products and pharmacologically active compounds such as antiulcerative agent cimetidine[1], the proton pump inhibitor omeprazole[2] and the benzodiazepine antagonist flumazenil[3] are imidazole derivatives. In this work, synthesis of $Cu_{0.5}Zn_{0.5}Fe_2O_4$@ZnO magnetic nanoparticles was performed by the green sol–gel method using natural gel. The sample was characterized by Fourier transform infrared spectrophotometer (FTIR), X-ray powder diffraction (XRD), vibrating sample magnetometer (VSM), Transmission electron microscopy (TEM), Field emission scanning electron microscopy (FESEM) and energy dispersive X-ray analysis (EDX). XRD results show that $Cu_{0.5}Zn_{0.5}Fe_2O_4$@ZnO MNPs corresponds to the hexagonal of ZnO and the spinel cubic structure of $Cu_{0.5}Zn_{0.5}Fe_2O_4$. $Cu_{0.5}Zn_{0.5}Fe_2O_4$@ZnO magnetic nanoparticles were used as a reusable and robust heterogeneous catalyst for one-pot three-component reaction of benzyl, aldehydes, and ammonium acetate in solvent free condition under microwave irradiation (scheme 1). The final product was investigated by ^1H NMR and ^{13}C NMR spectroscopy. The present methodology offers several advantages, such as excellent yields, shorter reaction times, economic availability, and reusability of catalyst.



Scheme 1. Synthesis of 2, 4, 5-triarylimidazole derivatives

Keywords: Multicomponent reactions, Magnetic nanoparticles, Green synthesis.

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Green synthesis of $Zn_{0.5}Ni_{0.5}AlFeO_4$ magnetic nanoparticles: Catalysis efficiency for synthesis of synthesis of 1,8-dioxo-octahydroxanthene derivatives

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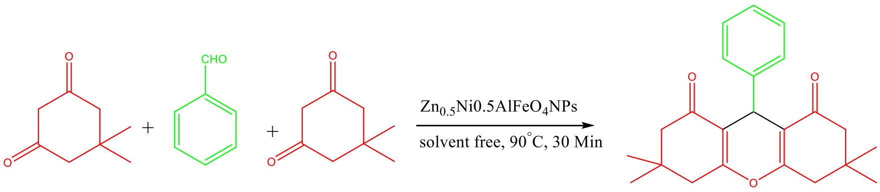
Nanotechnology is the science related to the synthesis and utilization of nanopaticles in diverse fields for example environment, food, health, chemistry, physics, biology, drug delivery, cosmetics, engineering, etc[1,2]. Diverse methods have been offered for the prepatio of nanoparticles such as physical, chemical, and green methods. In recent years, spinel structures have appealed kindness for their efficency as catalyst. A large class of mixed valence metal oxides crystallizes in spinel structure with a general formula of AB_2O_4, that, for the most spinels, A and B are di- and trivalent cations (2–3 spinels), respectively [3]. In this work, $Zn_{0.5}Ni_{0.5}AlFeO_4$ MNPs were synthesized using green methods without using any organic chemicals and were used as efficient magnetic catalyst. Henceforth, 1,8-dioxo-octahydroxanthene derivatives were prepared via solvent free multi-component reactions. 2 mmol dimedone and 1mmol benzaldehyde were used as starting materials (scheme 1). This method has numerous advantages such as environment friendly, high yields and simple work-up technique. The molecular structure of products has been determined by IR, ^{1}HNMR, and ^{13}CNMR techniques.



Scheme 1. Synthesis of 1,8-dioxo-octahydroxanthene derivatives

Keywords: Green synthesis, Spinel nanoparticle, 1,8-dioxo-octahydroxanthene.

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Synthesis and characterization of $MgFe_2O_4@\gamma{-}Al_2O_3$ magnetic nanocomposite as an efficient catalyst for synthesis of 3,4-dihydropyrimidin2-ones

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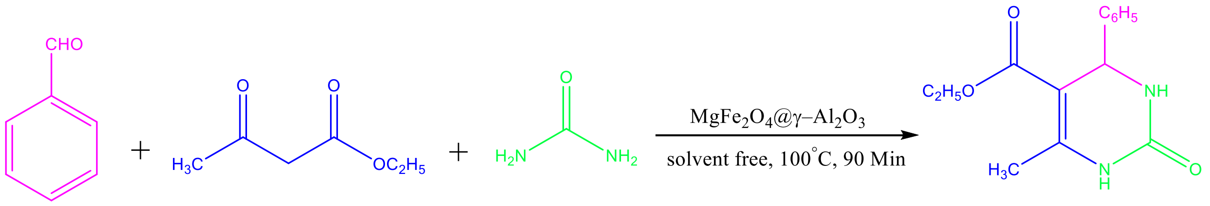
One-pot multicomponent condensation reactions represent an efficient tool to perform efficient synthesis, because they allow the assembly of complex molecules with maximum simplicity and brevity. Dihydropyrimidinones (DHPMs) are important substructures present in a wide variety of biologically active natural products[1]. The magnetic nanocomposite (MNCs) have attracted much consideration due to their rapid and easy separation, economic viability, reusability and recoverability[2,3]. In this study, $MgFe_2O_4@\gamma{-}Al_2O_3$ magnetic nanocomposite was characterized by FTIR, FESEM, EDX, VSM, TEM, and XRD. Synthesised catalyst was used for the synthesis of 3,4-dihydropyrimidin-2-ones derivatives via solvent free multi-component reactions (scheme 1)and structure of products has been determined by IR, ^{1}HNMR, and ^{13}CNMR techniques.



Scheme. 1. Synthesis of dihydropyrimidin derivatives

Keywords: Magnetic nanocomposite, Multicomponent reactions, Dihydropyrimidin.

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Preparation of new 1-phenyl-1H-tetrazole-5-thiol derivatives using michael reaction under solvent-free conditions

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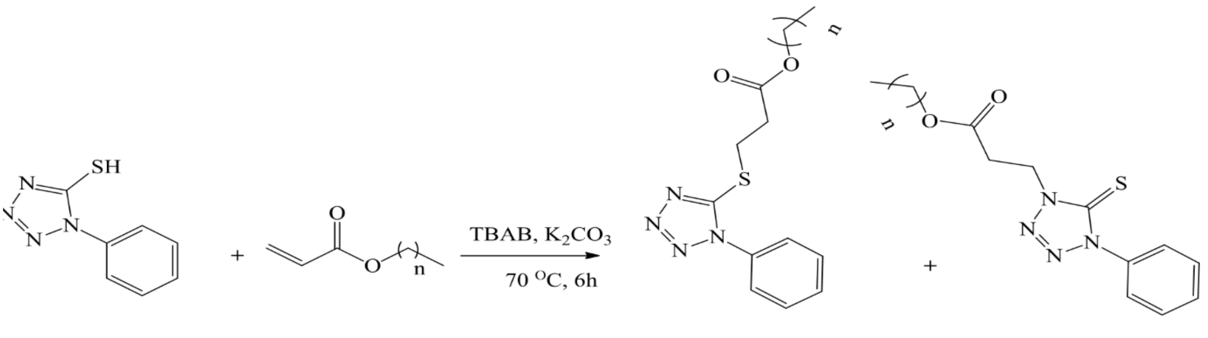
In this research, the reaction of PHtt with α,β-unsaturated esters has been investigated. Considering the use of 1-substituted 1H-tetrazole-5-thiols in the synthesis of pharmaceuticals, we decided to study the Michael addition reaction of PHtt with acrylate [1]. in an alkylation reaction by nucleophilic substitution method, S is used in the reaction. In the alkylation reaction by Michael method, depending on the reaction conditions, the product can be S-Michael, N_4-Michael or both. Therefore, considering the medicinal applications of the derivatives of this compound, we decided to synthesize new PHtt derivatives in solvent-free (green) conditions. due to the presence of tautomerization in PHtt, the reaction can be carried out from the S and N_4 positions. in the reaction with acrylate esters, at room temperature, the reaction is syntactic and the increase of Michael takes place from the S position, but at 70 °C, the reaction proceeds thermodynamically and the S-Michael product is neutralized and takes longer location from position N_4 [2].

Keywords: PHtt, Michael, Green, Solvent-free conditions



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Dimers of aromatic and aliphatic hydrazides with the aim of inhibiting cathepsin B

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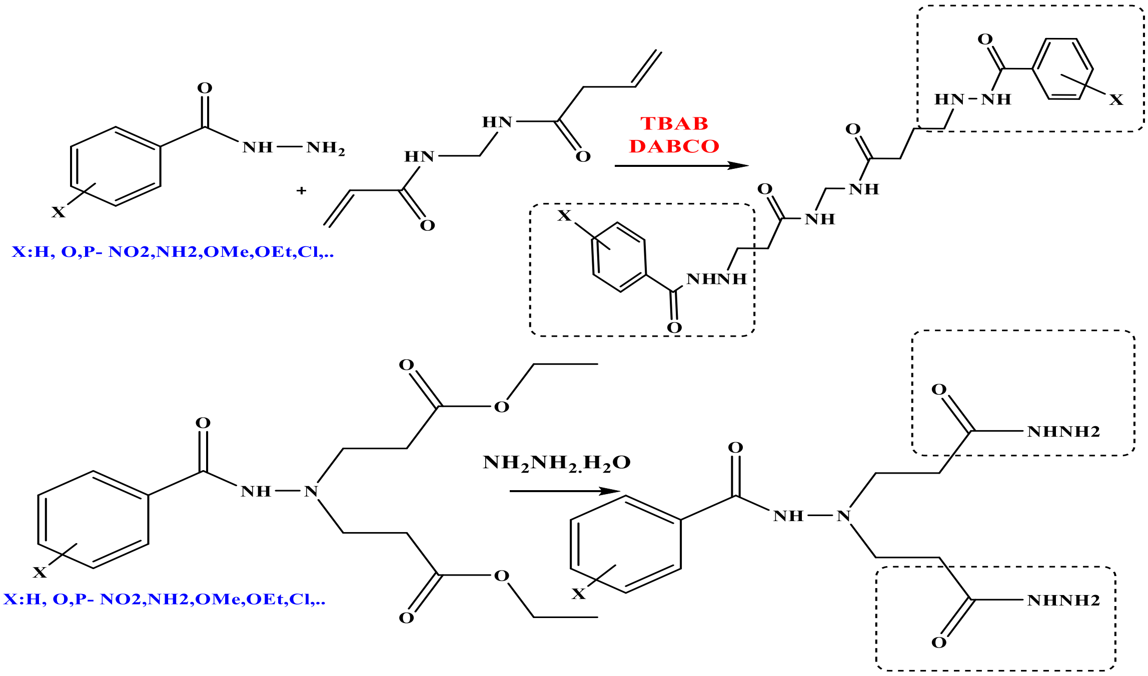
Recent studies showed that cathepsin B is roled in tumor extracellular matrix remodeling, cell invasion, and metastasis. It is recognized that a misbalance between cathepsins and their natural inhibitors is a sign of disease progression [1]. some acyl hydrazides and triazoles have been reported as inhibitors of mammalian cathepsin B and cathepsin H [2]. With attention to the above, we decided to synthesize new dimers of hydrazides as potent inhibitors of cathepsin B. for this purpose, we use n n'-methylene acrylamide as a Michael receptor for aromatic hydrazides to synthesize dimers with peptide bonds under solvent-free conditions. and aliphatic dimers have obtained with the reaction of Michael products of our previous work [3] with hydrazine hydrate in ethanole.



Keywords: Dimer- hydrazides- cathepsin B- solvent free conditions

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Novel Isatin-Dihydropyrimidinones hybrids and their Cu(II) complexes as potent anticancer agents

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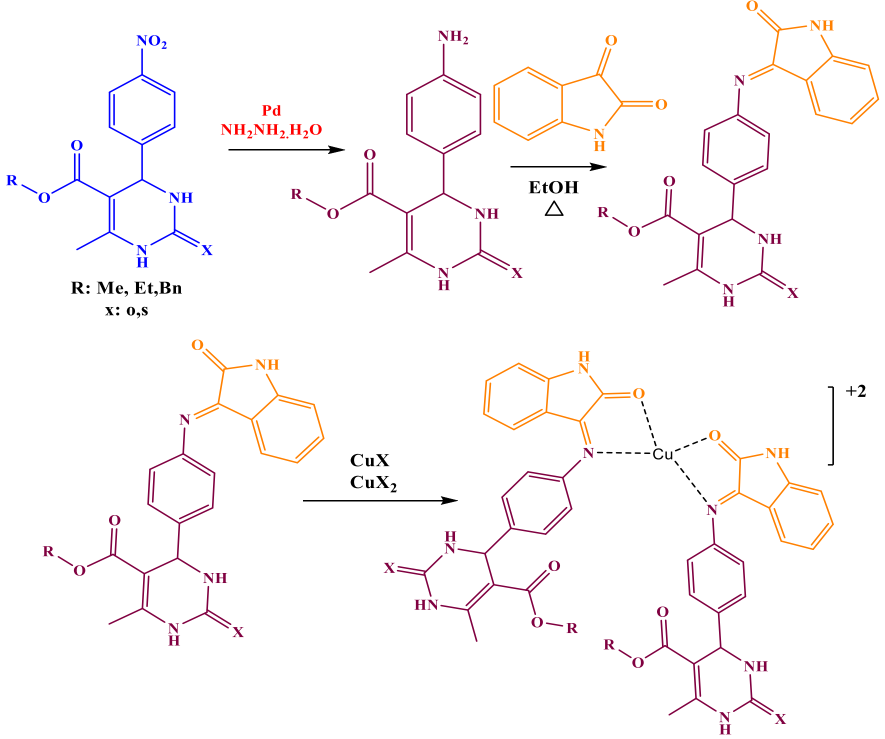
Because of its biocompatibility and versatility in coordination copper is one of the best choices for chemists in designing anticancer agents. It is likely that copper like endogenous metals may be less toxic for normal cells than cancer cells [1]. There are many copper contain complexes that show potential antitumor, anticancer activities [2]. On the other hand, the incorporation of two or more potent pharmacophores into a single hybrid molecule shows biological activities higher than those of the corresponding precursors together with much lower toxicity and reduced side effects. This recent tendency in drug design becomes particularly visible in the field of isatin and Dihydropyrimidinones chemistry. [3, 4]. In this work, we synthesized new Cu(II) complexes of Isatin-Dihydropyrimidinones hybrids and evaluated theirs in vitro anticancer activity.



Keywords: Cu(II) complexes -Isatin- Dihydroprimidinone- hybrid molecules- anticancer activity

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Microextraction by Packed Sorbent Based on Montmorillonite Bonded on Filter Paper for Determination of Carvedilol in Biological Samples

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In this work, a novel nano-structured sorbent was introduced for microextraction by packed sorbent (MEPS), which has been prepared based on grafted montmorillonite on a cellulosic paper (MMT/Cell) by chemically bonding to the surface of a cellulosic paper by glutaraldehyde as a cross linker. The prepared MEPS device was used for extraction of carvedilol (CAR) from biological samples followed by high performance liquid chromatography-ultra-violet absorption (HPLC-UV) detection. Scanning electron microscopy (SEM) was applied to investigate the morphology and the surface characteristics of the prepared thin layers and their elemental analysis was studied by energy dispersive X-ray spectroscopy (EDX). To study the presence of various functional groups on the MMT/Cell surface, Attenuated total reflection-Furier transform infrared spectroscopy (ATR-FTIR) was employed. Important parameters affecting the MEPS method including extraction draw-discard cycles, sorbent layers, desorption draw-eject cycles, pH, elution solvent and its volume were optimized. Based on the method validation, the calibration graphs for carvedilol is linear in the concentration range of 1.5 to 300 ng mL^{-1} and the limit of detection (LOD) was 0.5 ng mL^{-1}. The MEPS-HPLC-UV method precision (RSD %) considering three replications of extraction from spiked deionized water (100 ng mL^{-1}) was 6.8%. Standard addition method was applied to determine CAR in urine and plasma samples, and the relative recoveries (RR%) were 90.2 % and 80.0 % for urine and plasma samples, respectively, indicating the capability of the developed MEPS-HPLC-UV method to extract and determine CAR in biological samples [1-3].

***Keywords**:* Microextraction in packed sorbent, Montmorillonite, Mellulosic paper, Biological and environmental samples

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Preparation of biodegradable film based on modified marshmallow root mucilage with xanthophyll pigment nanoliposomes and vanadium oxide nanoparticles

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In recent years, packaging made from natural and changeable polymers has received a great deal of attention due to its high performance. Therefore, the aim of this study was to prepare a biodegradable film based on marshmallow root mucilage modified with xanthophyll pigment nanoliposomes and vanadium oxide nanoparticles [1]. For this purpose, the central composite design was evaluated to investigate the effect of marshmallow root mucilage and vanadium oxide nanoparticles modified with xanthophyll pigment nanoliposomes on physicochemical and structural properties of the produced film. Properties of the prepared nanocomposite include thickness, water vapor permeability, solubility, moisture, antioxidant properties, color indicators, transparency, mechanical properties, antimicrobial properties FTIR / FESEM / XRD / TGA tests were evaluated [2]. The results showed that the addition of marshmallow root mucilage led to an increase in thickness, moisture and index a of the samples and on the other hand a decrease in moisture from index a was observed by adding nanoparticles. With increasing replacement of marshmallow root mucilage, index b of samples decreased slightly and with increasing nanoparticles, yellowness increased. In the images obtained from FESEM, films containing nanoparticles and nanoliposomes showed a homogeneous and homogeneous film with low grain state. According to TGA results, film samples containing nanoliposomes and nanoparticles had better thermal stability than the control sample and the results of XRD showed that by adding nanoparticles and nanoliposomes to the films, there was not much change in the position of the peaks, but the intensity of the peaks was reduced.

Keywords: Nanoliposomes, xanthophylls, packaging films, nanocomposites, mucilage.

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A STUDY OF COMPLEX FORMATION OF COBALT(II) AND NICKEL (II) WITH 1-(2-PYRIDYLAZO)-2-HYDROXY-4-MERCAPTOPHENOL AND DIPHENYLGUANIDINE

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Here are the results of systematic studies of the extraction-chromogenic system, cobalt and nickel with 1-(2-pyridylazo)-2-hydroxy-4-mercaptophenol (PHMP) AND diphenylguanidine (DPG).

At pH 5-6, the cobalt-nickel complex {Me-PHMP-DPG (Me=Co or Ni)} is not extracted with inert organic solvents. To determine the charge sign of the complex, ion-exchange chromatography was used: the AV17 anion exchanger in chloroform absorbs part of the solution; the chromatographic column is colored orange; Ni(II) and Co(II) are not detected in the filtrate. The anionic complex is extracted in the presence of a hydrophobic amine, while the stability of the complex increases and the color becomes more saturated. To neutralize the charge of the anionic complex, diphenylguanidine was used as a hydrophobic amine.

The spectra of mixed ligand complexes (MLC) Me (II)-PHMP-DPG, extracted in chloroform. Complexes of cobalt and nickel are formed and extracted at pH 2.2-8.4 and 2.5-10.8, respectively. It could be seen that Co(II)- PHMP - DPG species are extracted in a great extent at pH values in the range 5.5–7.8. Ni(II) complexes are extracted at lower pH: 4.4–6.7. The best extractants were $CHCl_3$, $C_2H_4Cl_2$ and C_6H_5Cl. All further studies were carried out with $CHCl_3$ (extraction ratio (R,%) R=98.3-98.6%).

Co-HITP-DPG cobalt complex absorption is higher than that of the Ni-HITP-DPG nickel complex. The maximum values are recorded at 560 nm for Co (II) compounds and at 480 nm for Ni (II) compounds. For the formation and extraction of MLC, $(1.2\text{-}2.0) \times 10^{-3}$ M PHMP and $(2.0\text{-}2.5) \times 10^{-3}$ M DPG are required. Extracts of Ni-system and Co-system are achieved within approximately 2 minutes and 4 minutes respectively. A longer shaking time does not affect absorption. The molar ratios between the components of the MLC were found by several methods: relative yield method, straight line method and equilibrium shift method. The results suggest the complex composition of 1:2:2 (Me : PHMP : DPG).

To evaluate the complex applicability for photometric determination of cobalt and nickel, we examined the influence of foreign ions and reagents. The results showed that great excesses of alkali, alkali earth, and rare earth elements, as well as NO^{3-}, ClO^{4-}, SO_4^{2-} and CH_3COO^{-} do not interfere determination of cobalt and nickel with PHMP and Am. Interference of most cations masked by the addition of complexone III. Tartrate mask the milligram quantities of Ta, Ti, W and Mo. Zr fluorides should mask, and copper-thiourea.

Based on the results of spectrophotometric studies of cobalt (II) with L, methods have been developed for the determination of cobalt and nickel in plants (beans: 0.20 ± 0.0053 μg/kg Co; 0.28 ± 0.0042 μg/kg Ni; peas: 0.11 ± 0.0040 μg/kg Co; 0.31 ± 0.0041 μg/kg Ni).

Keywords: Cobalt, nickel, 1-(2-pyridylazo)-2-hydroxy-4-mercaptophenol, extraction-photometric method

Adsorbents used in the purification of phosphate ions from drinking waters

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Phosphorus stimulates plant growth (eutrophication) in rivers, lakes, streams and oceans. A significant part of the phosphorus in natural reservoirs enters them through wastewater. Due to the globalization of the problem of eutrophication, the need for the removal of phosphorus from wastewater is increasing [1].

Currently, the application of nanotechnology for water and sewage treatment has become a topic of great attention and care. Nanoparticles are one of the most important structures in nanotechnology. The most important feature of nanoparticles is their high reactivity due to their large surface-to-volume ratio, which can be used for a variety of applications in many fields. Among the different nanoparticles, iron nanoparticles have aroused great interest due to their superparamagnetic, high reactivity and non-toxic properties. These nanoparticles are used in various fields such as terabit magnetic storage devices, catalysis, sensors, high-sensitivity biomolecular magnetic resonance imaging (MRI) and wastewater treatment. Iron nanoparticles have been used as adsorbents for the extraction of heavy metals, the recovery of precious metals and the removal of dyes. These nanoparticles can also be used to modify commercial adsorbents [2].

Activated carbon has long been the preferred adsorbent in major industrial applications, especially in water and wastewater treatment processes, due to its high adsorption capacity, high adsorption rate and good abrasion resistance. Purification of solutions containing phosphorus compounds is based on the adsorption process. In this study, we calculated the thermodynamics of the process at 25°C, 35°C, 45°C using Fe-AC nanocomposites. we mixed in mixer. Then we filtered and measured the result of experiments - 50 ml parent solution + 0.5 g Fe-AC. Results of experiments performed that at different times at 35°C: 30 min−400 mg/g; 60 min−425 mg/g; 120 min −462mg/g phosphate anions were adsorbed by Fe-AC nanocomposites

Keywords: nanocomposite, adsorption, phosphate, drinking water

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Spectrophotometric determination of copper(ii) with 2,6-dimercapto-4-methylphenol and phenanthroline

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Copper shows a strong affinity for ordinary donor atoms (O, N, S). In addition to amines, phenolic or alcoholic oxycompounds, mercaptans, thioacids and other compounds are used. S-analogues of oxygen-containing compounds are the most reactive with respect to copper [1].

This work is devoted to studying the interaction of copper(II) with 2,6-dimercapto-4-methylphenol (DMMP) and phenantroline (Phen). The optimal pH, at which the optical density is maximum and constant, is at pH 6.7-7.9. At a solution pH of 9, the extraction of the mixed-ligand complex (MLC) is practically not observed, which, apparently, is associated with an increase in concentration in an aqueous solution of the non-extracting $[CuR_2]^{4-}$ complex, since the dissociation of H3R along the second sulfhydryl group continues to increase. Chloroform was used as an extractant (the degree of extraction is 98.2%). The optimal condition for the formation and extraction of MLC is $0.8 \cdot 10^{-3}$ mol/l and $1.0 \cdot 10^{-3}$ mol/l concentrations of DMMP and Am, respectively. Copper SLK with DF and Am are stable in aqueous and organic solvents and do not decompose within three days, and after extraction - more than a month. The maximum optical density is reached within 5 minutes. The maximum analytical signal during the complex formation of copper with dithiolphenols and Am is observed at 630 nm ($\varepsilon_к = 3.45 \cdot 10^4$). The stoichiometry of the studied complexes was determined by the methods of equilibrium shift and relative yield. The ratio of components in MLC is as follows: Cu : DMMP: Am = 1:1:1. It was established by the Nazarenko method that the complexing form of copper is Cu^{2+}. In this case, the number of protons displaced by it from one DMMP molecule turned out to be equal to 1. The disappearance of a pronounced band at 2580 cm^{-1} observed in the spectrum of DMMP and the appearance in the spectra of the complex of two absorption bands, one of which is shifted towards smaller frequencies, indicates that one of the –SH groups is involved in the formation of the complex. The disappearance of the absorption band at 3460 cm^{-1} indicates that the hydroxyl group takes part in the formation of a bond with the metal. The detection of absorption bands at 1370 cm^{-1} indicates the presence of coordinated phenanthroline.

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Extraction of valuable components from poor ore wastes

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Экономическое развитие страны во многом зависит от степени эффективного использования природных запасов, в том числе, запасов месторождений полезных ископаемых и развития отраслей промышленности, занимающихся их переработкой. Кучное выщелачивание, в настоящее время, является очень распространенной практикой, проводится на руднике с низкой капиталоёмкостью, что позволяет удовлетворительно управлять остатками производства [1]. На кучное выщелачивания руд и отвалов приходится порядка 20% годового мирового производства меди [2].

На образцах текущих хвостов обогащения Дашкесанского горно-обогатительного комбината Азербайджана с содержанием Al, Ca, Fe, Si, Co, Cu, Zn, Mn, V, Ga, In проведено исследование процесса кучного выщелачивания – наиболее простого и дешёвого способа переработки такого вида сырья. Предварительные эксперименты на перколяционных колоннах кучного и подземного способа промывки железорудных отходов с целью подбора типа растворителя, который эффективно вымывал бы металлы в отходах (Co, Cu, Zn и Mn), показали, что в ряду растворителей - H_2O, H_2SO_4, NaOH, NH_4Cl, $(NH_4)_2SO_4$, CH_3COOH - наиболее эффективным реагентом для размыва отходов является раствор серной кислоты. Учитывая, что на промывку 1 тонны отходов (по нашим расчетам) расходуется не менее 600 л H_2SO_4 (1 N), серную кислоту получали электролизом солевых растворов K_2SO_4 и Na_2SO_4 из продуктов переработки алунита для предотвращения реактивной экстракции.

Основную часть отходов составляют алюмосиликатные соединения (рис. 1). Сложный минералогический состав отходов и низкое содержание кобальта, меди, цинка и марганца в такой многокомпонентной системе не позволяет определять эти микроэлементы с помощью РФА.

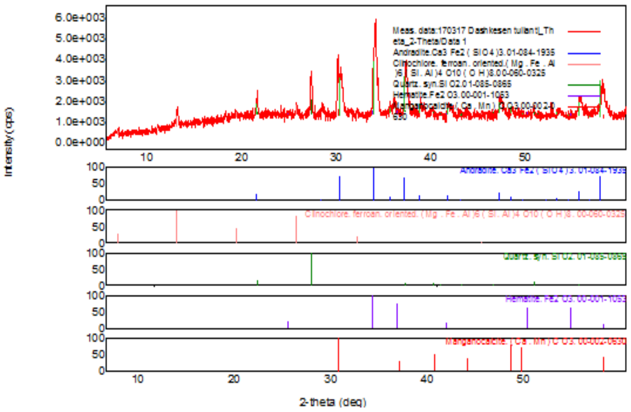

Рис. 1. Рентгенофазовый анализ сухих отходов в северной части пляжной зоны

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The study the behavioural fuctions of miopardalis pardalina under simulators pheromone influence

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Melon fly (Miopardalis pardalina) is widespread in Asia and some European countries, in particularly Azerbaijan, Armenia, Georgia, Cyprus, Turkey, and Ukraine. Afghanistan, Israel, India, Jordan, Iraq, Iran, Kazakhstan, Kyrgyzstan, Lebanon, Pakistan, Saudi Arabia Arabia, Syria, Tajikistan, Turkmenistan, Uzbekistan. It mainly damages wild and cultivated plants from the Cucurbitaceae family: melon, watermelon, sometimes - pumpkin and cucumber, prefers melon Cucumis melo. During the year Miopardalis pardalina gives 3-4 generations. Flies appear at the time of melon flowering. Female laid their eggs in the skin of ovaries and young fruits, as well as on leaves. The larvae penetrate the pulp of the fruit, where they feed on seeds, then leave the fruit and go to pupate in the soil. Spring years coincide with the period of fruit formation in the plants. At this time, the temperature of the soil where insects hibernate reaches + 20°C. The period of pest insects flying are observed from early June to mid-October. They feed on fruit juice. The period of imago life prolonged about 2 months. The puncture sites of the pulp can serve as a medium for the viral and fungal diseases. The first signs of melon damage are the appearance of small tuberculous spots or just tubercles in places where the fruits are bitten. Later, after the appearing of the larvae, begins internal decay of the fruit. And after, damaged fruits become unsuitable for further usage. For the limiting of the further pest insects spreading, strict quarantine restrictions taking place. One element of a pest management program is the elimination of males, or the reducing of fruit damage, the capture of female is equally important. According to main the pheromones importance for for the vital insects activity, we carried out biological tests of the sum pheromones mimics substances of Miopardalis pardalina, in various behavioral functions of the insect, in particular, in a time of copulation or time for choosing a place for laying eggs.

To study of the pheromone mimics effect on the Miopardalis pardalina behavior, we synthesized 4-(4'-hydroxyphenyl)-2-butanone acetate. We used anisaldehyde as the starting compound. From which they were successively obtained - anisalacetone - by a coupling reaction with acetone; - anisylacetone - as a result of hydrogenation; to protect the existing keto group, diethylene glycol was used; - 4-(4'-hydroxyphenyl)-2-butanone - according to the etherification reaction; and in the final result of acetylation reaction was - 4-(4'-hydroxyphenyl)-2-butanone acetate.

The synthetical product with an additional attractiveness synergist for Miopardalis pardalina, have been testing on farms in the Karakalpak region of Uzbekistan.

Selection of an effective sorbent for the disposal of arsenic from arsenic ore wastes and study of physical and chemical parameters of the sorbent

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Arsenic, found in ore wastes and groundwater, is currently one of the world's most pressing problems. The chemical compounds of this element have a negative effect on millions of people. Therefore, the European Union and the International Agency for Research on Cancer have classified arsenic as the No. 1 carcinogen (67/548 / EEC directive) [1].

It is necessary to develop an effective and environmentally friendly technology for the processing of arsenic ores. A modern solution to this problem can be found by complex processing. Currently, the conditions for maximum arsenic deposition from the residues after the extraction of the main components (Au, Co, Cu) during ore processing should be studied and the factors influencing the process (pH, temperature, concentration, etc.) should be studied. Or the choice of an effective adsorbent remains relevant. World-class arsenic utilization has not yet found a solution, either scientifically or technologically [2]. The toxicity of arsenic compounds is as follows: As (III) > As (V) > Organic As compounds

As found in ores and waters, it is inorganic, so catching it with organic carriers is important to reduce its toxicity. The most effective sediment used in world practice is iron and its compounds. The use of peanut shells as an adsorbent has been experimented with. Thus, peanut shells impregnated with iron compounds provide both effective sedimentation and effective sorption. Enrichment of shells with coal increases the efficiency by 99.9% (Fig 1).

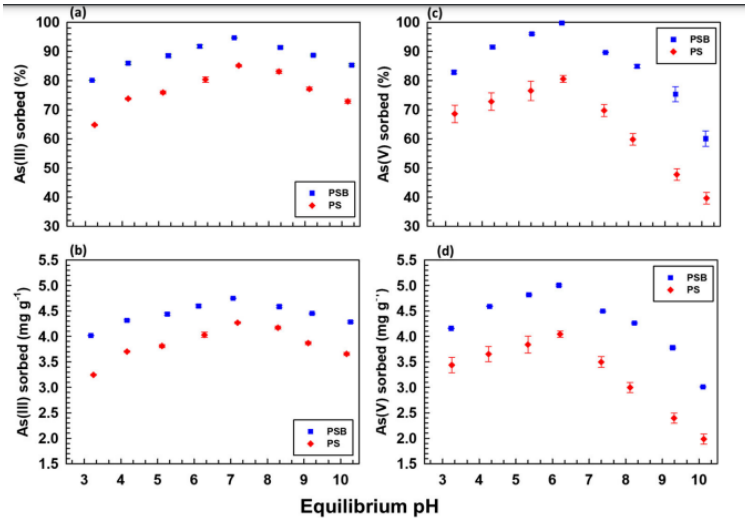

Fig.1 As sorption by peanut shell and peanut shell biochar doped with iron compounds.

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Precipitation of vanadium in the form of ammonium vanadate

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As a result of alkali solubility in alkali, in addition to the main component $NaAlO_2$, other micro-mixtures $NaVO_3$ and Na_2SiO_3 were present in the solution. Vanadium is precipitated from aluminate solutions in the form of polyvanadate and metavanadate. NH_4Cl, $(NH_4)_2SO_4$, CaO, $Ca(OH)_2$, $CaCl_2$ [1, 2] are used as precipitating reagents.

The precipitation of vanadium in the solutions obtained from the processing of alunite, due to the presence of large amounts of alkali metal sulfates in the solution (ie due to the abundance of SO_4^{2-} ions), we precipitated vanadium not with NH_4Cl, but with $(NH_4)_2SO_4$. Due to the absence of Cl^- ions in the solution during the production of alunite, the transfer of foreign Cl- ions to the solution emphasizes the purification of solutions from this ion in the subsequent processing stages.

Air containing 10-12% CO_2 in sodium aluminate solution is brought to pH = 9.0-10.5 at a rate of 3 l/min for 8-10 hours. At this pH, the bulk of $Al(OH)_3$ (90%) is precipitated. Along with aluminum, $Ga(OH)_3$ precipitates in the new sediment. After the separation of aluminum, phosphate and gallium compounds, the solution consists of alkali metal sulfates (Na_2SO_4, K_2SO_4) and sodium vanadate. Ammonium sulfate is added to such a solution (NH_4) until the molar ratio of $2SO_4:V_2O_5$ reaches 2.5:1. Add different amounts of $(NH_4)_2SO_4$ to 100 ml of sodium vanadate solution and mix until the salt is dissolved. If sedimentation is not observed at first, sedimentation is observed after a certain period of time. Initially, the precipitant dose was determined by adding different amounts of ammonium sulfate to sodium vanadate solutions.

When the mass ratio of V_2O_5 oxide to $(NH_4)_2SO_4$ is 1:2.6, vanadium can precipitate 99%. The composition of the ammonium vanadate sample was confirmed by X-ray phase analysis (Fig. 1).

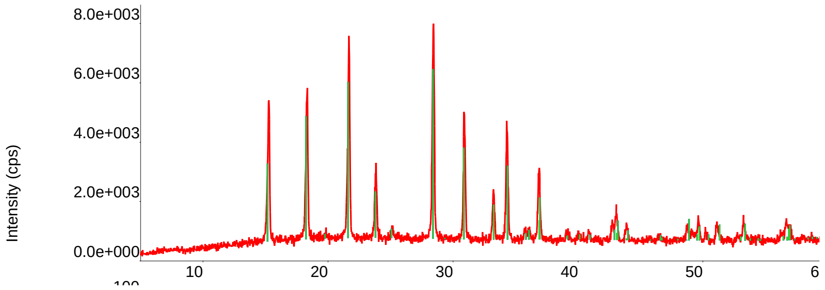

Figure 1. X-ray phase analysis of ammonium vanadate

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A study of the impact of clay minerals on the ecological condition of the soil

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At present, the soil, in the ecological sense of the word, is subjected to the greatest anthropogenic pollution. During the intensive work of various industries: energy, industrial and agricultural construction, transport, etc. there is one or another negative impact on the eco-balance of the environment [1]. The greatest danger in this aspect is and chemical, metal processing, oil, metallurgical and some other industries which intensively pollute the biosphere by gas emissions, solid wastes and wastewater.

The main toxic component polluting wastewater are aromatic compounds, ions of some heavy metals such as: chromium (VI), cadmium, lead and other toxic substances. Non-ferrous metallurgy is also one of the industries that contributes most significantly to environmental degradation. When processing ores, non-ferrous metallurgy enterprises generate solid waste such as red mud, which is accumulated over large areas, causing irreparable damage to the fertility of agricultural land. It should be noted that red mud contains a significant amount of toxic elements, such as oxides of iron, aluminum and titanium. Questions of processing of waste products are still very urgent, which is due to the need for disposal of man-made waste as toxic elements negatively affect the environment, which is closely related to industrial ecology and safety of life of living organisms.

This work is devoted to the study of the impact of natural minerals on the ecological state of the soil. Clay minerals, from the group of smectites, are used in crop production when used as a substrate, as well as in the saturation of plants with useful minerals. In this case, it was of interest to study their behavior when applied to the soil along with mineral fertilizers. The fact that the structural composition of aluminosilicates is saturated with a number of inorganic elements which actively participate in sorption processes was taken into account. The structure of aluminosilicates and their mineralogical and elemental composition are described. It is shown that they are able, depending on temperature and humidity, to give and re-absorb water, as well as to ionic exchange, i.e. to selectively release and re-absorb various substances. The main natural physical condition of clay minerals is their high dispersion, the size of microcrystals of such minerals does not exceed a few micrometers, therefore they are referred to nanoscale materials.

Specific properties are due to the structure of the crystal lattice of the minerals composing these clays. It has been established that when clay minerals are introduced into the soil, they contribute to the preservation of Mg^{2+},Ca^{2+}, K^+ cations for several years. Indicators of the granulometric method of studies of the composition of clean and contaminated soils with toxic elements are given. Bentonite clays together with superphosphate when applied to the soil improves not only the ecological condition of the soil, but also increases plant growth and has a positive effect on the absorbed phosphorus in the soil.

Keywords: *clay minerals, soil, ekologi,* aluminosilicates,cations

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Determination of molybdenium (vi) and tungsten (vi) with tetrahydroxyazon sn in a micellar medium

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The reactions of molybdenium (VI) and tungsten (VI) with tetrahydroxyazon SN (2,2,3,4 - tetrahydroxy - 3 - sulpho - 5 - nitroazobenzene) in the presence of catonic, anonic and non - ionic surfactans were investigated spectrophotometrically. Maximum enhancement of the absorbance of the complexes is obtained with the catonic surfactant CTMAB (cetyltri methylammonium bromide), anonic surfactant SDS (sodium dodecyl sulphate) and non-ionic surfactant Triton X - 100.

The binary complexes is formed with tetrahydroxyazon SN was obtain when their solutions were acidium medium the range 0,01 — 4 M sulphonic acid that the maximum absorbance 500 nm, with molar absorbtivities 1.7-10^4 L mol^{-1} cm^{-1}of molybdenium and of tungsten the range 0,01 -2 M HCI acid the maximum absorbance 490 nm, with molar absorbtivities 3,2-10^4 L mol^{-1} cm^{-1}.

Investigation of the effect of acidium medium the maximum absorbance of the ternary complexes revealed maximum and constant values in the acidium medium ranges 0,1 - 2M sulphonic acid, 540 nm, with molar absorbtivities 1,25 -10^5 L mol^{-1} cm^{-1}for molybdenium - tetrahydroxyazon SN - CTMAB; maximum absorbance 535 nm, ε = 3,72-10^4 L mol^{-1} cm^{-1}for molybdenium - tetrahydroxyazon NS - SDS; maximum absorbance 530 nm, ε= 5,17-10^4 L mol *A* cm' for molybdenium - tetrahydroxyazon NS -f Triton X-100 and 0,1 - 1M HCI acid 525 nm, with molar absorbtivities 1,38-10^5 1. mol^{-1} cm^{-1} for tungsten - tetrahydroxyazon SN - CTMAB; 510 nm, with ε = 4,00 • 10 ^{4} L mol^{-1} cm^{-1}for tungsten - tetrahydroxyazon NS-SDS; 515'nm, with ε = 5,12 -10^4 L mol cm'^{1} for tungsten - tetrahydroxyazon SN -Triton X-100. Therefore, 2M sulphonic acid acid 1M HCI acid are recomended for the determination of molybdenium (VI) and tungsten (VI) with tetrahydroxyazon SN in a micellar medium.

Under the optimum conditions, Bees law was obeyed over the range 0,04 - 0,09 µg • ml^{-1}f molybdenium (VI) and 0,04 -1,6 mg ml^{-1} tungsten (VI). In the presence of CTMAB the ratio of Mo to tetrahydroxyazon SN and the ratio of tungsten - tetrahydroxyazon SN-CTMAB obtained by the mole ratio method with'the final concentration of tetrahydroxyazon SN fixed 2; 10 mol L^{-1} were both 1:1.Thus the composition ratio of the molybdenium (VI) and tungsten (Vi) complexes was metal, tetrahydroxyazon SN : CTMAB= 1:1:2.Effects of some other foreign ions. The results, together with the effects of the reducing agents and complexing agents Zn, Mn, Ni, Co, Cu, Cd, Hg, Pb, Al, Cr, Ti, Zr, Bi, U, absorbinic acid, salicil acid, etc. interfere, in varging degree, with the determination of molybdenium (VI) and tungsten (VI).

The selectivity and sensivity the propose method was applied to the direct determination of molybdenium and tungsten in steel, alloys, in natural water, waste water, in plants and seeds. The obtained analytical results were in good agreement with the certified values.

Spectrophotometric determination of thorium (iv) with tetradyroxyazon sci in the earth minerals

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Thorium is an important element. It is often used as a fuel for nuclear reactors besides its industrial applications. Thorium(IV) occurs in nature in the Earths crustin the form of the mineral monazite with different proportions of most of the rare earth minerals. The determination of Thorium (IV) in the presence of these ions is of special interest. An effort has been made to develop a selective, reproducible and sensitive method for the determination of Thorium (IV) with.

In this paper a spectrophotometric study on the interaction of Thorium(IV) with 2,2,3,4 -Tetrahydroxy-3 -sulpho-5 -nitroazobenzene (tetrahydroxyazon SN) and 2,2,3,4-Tetrahydroxy-3 -sulpho-5 -chlorazobenzene (tetrahydroxyazon SCI).

The purple coloured complex formed between Thorium(IV), tetrahydroxyazon SN and tetrahydroxyazon SCI in acidic medium was investigated spectrophotometrically. Results obtained revealed the formation of Th : R = 1:2 complex in aqueous solution at pH 2 and pH 1 with a Logarithmic conditional stability constant of 18, 16 ±0.08. The color of the complex was used for the determination of Thorium(IV) in the range 0,1-3,6 µg ml^{-1} Th^{4+} with there tetrahydroxyazon SN at 520 nm and 0,08-2,8 µg ml^{-1} Th^{4+} with there tetrahydroxyazon SCI at 500 nm. Beside its high sensivity, the reaction was also proved to be highly selective for Thorium (IV). Thorium(IV) was determined in presence of great number of transition metal ions, rare earths.

The complex tetrahydroxyazon SCI solution at pH 1 a maximum absorbance at 500 nm, with a molar absorptivity of $7{,}06\text{-}10^{4}$ 1 mol^{-1}cm^{-1} and tetrahydroxyozone SN solution at pH 2 a maximum absorbance at 520 nm, with a molar absorptivity of $6{,}30\text{-}10^{4}$1 mol^{-1}cm^{-1}. The detection limit of the method is 0,1 µg Th (IV) ml^{-1}, the RSO (n=8) is 1,6 %. The method has been successfully employed for the determination of Thorium (IV) in various standart and monazite samples.

The procedure does not require separation of Thorium (IV), and alloys the determination of both metals in the presence of alkaline - earth metals and but lantanides interfere.

Kur river in Azerbaijan and assessment of its environmental pollution

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One of the urgent global challenges of today's time is water supply to the population and various sectors of the economy. Today, water has become one of the decisive factors of sustainable development in the countries. The population of the Kur River in Azerbaijan has historically used river water for various purposes, including drinking water supply. As a result, along with the natural transformation of the river flow, anthropogenic transformation took place.

Kura is a source of drinking water for 60-70% of the republic's population. It is a vital factor for the population, agriculture and industry of our republic. From this point of view, the analysis of the contamination of the Kura river in Azerbaijan is of great importance.

The Kur River, the largest trans-boundary river in the Caucasus, is located in five countries, and its water is used for various purposes.

The Kura River is exposed to severe pollution primarily due to industrial and municipal waste from other settlements in Georgia. As a result, the Kura river enters our republic as a highly contaminated river, which is dangerous for human and aquatic organisms. Anthropogenic impacts on the Kura River in Azerbaijan occur at the expense of reservoirs built on the basin.

Drinking water samples were collected from Kur River for the analysis of their physicochemical parameters. Six samples of water were collected from the Kur River in a plastic bottle. Samples taken to the laboratory have been analyzed some physico-chemical parameters such as pH, Electrical conductivity (EC), Total dissolved solids (TDS), Total alkalinity (TA), Chloride (Cl^-), fluoride (F^-) and others. The results were compared with the requirements of the World Health Organization and Directive 98/38 / EC on potable water. Based on the analysis results, the water samples taken are suitable for drinking. pH 8.07-8.30 in the samples; TA 2.6-3.58 mg / L; TDS was 486-724 mg / L, TH 239-348 mg / L, sulfates 165 -275 mg / L, chlorides 37.5-92 mg / L, nitrates 3.1-4.5 mg / L. Although sulfate levels are slightly high, they are not harmful to health. Although it breaks down the intestines in non-habitual people, the digestive system is accustomed to it over time. In addition, calcium, magnesium and ammonium ions were also analyzed in the water samples taken.

Improvement of the Graphitic-Carbon Nitride Photocatalytic Activity Using Plasmonic Nanoparticles

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Today, much attention has been paid to graphite nitride carbon frames with 3:5 (g-C_3N_5) C: N stoichiometry to reduce the bond gap and increase photocatalytic activity. In this research work, first g-C_3N_5 nanomaterials were prepared by heat treatment of 3-amino-1,2,4-triazole and NH_4Cl and then by protonation with acid method, the adhesive plates of g-C_3N_5 graphite structure were separated and thin nanofibers. g-C_3N_5 was formed [1]. Systematic study of phase structure, morphology, optical properties, chemical surface conditions of nanomaterials was performed using different analyzes. The characterization results showed that the protonation process could contribute to the peeling of g-C_3N_5 with a large surface area (3.75 for g-C_3N_5 bulk and 45.78 for g-C_3N_5 nanoparticles), more efficient charge transfer capability, and a modified band structure. In order to improve the photocatalytic activity of the synthesized g-C_3N_5 nanoparticles, we compared it with Ag@Au coupled core/shell nanoparticles and its structural properties [2]. Photocatalytic activity of synthesized nanocomposites in photocatalytic degradation of methylene blue and tetracycline was investigated as an example of organic pollutants and the effect of various factors and their optimal amount including photocatalyst content, g-C_3N_5 to nanoparticle ratio, and dye concentration were studied took. Addition of nanoparticles to g-C_3N_5 nanoparticles improved photocatalytic degradation efficiency. For example, the removal efficiencies of methylene blue at 10 mg/L and tetracycline at 100 mg/L by g-C_3N_5 for 60 minutes under xenon light are about 47.5% and 30.5%, respectively, but the removal efficiencies at the same concentration and duration by g-C_3N_5-Ag@Au composite are about 99.7% and 82%, respectively. The mechanism and synthesis of photocatalytic reactions were studied and it was found that cavities as active species play an effective role in the degradation process and the reactions follow the first-order synthetics. The high photocatalytic activity of the composite compared to g-C_3N_5 nanoparticles can be related to the increase in high light absorption, smaller bandgap, high surface area, and low recombination velocity of the charge carriers.

Keywords: Graphite carbon nitride, Tetracycline, Methylene blue, Gold, Silver

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A Green Eutectic Solvent Used for High-yielded Thioamidation of Methyl Aryl Ketones: K_2CO_3-Glycerol as a Trapping Agent Captures most of H_2S

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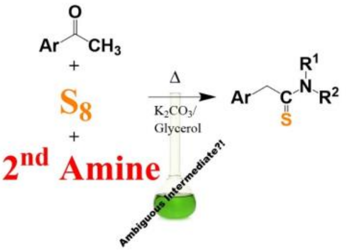
Abstract: This presentation is based on a green approach for the synthesis of products of the well-known reaction, namely Willgerodt-Kindler (W-K). Within this survey, an almost forgotten method of thioamidation, in which a shifting rearrangement (a ketone to an amide) could be seen, was conducted. What has considered the main point of this reaction is its internal oxidation using elemental sulfur. To enhance previous methods, we brought the world of homogenous activators into the W-K stage. As the main problem for this procedure includes sulfur or its organic derivatives, a malodorous byproduct releases out of a mixture of reactants. The existence of this corrosive agent, Dihydrogen Sulfide (H_2S), has formed numerous problems in both labs and industry. K_2CO_3-Glycerol (with the ratio of 1:10) resolved it, at least, for lab-scale works. Not only have this peripheral parameters improved the yield of reaction, but this DES also could maintain excess formed H_2S inside of itself. Furthermore, the durability of this simple, known medium was proven. As a result, the more it is alkaline, the more its trapping nature appears for H_2S. But it should not be neglected to keep the yield of the reaction as high as possible. To do this, 1 (mL) of this DES (1:10) was prepared for each step. In the following, the three-component oxidative thioamidation of W-K is done by this basic, dehumidifier medium. After setting the optimized condition for 2 h and at 80˚C, obtained yields were between close to 70% and just below 90%.



Keywords: Deep Eutectic Solvent, Green Medium, Thioamidation, H_2S Trapping, Willgerodt-Kindler

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Cold plasma effect on cyclotides extraction

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Cyclotides, a large family of plant derived peptides, consist of 28-37 amino acids in a circle skeleton with three disulfide bonds donating cystine knot motive. Cyclotides are resistance to heat and enzymatic digest because of stable cysteine knot motive. A broad range of biological activities have been reported such as insecticide, anti-HIV, anti-cancer, anti-bacterial, immiunomodulatory effect, etc. In this study a pre-treatment as cold Plasma used to investigate extraction yield of cyclotides from Viola ignobilis. Here we use cold plasma, or non-thermal plasma, which is created by sending super-fast electrons through gases such as helium and oxygen with two electrods including Jet and BDB. Areal parts of plant were treated with cold plasma by two electrods and then extracted with ACN/H2O by maceration method to obtain cyclotides. Also a none-treated plants was extracted with ultrasound-assisted method. After extraction of cyclotides LLE and SPE were used for clean-up and purification. Cyclotides fractions from 50% ethanolic elutions of SPE were analyzed by HPLC and compared with none-traded one. The obtained results showed that the cold plasma could not increas the extraction yield and ultrasound-assisted was more effective method for extraction of cyclotides.

Keywords:

Peptides, Cyclotides, Maceration, Cold plasma,Ultrasound-assisted extraction,

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Workshops

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(داروسازی هسته ای)

بیست و یکمین کنگره بین المللی شیمی انجمن شیمی ایران
۶-۴ مرداد ماه ۱۴۰۱
ویژه متخصصان و دانشجویان داروسازی، پزشکی و شیمی
حضوری و مجازی

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رئیس بخش رادیوفارماسی دپارتمان طب هسته ای
دانشگاه فیلیپس ماربورگ آلمان

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