دانشگاه زابل

بیست و ششمین سمینار شیمی آلی انجمن شیمی ایران

دانشگاه زابل - گروه شیمی

۲۱-۲۳ اسفند ۱۳۹۷

26th ISOC, University of Zabol
March 12-14, 2019

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محورهای همایش

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نشانی: زابل، دانشگاه زابل، دانشکده علوم، گروه شیمی، دبیرخانه بیست و ششمین سمینار شیمی آلی ایران

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In name of Allah, the compassionate, the merciful

The 26th Iranian Seminar of Organic Chemistry
University of Zabol
12-14 March, 2019

University of Zabol

26th Conference on Organic Chemistry

March 12-14, 2019

University of Zabol, Iran

By:

University of Zabol

Department of Chemistry,
Faculty of Science, University of Zabol

In collaboration with:

Iranian Chemical Society

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WELCOME MESSAGE

Dear Colleagues

On the behalf of our hosts and of the Organizing Committee, it is my great pleasure to welcome you all to the 26th Iranian Seminar of Organic Chemistry to be held in the University of Zabol from March 12 to 14, 2019.

I would first like to thank our sponsors for their generous support for the 26th Iranian Seminar of Organic Chemistry. I would also like to convey my sincere gratitude to the Advisory Committee and to the members Organizing Committee especially my kind colleagues in Department of Chemistry as well as the MSc Students, staffs, the Iranian Chemical Society for their tremendous efforts, on which the success of this venture depends. This conference would not have been possible without them.

For the 26th conference, we have planned a scientific program consisting of 20 invited lectures and 195 poster presentations. Filled with brilliant presentations on the latest issues and recent developments in the field, we anticipate an intellectually demanding and stimulating experience for all participants. We believe that the lectures and poster sessions, which will take place in the main hall in the center of the conference site, will be lively and stimulating and will leave a lasting impression on all participants.

As organizers of the conference, it is our hope that you, the participants, thoroughly enjoy the 26th Iranian Seminar of Organic Chemistry; that you benefit from the rich scientific program, strengthen your professional network and take home lasting memories of your experiences here. We also hope you take pleasure in the venue, the beauties and culture of Zabol. We truly hope you enjoy the conference!

Dr. M. Bohlooli
Chairman of ISOC26
March 2019

PROGRAM OVERVIEW

Time	*Tuesday, 12 March, 2019* سه شنبه، ۲۱ اسفند، ۹۷
8:00-13:00	Registration
13:00-14:00	Lunch Break
15:00-17:00	Opening Ceremony
17:00-18:00	Coffee Break & Poster Session A
Chairmen: *Prof. Babak Karimi, Prof. Kazem Saeedi & Dr. Ashraf Moradi*	
18:00-18:30	**Prof. Ayoob Bazgir** Transition Metal Catalyzed Organic Transformations
18:30-19:00	**Dr. Reza Sheikhnejad** Chemistry's Role in the Treatment of Cancer
19:00-20:00	**Dr. Tayeb Kakeshpour** AMHB: (Anti)aromaticity-Modulated Hydrogen Bonding
20:00-21:00	Dinner
22:00-23:30	Swimming pool – Gentlemen
	Wednesday, 13 March, 2019 چهارشنبه، ۲۲ اسفند، ۹۷
Chairmen: *Prof. Hossein Eshghi, Prof. MohammadAli Naseri & Dr. Reza Aryan*	
8:00-8:30	**Dr. Meysam Yarie** *Applications of Phosphonium-based Ionic Liquids in Chemical Processes*
8:30-9:00	**Dr. Mohaddeseh Shahabinejad** *Fabrication of Ultra-Small Ruthenium Nanoparticles on Porous Modified Reduced Graphene Oxide and its Application in Solvent-Free Oxidation of Cyclohexene with Molecular Oxygen*
9:00-9:30	**Dr. Naeimeh Salehi** *Design, Synthesis and Biological Evaluation of Novel Ligands as Potential Anti-Alzheimer's Agents*
9:30-10:00	**Prof. Ali Khalafinezhad** *Polyethylene Glycol-bonded Tetraethyl Ammonium L-Prolinate: A New Highly Efficient Biodegradable Amino Acid-based Ionic Liquid for the Synthesis of Some DNA Binders as Anticancer Agents*
10:00-11:00	Coffee Break & Poster Session B
Chairmen: *Prof. Ali Khalafinezhad, Prof. MohammadAil Zolfigol & Prof. Sara Sobhani*	

11:00-11:30	**Dr. Ehsanorreza Poorhassan** *Continuous Flow Synthesis of Cyclopropanated Amino Acids Using Diazo Compounds*
11:30-12:00	**Dr. Neda Seyedi** *Fabrication of Nitrogen-enriched Graphene Oxide/Cu NPs as a Highly Efficient and Recyclable Heterogeneous Nanocatalyst for the Chan-Lam Cross-Coupling Reaction*
12:00-12:30	**Dr. Abdolhamid Bamoniri** *Synthesis of Heterocyclic Compounds Bearing Nitrogen and Oxygen Atoms using Nano- kaolin/BF3/Fe3O4 Based on Green Chemistry in Different Conditions*
12:30-13:00	**Prof. Massoud Kaykhaii** *Introducing the Corresponding Committee on Reference Materials of the Institute of Standards and Industrial Research of Iran (ISIRI/REMCO)*
13:00-14:00	Lunch Break
Chairmen: *Dr. Abdolhamid Bamoniri, Prof. HamidReza Shaterian & Dr. Alireza Samzadeh-Kermani*	
15:00-15:30	**Prof. MohammadAli Zolfigol** *Anomeric Based Oxidation*
15:30-16:00	**Dr. Reza Aryan** *Green Synthesis of Monocyclic and Fused Nitrogen Heterocycles with Promising Bioactivity Effects*
16:00-16:30	**Prof. Reza Ranjbar-Karimi** *Perhalopyridines: Synthesis and Synthetic Utility*
16:30-17:00	**Dr. Mahnoosh Rashidi** *Biochemical Synthesis of Ag@AgCl Nanoparticles and its Application in Photodegration of Azo Dyes*
17:00-18:00	Coffee Break & Poster Session C
Chairmen: *Prof. Reza Ranjbar-Karimi, Prof. Bi Bi Fatameh Mirjalili & Dr. Fereshteh Shiri*	
18:00-18:30	**Prof. AliReza Modarresi-Alam** Application of Conducting Polymers (Polyanilines) in Sustainable and Renewable Energies and Electronic Systems
18:30-19:00	**Dr. Ahmad Akrami** *Intelligent Chemical Passive Defense*
19:00-19:30	**Dr. Saba Daliran** *Metal-organic Frameworks as Heterogeneous (Photo-) Catalysts in Organic Transformation Reactions*
19:30-20:00	**Prof. HamidReza Shaterian** *Preparation and Characterization of New Organocatalysts Supported on Nanomagnetic Particles as Green Nanocatalysts and Their Applications in Organic Synthesis*
20:00-21:00	Dinner
21:00-22:30	Swimming pool – Ladies

Thursday, 14 March, 2019 ***پنج شنبه، ۲۳ اسفند، ۹۷***	
8:00-15:00	Sightseeing
16:00-17:00	Coffee Break
17:00-20:00	Closing Ceremony
20:00-21:00	Dinner

CHAIRMEN OF THE CONGRESS

Dr. Mousa Bohlooli
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Chairman of the Executive Committee

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Jamshid Mirshekar

SPONSERS

SPEECHES PROGRAM

Time	Lecturer & Title of the Lecture
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19:00-19:30	**Dr. Saba Daliran** Metal-organic Frameworks as Heterogeneous (Photo-) Catalysts in Organic Transformation Reactions
19:30-20:00	**Prof. HamidReza Shaterian** Preparation and Characterization of New Organocatalysts Supported on Nanomagnetic Particles as Green Nanocatalysts and Their Applications in Organic Synthesis

POSTER PRESENTATIONS

Poster Session A

Tuesday, 12 March, 2019

سه شنبه عصر، ۲۱ اسفند، ۹۷

NO.	*Code*	*Title*
1	1201-ISOC26	**Farzaneh Esmaili** Co(II) Immobilized on Functionalized Magnetic Hydrotalcite: A Green and Magnetically Recyclable Bifunctional Nanocatalyst for the Synthesis of Xanthenes
2	1155-ISOC26	**Mehri Mohammadpour** CoFe2O4@SiO2-NH2-CoIIMagnetic Nanoparticles as a Highly Efficient Nanocatalyst for the Synthesis of Spirooxindole Derivatives
3	1156-ISOC26	**Mehri Mohammadpour** $CoFe_2O_4$@SiO_2-NH_2-Co(II) magnetic NPs as a novel, inexpensive and highly efficient magnetic nanocatalyst for aldol-condensation reaction
4	1151-ISOC26	**Elaheh Naghdi** Co(II)@KCC-1 as a Novel Metal Salen Complex for the Synthesis of Spirooxindole Derivatives
5	1205-ISOC26	**Nafise Ayati** The Study of Performance of Trachyspermum Ammi and Dimethicone in Bloating
6	1131-ISOC26	**Meysam Yarie** Synthesis of Polycyclic 1,4-Dihydropyridine Derivatives in the Presence of a Ionically Tagged Nanomagnetic Catalyst
7	1148-ISOC26	**Mohammad Reza Anizadeh** Magnetic Nanoparticles-Supported CuI-Caffeine: ARecyclable and Ecofriendly Catalyst for Green Synthesis of 1,2,3-Triazols from Organic Halides

8	1149-ISOC26	**Mohammad Reza Anizadeh** Synthesis of Quinoline-3-carbonitrile Derivatives in the Presence of a Novel and Reusable Nanomagnetic Catalyst
9	1124-ISOC26	**Saeed Babaee** Application of MIL-101(Cr) in the Synthesis of N-Amino-2-pyridones and 1,4-Dihydropyrano[2,3-c]pyrazoles
10	1122-ISOC26	**Saeed Babaee** Synthesis of Pyridinioum Based Nano Molten Salts as Dual Role Catalysts: Application for the Synthesis of O-Heterocycle Compounds
11	1023-ISOC26	**Farbod Tabesh** Purgation of the Environment Using Natural Materials from the Environment: Study of the Recent Development in Isotherms, kinetics, and Thermodynamics of the Adsorption
12	1140-ISOC26	**Morteza Torabi** Novel Phosphonium Based Ionic Liquid Catalyzed One-Pot Multicomponent Synthesis of 2-Oxo-4,6-diphenyl-1,2-dihydropyridine-3-carbonitrile Derivatives
13	1139-ISOC26	**Morteza Torabi** Synthesis of a Novel and Reusable Acidic Nanomagnetic Catalyst: Application for the Synthesis of New 2-Amino-3-cyanopyridines via Vinylogous Anomeric Based Oxidation
14	1150-ISOC26	**Amirmahdi Tavassoli** Biological Based DES Shows Brilliant Catalytic Activity at the Synthesis of Linked Pyridine Derivatives
15	1089-ISOC26	**Omid Jawhid** Synthesis and Characterization of Crosslinked Cellulose Schiff base as a Novel Bio Based Polymer Ligand
16	1090-ISOC26	**Omid Jawhid** Synthesis of Reduced Graphene oxide/Silicate from Industrial Grade Graphite Flakes
17	1030-ISOC26	**Masoud Hatami** Efficient Elimination of Methyl Orange Dye from Wastewater through Recyclable Bio-intercalate LDH-Fe3O4/PVA Nanocomposite
18	1126-ISOC26	**Zeinab Hataminegzad** Co(NO3)2 Efficiental Catalyst fo Synthsis of Dihydropyrimido[4,5-b]quinolinetrione Derivatives Using a Multi-Component Reaction
19	1198-ISOC26	**Zahra Habib Zadeh Chenari** Nano Polymeric Biodegradable of Alginate-Arginine for Breast Anticancer Drug Delivery
20	1187-ISOC26	**Hadis Hosseini Moghadam** A New Nanomagnetic Cobalt Catalyst for Copper-free Sonogashira Coupling Reaction in Water at Room Temperature

21	1111-ISOC26	**Mohammad Dashteh** 1,10-Phenanthrolin-1-ium trinitromethanide (1,10-PHTNM) as a Nano Molten Salt Catalyst with Y-Aromatic Counter ion: Applications for the Synthesis of Organic Compounds
22	1061-ISOC26	**Mohammad Dashteh** Application of Cobalt Phthalocyanine as a Nanostructured Catalyst for Synthesis of Biological Henna-Based Compounds
23	1218-ISOC26	**Esmat Rahmanifar** Removal of Pb(II) Ion from Aqueous Solution by an Engineered Novel Chitosan Functionalized Schiff-Base Adsorbent
24	1119-ISOC26	**Mahmoud Zarei** Design, Synthesis and Application of a Novel Nanomagnetic Function-alized Acetic Acid as a Catalyst for theSynthesis of Amidoalkyl phe-nols
25	1120-ISOC26	**Mahmoud Zarei** Synthesis of New (3´-Indolyl)pyrazolo[3,4-b]Pyridine via Vinylogous Anomeric Based Oxidation under Mild and Green Conditions
26	1153-ISOC26	**Sara Sobhani** A New Schiff Base Complex of Aminoguanidin Established on γ-Fe2O3 for the Synthesis of Hexahydroquinolins
27	1118-ISOC26	**Hassan Sepehrmansouri** Multilinker Phosphorous Acid Anchored En/MIL-100(Cr) as a Novel Nanoporous Catalyst for the Synthesis of New N-heterocyclic Pyrim-idoquinolines
28	1121-ISOC26	**Hassan Sepehrmansourie** Synthesis and Application of a Novel Ionically Tagged Polymer as a Nano-Heterogeneous Catalystfor Synthesis of N-Heterocycle Spiropy-rans under Mild and Green Conditions
29	1224-ISOC26	**Hesam Sotoodeh** Tautomerism in Phenytoin: A Theoretical Study in Gas Phase
30	1027-ISOC26	**Banafsheh Seyfi** Poly(vinyl alcohol)/TiO2@Folic Acid Nanocomposite Films: Survey of Optical, Thermal and Antibacterial Properties
31	1049-ISOC26	**Iman Sargazi** Solid-State Synthesis of Nanocopolymer of Aniline and 3-Aminobenzenesulfonic acid in the Presence of p-Toluene sulfonic acid and its Application in Solar Cell
32	1050-ISOC26	**Iman Sargazi** Solid-State Synthesis of Nanocopolymer of Aniline and 3-Aminobenzenesulfonic acid in the Presence of p-Toluene sulfonic acid and its Application in Solar Cell

33	1207-ISOC26	**Mehri Salimi** Magnetic Cellulose Nanofibers Supported Imidazolium-Based Ionic Liquid as a Biodegradable Catalyst for the Synthesis of Quinoline Derivatives
34	1249-ISOC26	**Ziba Sori Nezami** Gold Nanoparticles: Synthesis and Application in Drug Delivery
35	1082-ISOC26	**Hoda Davoodi** Gold Nanoparticles: Synthesis and Interaction Studies with Calf Thymus DNA
36	1162-ISOC26	**Sara Sheikhi** An Efficient Regioselective Synthesis of Functionalized Spiropyrrolizidines through Azomethine Ylides Intermediate
37	1028-ISOC26	**Fatemeh-Sadat Sadeghi** A Benign Route for the Production of Polymer Nanocomposite Films Based on Poly(vinyl alcohol) and SiO2–Folic Acid Nanoparticles
38	1219-ISOC26	**Ali Kakeshpour** Application of Modern Computers in in-silico Chemical Simulations
39	1085-ISOC26	**Elahe Hojatnia** Computational Study Regards Inhibitory Effects of Some Pyrimidine Based Drugs against Kinase Protein for Treatment of Cardiovascular Disease
40	1084-ISOC26	**Motahare Kiyanee-Ghaleno** Theoretical Study on Some Substituted Hydrazones as Anti-Depressant Agents
41	1074-ISOC26	**Morteza Karimi Seresht** Mixed Metal Oxides Modified Mesoporous Silica with Magnetic Core: A Reusable Catalyst for the Synthesis of 2-Substituted Pramipexole Dihydrochloride
42	1230-ISOC26	**Zahra Garkani Nezhad** Synthesis and Antibacterial Activity of a New Bipyridyl Complex
43	1026-ISOC26	**Maryam Lormehdiabadi** Influence of ZnO-Folic Acid Nanoparticles on the Bioactivity Property of Polycaprolactone in the Simulated Body Fluid
44	1206-ISOC26	**Sajad Mohammadian Souri** Salen Complex of Cu(II) Supported on Superparamagnetic Fe3O4@SiO2Nanoparticles: An Efficient and Magnetically Recover ble Catalyst for the Synthesis of 1,4-Dihydropyridines
45	1005-ISOC26	**Reza Mohammadi Pour** One-Pot Synthesis of 1,4-Dihydropyridines via Hantzsch Reaction U ing Nano-kaolin/BF3/Fe3O4 as a Green Catalyst under Solvent-Free Conditions

46	1058-ISOC26	**Samaneh Mahmoudi-GomYek** Fe3O4-Supported Macroacyclic Schiff-Base Copper Complex: A valuable Heterogeneous Nanocatalyst for One-Pot Synthesis of New Pyrano[2,3-b]pyridine-3-carboxamide Derivatives
47	1186-ISOC26	**Mujib Miri** The Aromaticity of Rings in Some Pterin-Based Inhibitors of Dihydropteroate Synthase
48	1193-ISOC26	**Sanaz Naderi** Application of Schiff Base Mn(III) Complexes Grafted to Crown Ether Rings as Catalysts for Oxidation of Benzyl Alcohol Derivatives by Oxone
49	1197-ISOC26	**Sanaz Naderi** Synthesis and Application of Schiff Base Mn(III) Complexes Containing Crown Ether Rings as Catalysts for Oxidation of Sulfides by Oxone
50	1152-ISOC26	**Amir Mohammad Naseri** Zr-based MOF as a Novel Nanoporous Catalyst for the Synthesis of Dihydropyrido[2,3-d]pyrimidines
51	1243-ISOC26	**Ameneh Heydari** New Complex Based on Zn(II) and Quinoline: A Supra Precursor for Fabrication of ZnO Nanoparticles
52	1242-ISOC26	**Ameneh Heydari** Superparamagnetic Fe3O4 Nanoparticles Applicable in the Removal of Cd^{2+}
53	1248-ISOC26	**Vajiheh Behranvand** Development of Carbon Quantum Dot Decorated Multi-Walled Carbon Nanotubes Incorporated into the Recycled PET Nanocomposites for Dye Remediation
54	1251-ISOC26	**Majid Nasiriboroumand** Green Synthesis of Silver Nanoparticles using Grape Leaf, Stability and Antimicrobial Evaluation
55	1250-ISOC26	**Majid Nasiriboroumand** Michael Addition Reactions in Dyeing of Protein Fibers with Quercetin
56	1244-ISOC26	**Hossein Tavakol** Doped Carbon Nanostructures; Synthesis by Chemical Vapor Deposition and Their Applications as Sensor, Catalyst and Adsorbent
57	1232-ISOC26	**Saba Daliran** Defect Engineering of a Chromium-Based Metal–Organic Framework for Catalysis
58	1233-ISOC26	**Ali Reza Oveisi** Post-modification a Mesoporous Metal-Organic Framework: Synthesis and Structural Studies

59	1241-ISOC26	**Ali Reza Oveisi** Zr-Based Metal-Organic Framework as an Efficient Nanocatalyst for Three-Component Synthesis of Quinazolin-4(1H)-one Derivatives
60	1065-ISOC26	**Mahdiye Poorsargol** Self-Assembly of Surfactant Mixtures on GrapheneNanosheets: In-sights from Molecular Dynamic Simulation

Poster Session B

Wednesday, 13 March, 2019

چهارشنبه صبح، ۲۲ اسفند، ۹۷

NO.	*Code*	*Title*
1	1247-ISOC26	**Shiva Teylaghi** Fabrication and Study of Nigella sativa-Loaded Electrospun Nanofiber
2	1245-ISOC26	**Atefeh Kadkhodaie** Preparation and Assesment of Althaea Officinalis -Loaded Electrospun Nano Fiber
3	1246-ISOC26	**Salehe Honarmand** Preparation and Evaluation of Electrospun Nanofiber Membrane Load-ed with Green Tea Extract
4	1080-ISOC26	**Sattar Ebrahimi** Tannic Acid-Functionalized Fe3O4/SiO2 Magnetite Nanoparticles as an Efficient, Reusable and Magnetically Separable Catalyst for the Synthe-sis of Acridinone Derivatives under Solvent-Free Conditions
5	1079-ISOC26	**Sattar Ebrahimi** A Novel Method for the One-Pot Synthesis of Imidazole Derivatives in the Presence of Potassium Persulfate (KPS) as a Free Radical Initiator
6	1060-ISOC26	**Tayebe Talebi Meymand** Survey Reaction of Benzoimidazolo/Benzooxazolo/Benzothiazolo 2 thioacetophenone Derivatives Using TiO2-Nanoparticles
7	1099-ISOC26	**Hossein Eshghi** Uniform Copper Nanoparticles on Tunable Porous N-Doped Carbon Nanospheres for Esterification of Various Aryl Aldehydes with Alco-hols
8	1142-ISOC26	**Mojtaba Namroudi** Multi-Component Reactions for the Synthesis of Arylsulfonyl hydra-zide Derivatives

9	1209-ISOC26	**Mojtaba Namroudi** Synthesis of Sulfonamide Derivatives Using Electrochemistry
10	1052-ISOC26	**Moones Honarmand** Synthesis and Characterization of 3-Aminopropylammonium Hydrogensulfate as a Nano Aliphatic Quaternary Ammonium Salt
11	1051-ISOC26	**Moones Honarmand** Three-Component Process for the Synthesis of 4H-Pyrans Using a Recyclable Ionic Liquid in Aqueous Media
12	1176-ISOC26	**Azam Habibollahi** Application of Hydrophilic Palladium Complex in Cyanation Reactions
13	1097-ISOC26	**Younes Khademi** Design and Synthesis of Acidic Deep Eutectic Solvents Based on Choline Chloride and Discovery of a Highly Efficient Catalyst for the Synthesis of Benzoazepinones
14	1096-ISOC26	**Younes Khademi** Iron(III) Chloride Hexahydrate as an Efficient Heterogeneous Recyclable Catalyst for the Synthesis of 2-Substituted Quinazolinones
15	1228-ISOC26	**Maryam Khorsandi** Synthesize and Functionalize of a Novel Organic-Inorganic Hybrid Material Based on Heteropoly Acid for Gene Delivery into the HEK-293T Cells
16	1227-ISOC26	**Maryam Khorsandi** Synthesize and Functionalize of the Novel Choline Chloride/2 Chloroacetylchloride/PEI Derivatives for Applications inEnzyme Stabilization
17	1094-ISOC26	**Mariya Dehvari** Theoretical Studies to Examine the Inhibition of Two New Thiourea Derivatives
18	1095-ISOC26	**Mariya Dehvari** A DFT Study of the Cheletropic Reaction between Diacetyl and Trimethylphosphite
19	1044-ISOC26	**Ziba Daroughehzadeh** Triphenylphosphane: An Efficient Catalyst for Three-Component Synthesis of Arylmethylidene-isoxazole-5(4H)-ones in Green Medium
20	1147-ISOC26	**Mohadeseh Goli** Green and Expeditious Synthesis of Isoxazol-5(4H)-ones via Three-Component Reaction
21	1145-ISOC26	**Mohadeseh Goli** Organocatalyzed Synthesis of Dihydropyrimidinone/Thiones via Biginelli Condensation Reaction
22	1161-ISOC26	**Mahboobeh Dowlati** Alcohol Oxidation by TBHP Using Molybdenum Oxide Immobilized on Mesoporous Silica

23	1220-ISOC26	**Mahboobeh Dowlati** Oxidation of Alcohols by TBHP Applying Fe(III) Complexes on the Magnetic Nanoparticles
24	1014-ISOC26	**Mahboobeh Rezaie Khahkhaie** One-Pot Condensation Approach for the Synthesis of Tetrahydrobenzo[b]pyran Derivatives Utilizing Salicylic Acid as an Efficient and Eco-friendly Catalyst
25	1016-ISOC26	**Mahboobeh Rezaie Kahkhaie** $Co(NO_3)_2.6H_2O$: A mild, efficient and novel catalyst for the One-pot synthesis of tetrahydrobenzo[b]pyran derivatives
26	1041-ISOC26	**Zinat Rezazadeh** One-Pot Three Component Synthesis of 2,3-Dihydroquinazolin-4(1H)-ones by a Heterogeneous and Reusable Polyvinyl Alcohol Immobilized Cu(II) Schiff base Complex
27	1031-ISOC26	**Zinat Rezazadeh** Selective and Efficient Oxidation of Benzyl alcohols to Benzaldehydes by Polydoxirane in the Presence of Molecular Oxygen at Room Temperature
28	1130-ISOC26	**Mohammad Rezaei-Gohar** Synthesis of 3,4-Dihydropyrimidin-2(1H)-ones using Boric Acid Aqueous Solution System
29	1046-ISOC26	**Mohammad Zarei** Green Synthesis of Silver Nanoparticles Supported on Magnetic Functionalized Graphene oxide and its Application as Recoverable Catalyst for Reduction of the Dye Pollutants in Water
30	1047-ISOC26	**Mohammad Zarei** Preparation of Functionalized Graphene Oxide Loaded with Silver Nanoparticles and Investigation of its Antibacterial Activities
31	1057-ISOC26	**Bardia Zamani** Application of the Immobilized Sulfonic Acid on the Magnetic Cobalt Ferrite Nanocatalyst ($CoFe_2O_4/SiO_2/SO_3H$) in the Synthesis of Organic Materials
32	1053-ISOC26	**Jamil Sheykhahmadi** A Convenient Synthesis of Functionalized 2,3-Diazaspiro[4.4]nona-1,6,8-trienes
33	1045-ISOC26	**Sina Shaabanzadeh** Electrochemical Synthesis of 4-Aryl-2-styryl-1H benzo[b][1,4]diazepines from o-Phenylenediamine and 1,5-Diarylpenta-2,4-dien-1-ones
34	1192-ISOC26	**Maryam Shokoohian** Synthesis of New[1,2,4]triazolo[1,5-a]pyridine Derivatives by Reaction Pyridine-2-(1H)-ones and Aldehydes in the Presence of Acetic Acid

35	1191-ISOC26	**Maryam Shokoohian** Ultrasound-Promoted One-Pot, Four-Component Synthesis of 1,6-Diamino-2-oxo-1,2,3,4-tetrahydropyridine-3,5-dicarbonitriles Using 4-Dimethylaminopyridine (DAMP) as Catalyst
36	1056-ISOC26	**Maryam Safaei** Formation of Trichloromethylated-1,3,5-triazines from Guanidine, Trichloroacetonitrile, and Isothiocyanates
37	1223-ISOC26	**Zohreh Taheri** A Convenient Synthesis of Tetrasubstituted Pyrazoles from Nitrile Imines and 2-(Thioxothiazolidin-5-ylidene)acetates
38	1037-ISOC26	**Seyyedeh Ameneh Alavi Gol** $CuFe_2O_4@SO_3H$: A Mild, Efficient and Reusable Heterogeneous Catalyst for the Synthesis of Highly Functionalized Piperidines
39	1036-ISOC26	**Seyyedeh Ameneh Alavi Gol** One-Step, Three-Component Synthesis of Highly Substituted Pyridines Using $CuFe_2O_4@SO_3H$ as Reusable Catalyst
40	1009-ISOC26	**Homayoun Faroghi Niya** Lactose: A Novel and Green Catalyst for an Environmental Synthesis of Medicinally Important Pyrano[3,2-c]pyrazoles
41	1020-ISOC26	**Mahyar Karimi** Influences of Decor Raw Paper and Type of Thermosetting Resins on the Quality of Laminated Wood Panel
42	1021-ISOC26	**Mahyar Karimi** Investigation of Melamine Formaldehyde (MF) and Rubber Blending on Some Quality Effect of Composite Product
43	1188-ISOC26	**Maryam Kochakzay** Diasteroseletive Synthesis of Functionalized Cyclohexanones by Condensation of Acetoacetanilide and Various Aldehydes in the Presence of DMAP as Catalyst
44	1190-ISOC26	**Maryam Kochakzay** PTSA: A FacileCatalyst a One-Pot Synthesis of 2-Arylpyrrolo[2,3,4-kl]-1(2H)-one under Mild Conditions
45	1229-ISOC26	**Soma Majedi** Synthesis of Novel Bioactive Candidates 4-Aryl-1H-indeno [1,2-d]pyrimidine-2,5-diones using $\{[HMIM]C(NO_2)_3\}$ as a Dual Role Ionic Liquid Catalyst: An Experimental and Theoretical Evaluation of Their Corresponding Antioxidant Activities
46	1070-ISOC26	**Tina Mirzaei** One-Pot Three-Component Synthesis of 1-Amidoalkyl-2-naphthols Derivatives by using Sulfamic Acid-Functionalized Fe_3O_4 Nanoparticles as Highly Efficient and Recyclable Catalyst

47	1100-ISOC26	**Atiyeh Marzban** N-Sulfopiperidine-4-Carboxylic Acid Functionalized Fe_3O_4 Nanoparticles as Catalyst for One-Pot Synthesis of Dipyrromethanes under Solvent-Free Condition
48	1195-ISOC26	**Sahar Marghzari** Simultaneous Removal of Organic Dyes from Environmental Samples by Using Sistan Sand as an Effective Sorbent
49	1203-ISOC26	**Mahdieh Mozaffari Majd** Effect of Vitamin C Template on Morphology and Structure of α–Alumina
50	1166-ISOC26	**Sepideh Masoomifar** Chlorosulfonic Acid Supported Piperidine-4-carboxylic acid Functionalized Fe3O4 Nanoparticles: A Green Catalyst for the Synthesis of 2-Arylbenzimidazoles under Solvent Free Condition
51	1098-ISOC26	**Eideh Mofarrah** Polyphenols in Pistachio Hulls
52	1144-ISOC26	**Fouziyeh Mollazehi** Application of Dendrimer-Coated Magnetic Nanoparticles as a Heterogeneous and Reusable Catalyst for the One-Pot Synthesis of Acridinedione Derivatives
53	1154-ISOC26	**Faheimeh Haghbeen** Synthesis of 2-Amino-5-hydroxy Pyrimidines as the Novel Analogues of Tyrosinase Substrate
54	1038-ISOC26	**Alae Mousavi Tabar** Synthesis of a 3D-Network Polymer Based on a Calix[4]resorcinarene Containing N3Anion: A Green and Reactive Solid Supported Reagent
55	1040-ISOC26	**Ala Mousavi Tabar** Synthesis of the 2,4,6-Triarylpyridines and 2,5,7-Triaryl-1,3-thiazepine Derivatives by Using a Green and Reactive Polymer Supported Reagent Based on Calix[4]resorcinarene
56	1011-ISOC26	**Firouzeh Nemati** Organoselenium-Palladium(II) Complex Supported on Modified Magnetic Nanoparticles as an Efficient Catalyst for Suzuki Reaction
57	1012-ISOC26	**Firouzeh Nemati** Synthetic Application of Palladium(II) Anchored on a Magnetic Mesoporous Polymelamine-formaldehyde as a Heterogeneous Nanocatalyst with Excellent Regeneracy Performance in Suzuki Coupling Reactions
58	1103-ISOC26	**Farzaneh Nehzat** Synthesis and Characterization of Two Transition Metal Ionic Schiff Base Complexes and Investigate the Anticancer Activity

59	1185-ISOC26	**Marzieh Hashemi** 1,3-Dipolar Cycloaddition Reactions on Medicine Dimethisterone: A Computational Insight
60	1183-ISOC26	**Marzieh Hashemi** Theoretical Investigation of Methylpentynol-AzideIntermolecular H-Bonding and Regiochemical Outcome of Its 1,3-DC Reactions

Poster Session C

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2	1179-ISOC26	**Zahra Aelami** Acetic Acid as a Green Catalyst for the Synthesis of N-Aminotriazolethione Azomethine Derivatives
3	1055-ISOC26	**Hamed Saffarian** A Convenient Synthesis of Functionalized Pyrazolones Bearing a Highly Twisted 1,3-Butadiene Moiety with Skew Geometry
4	1008-ISOC26	**Zohreh Razmara** A di-Nuclear Copper(II) Complex as a Precursor for Octahedron-Like CuO Nanoparticles
5	1007-ISOC26	**Zohreh Razmara** Preparation and Characterization of Ferromagnetic Nanoparticles of La2O3 by Thermal Decomposition Approach
6	1196-ISOC26	**Somaye Shahraki** Adsorptive Schiff Base-Chitosan Nanocomposite for Removal of Pb(II) Ion from Aqueous Solutions
7	1234-ISOC26	**Ashraf Moradi** Advanced Computational Methods for Investigating in Liquid Phase
8	1043-ISOC26	**Maryam Ghanbari Kudeyani** A Green Multi-component Synthesis of 3-Substituted 1,2,4-triazol-5-amines as Potential Antimicrobial Agents
9	1042-ISOC26	**Maryam Ghanbari Kudeyani** Green Synthesis of Novel 1,2,4-Triazole-3-thione Derivatives in Natural Deep Eutectic Solvent

10	1063-ISOC26	**Fahimeh Assadzadeh** A Green Procedure for One-Pot Synthesis of Quinazolinone Derivatives Using CuFe2O4@SO3H as an Efficient and Reusable Catalyst under Solvent-Free Conditions
11	1062-ISOC26	**Fahimeh Assadzadeh** One-Pot Synthesis of β-Amino Ketones via Direct Mannich-type Reaction Catalyzed with CuFe2O4@SO3H
12	1048-ISOC26	**Saeed Asadi** A Green Protocol for Direct Esterification of TMS and THP Ethers with Aldehydes Using KCN and Air as the Simplest Available and Free of Cost Oxidant
13	1067-ISOC26	**Mahdi Hussain Zadeh** An Efficient, High Yielding Protocol for the Synthesis of Functionalized Quinolines via the Tandem Addition/Annulation Reaction of O-Aminoaryl Ketones with α-Methylene Ketones
14	1066-ISOC26	**Mahdi Hussain Zadeh** Conjugate Addition of Indoles to Electron-deficient Olefins Catalyzed by CuFe2O4@SO3H Under Mild Conditions
15	1035-ISOC26	**Morvarid Najjar** An Efficient Synthesis of Benzimidazole Derivatives Using a New Binuclear Cu-Bis-Salen Complex at Room Temperature
16	1034-ISOC26	**Morvarid Najjar** One-Pot Three Component Synthesis of 2,3-Dihydro-1H-1,5-benzodiazepines by a Magnetically Recyclable Nanocatalyst Fe3O4@SiO2-Cu-salen
17	1125-ISOC26	**Naser Salehi** A New Ecofriendly Methodology for the Synthesis of Spiro-Oxindole Derivatives via Alcoholic Extract of Angustifolia Leaves as the Solvent and Catalyst
18	1167-ISOC26	**Fatemeh Khosravi** Antibacterial Activity and DNA Binding Studies of Co^{3+}, Cu^{2+}, Zn^{2+} an Pd^{2+} Complexes: Investigating Antibacterial Combination Therapy o These Complexes
19	1215-ISOC26	**Fereshteh Shiri** Antioxidant Function and β-LG Interactions of Zinc(II) Dithiocarbamate Complex
20	1216-ISOC26	**Fereshteh Shiri** Pd(II) Complex Based on the Propylenebis (Dithiocarbamate) Bridging Ligand: Synthesis, Characterization, Antioxidant Activity and Investigation on the Interaction with Human Serum Albumin

21	1069-ISOC26	**Seddigheh Sheikhi-Mohammareh** A One-Pot Procedure for the Synthesis of Highly Functionalized Derivtives of a Novel Five-Cyclic Scaffold: Pyrazlo[5",1":2',3']pyrimido[4',5':5,6][1,4]thiazino[2,3-b]quinoxaline
22	1072-ISOC26	**Ali Shiri** Synthesis of Various Derivatives of a Novel Heterocyclic System of Tetrazolo[1,5-a][1,2,3]triazolo[4,5-d]pyrimidine
23	1088-ISOC26	**Maliheh Safaiee** Biopolymeric Alginic acid: AnEfficient Recyclable Green Catalyst for One-Pot, Four-Component Synthesis of Pyrano[2,3-c]pyrazoles
24	1087-ISOC26	**Maliheh Safaiee** One-Pot, Four-Component Synthesis of Pyrano[2,3-c]pyrazoles Catalyzed by Vanadium Oxo Pyridinoporphyrazine
25	1117-ISOC26	**Ronak Afshari** Carbonaceous Materials Functionalization with Multicomponent Reactions: Novel Drug Delivery Platforms
26	1173-ISOC26	**Afsaneh Omidi** Classification and Discrimination of Pyridine-based Compounds with Various Substitutions Using Fluorescent Carbon-dots Sensor Array
27	1039-ISOC26	**Samira Ghasemi** Comparison the effects of ZnO nanoparticles and ZnO/Chitosan nanocomposites on Diabetes-induced Memory Impairment in Rats
28	1214-ISOC26	**Fateme Baghaei** Efficient and Facial Synthesis of Tetrahydrobenzo[b]pyrans using Sodium Cyclamate as a Green Catalyst
29	1170-ISOC26	**Omid Hashemi Akhourdi** Green Multi-Component Reaction of α-Haloketoneswith Acetylenic Esters in the Presence of Papaverine(Poppy alkaloid)
30	1127-ISOC26	**Fahimeh Sistani** Green Multicomponent Synthesis of Pyrido[2,3-d]pyrimidine Derivatives Catalyzed by a Novel LDH Modified Clinoptilolite Nanocatalyst
31	1159-ISOC26	**Farideh Malekraeesi** Green Synthesis of 1,2,4-Triazole Derivatives and Evaluation of their Antimicrobial Effects
32	1199-ISOC26	**Atefeh Darvishi** Magnetic Nanoparticles-Supported CuI-Caffeine: ARecyclable and Ecofriendly Catalyst for Green Synthesis of 1,2,3-Triazols from Organic Halides
33	1101-ISOC26	**Iran Sheikhshoaie** Nanosized Vanadium Oxide (V2O5/NPs): A Hetrogenous Catalyst for Direct Epoxidation of Some Alkenes Compounds

34	1093-ISOC26	**Zohreh Shirdel** One-Pot Synthesis of Succinimide-3-Carboxamide Derivatives Using Microwave and Mechanistic Insights and Kinetics Analysis by Computational Method
35	1106-ISOC26	**Elham Naeemikhah** Investigation of Dynamic Thermo-Mechanical Analysis on Epoxy/Silica Nanocomposites with Flexible Backbone
36	1107-ISOC26	**Elham Naeemikhah** Synthesis and Characterization of Magnetic Poly[St-co-CMS] Nanocomposites by ATRP Method
37	1104-ISOC26	**Aziz Ahmadikhaneghah** Polyoxyethylene-Based Epoxy/Graphene Oxide Thermosetting Materials with Enhanced Storage Moduli
38	1105-ISOC26	**Aziz Ahmadikhaneghah** Fabrication and Investigation of Poly[St-Co-CMS] Loaded by Modified SiO2 as Initiator via ATRP Method
39	1202-ISOC26	**Asma Parvizi** Preparation and Characterization of Ammonium-Based Ionic Liquids for Separation of Polycyclic Aromatic Hydrocarbons
40	1165-ISOC26	**Mehrdad Omidi-Ghalle Mohamadi** Preparation of New Hydrogels Based on Polyurethane/Polyoxyethylene/Silica Components via Click Chemistry
41	1164-ISOC26	**Fateme Heidari** Relative Stability of Clonidine Isomers
42	1018-ISOC26	**Fahimeh Doustzadeh** Study of Antioxidant Activity of Methanolic Extract of (Inula Salicina (L.)) and (Inula Thapsoids (M.B.ex Willd)) With FRAP and DPPH Methods
43	1123-ISOC26	**Ali Shahryari** Synthesis and Antibacterial and Antifungal Evaluation of Novel Dithiocarbazinate Derivatives
44	1059-ISOC26	**Fereshteh Fathi** Synthesis and Characterization of Iron Oxide Nanoparticles via co-Precipitation and Reverse Micelles Methods in the Biological Applications
45	1054-ISOC26	**Fereshteh Fathi** Synthesis and Characterization of Iron Oxide Superparamagnetic Nanoparticles (Magnetite) by co-Precipitation Method Coated with Biocompatible (Polymeric, Organic and Inorganic) Compounds and Evaluation of In vitro Toxicity of Synthesized Nanoparticles

46	1158-ISOC26	**Mohammadreza Moghaddam-Manesh** Synthesis, Antimicrobial and Antioxidant Evaluation of 3-(2-Phenylhydrazono)indolin-2-one Derivatives by $Co(NO_3)_2$ as Powerful and Efficient Catalyst
47	1071-ISOC26	**Ehsanorreza Poorhassan** Synthesis of Bi(cyclopropane) β-Amino Tricarboxylic Acids fro Fulvalene
48	1252-ISOC26	**Mehdi Zangene** Synthesis of Halloysite/Zein Nanocomposite for Controlled Drug Delivery of Phenobarbital Sodium
49	1129-ISOC26	**Mahmood Barani** Synthesis of Hydrophobin-Coated Niosome for Stealth Delivery of Anticancer Drugs
50	1236-ISOC26	**Zahra Malaie** Synthesis of Starch Nanocatalysts and Use in the Green Synthesis of Heterocyclic Naphthyropane Derivatives
51	1168-ISOC26	**Afsaneh Piri** The Aromaticity of Aromatic Rings in Pyrroloquinoline Quinone Isomers
52	1240-ISOC26	**Farahnaz Raji Dahmardeh** The Effect of Different Supports Calcineal at Different Temperatures on the Catalytic Activity for Fischer-Tropsch Synthesis
53	1221-ISOC26	**Roohollah Amanollahi** Synthesis of Novel Spiro Uracil-1,4-dihydropiridine via One-Pot, Three Component Reaction
54	1222-ISOC26	**Roohollah Amanollahi** Synthesis of Novel Tetrahydrospiro[1,4]diazepine
55	1253-ISOC26	**Mohammad Asadpour** Copper (II) acetate Intermolecular C (sp2)-H Amination of Directing Group with Electron-Rich Anilines
56	1169-ISOC26	**Soheila Heydari-Parastar** A Green Synthesis of Substituted Bis(indolyl)methanes Using Chlorosulfonic Acid Supported Piperidine-4-carboxylic acid (PCA) Functionalized Fe3O4 Nanoparticles (Fe3O4-PCA) as Recyclable Catalyst
57	1112-ISOC26	**Abolfazl Zakavat Moghanlu** Application of Pristine and Ni-Decorated Zigzag (8,0) Boron Nitride Nanotube for Adsorption of Methylamine and Ethylamine: A DFT Study
58	1128-ISOC26	**Masoumeh Taherimehr** Core-Shell Fe3O4@SiO2-SO3H Nanoparticles as Efficient Catalyst in the Synthesis of Dihydropyrano[3,2-c]chromenes

59	1092-ISOC26	**Mousa Khodadadi** Design and Synthesis a Self-Healing Polymeric Coating Formed through Diels-Alder Reaction between Bismaleimide and Furan-Modified Poly-ethyleneglycol
60	1091-ISOC26	**Mousa Khodadadi** Preparation and Characterization of Chitosan/Poly(vinyl alcohol) Injecta-ble Hydrogel as Drug Carrier
61	1004-ISOC26	**Morteza Ebrahimnejad** The Role of Formaldehyde Coagulation in the Production of Regenera-tive Fibers from Dairy Products
62	1081-ISOC26	**Hadi Kargar** MoO2(ONO) Schiff Base Complex: A Homogeneous Catalyst for the Synthesis of Benzimidazolesunder Various Reaction Conditions
63	1116-ISOC26	**Shafie Shokrollahzadeh Haghi** Optimization, Kinetics, and Equilibrium Studies on the Removal of Beta-Lactam Antibiotics from Industrial Waste Water Using Functionalized Magnetic Multi-Walled Carbon Nanotube as a Novel Adsorbent
64	1109-ISOC26	**Mahdi Afshar Torbati** Performance of Graphene Nanomaterial for Removal of Organophos-phate Pesticide from Aqueous Solutions
65	1238-ISOC26	**Aliyeh Barzekar** Preparation of Sulfamic Acid-Functionalized Fe3O4@Carbon as an Effi-cient Nanocatalyst for One-Pot Synthesis of 9,9-Dimethyl-12-phenyl-8,9,10,12-tetrahydro-11H-benzo[a]xanthen-11-one Derivatives
66	1177-ISOC26	**Ebtesam Saadi** Removal of Methyl Orange Dye by Absorbent Carbon Nanotubes with Response Surface Experimental Design and Genetic Algorithm
67	1231-ISOC26	**Sorosh Ziarati** Removal of *Orange* II *R and Red 12* Dyes from Water with Montmorillo-nite and Chitosan Nanosheets
68	1181-ISOC26	**Babak Vosoughi** Removal of phenol from Synthetic Waste Water by Fenton Method with Taguchi Test Design
69	1237-ISOC26	**Aliyeh Barzekar** Synthesis and Characterization of Copper-Salen Complex on Periodic Mesoporous Organosilica and its Application in Synthesis of Pyrano (2,3-d) Pyrimidine Derivatives
70	1102-ISOC26	**Iran Sheikhshoaie** Synthesis, Characterization and Theoretical Study on the Structural Prop-erties of a Tetradentate Schiff Base Compound

71	1115-ISOC26	**Mina Islami** Synthesis of a Novel Dendrimer Based on Poly Ethylene Glycol for Gene Transfection into the HEK-293T Cells
72	1073-ISOC26	**Hadi Kargar** Synthesis, Spectral Characterization and Antimicrobial Activity of Schiff Base Ligands Derived from 4-Amino-2,3-dimethyl-1-phenyl-3-pyrazolin-5-one
73	1006-ISOC26	**Azita Jafarnezhad** The Study and Compartion of Antioxidant Properties of Methanolic Extracts of Portulaca oleracea L. and Colutea buhsei (boiss.) shap from Northern Khorasan Province
74	1157-ISOC26	**Mahsa Haddadi** Efficient Synthesis of Some New Oxazolone Based Azo Dyes
75	1017-ISOC26	**Ali Mondanizadeh** Synthesis of Thiohydantoins with MCM-41-based in Solvent-Free condition and Microwave Irradiation

ABSTRACTS

Higher Education in Iran; from Dar-al-Funun to Payam-e-Noor

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Dar al-Funun, founded by Amir Kabir, originally was conceived as a polytechnic to train officers and civil servants to pursue the regeneration of the state that Amir Kabir had begun, but as the first educational institution giving instruction in modern learning, it had far wider impact. Among the subjects taught were medicine, surgery, pharmacology, natural history, mathematics, geology, and natural science. The school was established in 1851, training 287 students by 1889, and had graduated 1100 students by 1891. During this time, the faculty consisted of 16 European, and 26 Iranian professors. Dar al-Funun developed and expanded its mission over the next hundred years, eventually becoming the University of Tehran. During the last three decades, higher education in Iran has witnessed enormous expansion. Presently, more than 5 million students are enrolled in the universities. The admission of so many students of only average ability to higher education requires a decline in academic standards. The supply of graduates in many fields of study is exceeding the demand for their skills, which aggravates graduate unemployment, as well as educational inflation.

Application of Conducting Polymers (Polyanilines) in Sustainable and Renewable Energies and Electronic Systems

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Organic materials are most often insulating and only rarely discussed in the connection with metallic behavior. Nevertheless, one class of organic materials have turned out to possess conductivities that match those of the best crystalline metals like copper. This class of material, the conjugated polymers, has for that reason been coined 'synthetic metals'. Although the initial interest in those materials was related to the metal-like conductivity, the current researches focus more on exploiting the semiconducting properties of the conjugated polymers. Materials in which electrons are the charge transfer elements are intrinsically conducting polymers, where the electrical conductivity is a result of delocalized electrons along the polymer backbone. Today's conductive polymer workhorses are primarily derivatives of polypyrrole, PEDOT, polyaniline, and polythiophene. Polyaniline is considered as a prototype and among most popular conductive polymers. Already in 2000 Alan Heeger, Alan MacDiarmid, and Hideki Shirakawa were awarded the Nobel Prize in chemistry "for the discovery and development of conductive polymers". Nanotechnology and conductive polymers approximately have the same age, but contrary to the field of conductive polymers, which was abruptly introduced in a short communication, nanotechnology emerged gradually through the journey from microtechnology to smaller scales. Now structural entanglement at the nanoscale has provided rare opportunities for the formation of interesting nanocomposites. This lecture covers the remarkable range of applications emerging for nanostructured conductive polymers. These applications generally exploit the increased surface area of nanostructured materials, often to do something very new. One very important example is of polymer solar cells, where nanoscale phase separation lies at the heart of charge generation and extraction. Another exciting application domain is the use of nanostructured conductive polymers as biomaterials, including the development of neural interfaces. Other applications are sensors, actuators, corrosion protection, light-emitting diodes (LED), electrocatalysis and so on. It is our hope that the listeners will find inspiration and profit from looking into this lecture dedicated to the important and valuable conducting polymeric materials.

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Transition Metal Catalyzed Organic Transformations

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Transition metal-catalyzed reactions are some of the most attractive methodologies for synthesizing potentially active organic compounds, since a transition-metal catalyzed reaction can directly construct complicated molecules from readily accessible starting materials under mild conditions [1]. The transition-metal-catalyzed isocyanide insertion reaction as an important and modern strategy has received broad attention recently compared to traditional methods for the organic molecules synthesis which gives an atom economical, simple and direct synthetic strategy to complex and structurally diverse molecules using simple substrate [2]. Similarly, homocoupling reactions are the operators of the symmetrical compound productions within the synthetic chemist's repertoire. Typically, the metal-catalyzed synthesis of these reactions involves the reaction of (hetero) aryl halides or pseudohalides, oxidative-homocoupling of organometallic reagents and direct C–H bond functionalization (dehydrogenative homocoupling) [3]. In this lecture, new transition-metal-catalyzed isocyanide insertion reactions for the synthesis of new potentially active compounds will be discussed. In second part, some new transition-metal-catalyzed, CN-directed unsymmetrical synthesis of bithiophenes via an unprecedented homocoupling reaction will be described.

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Doped Carbon Nanostructures; Synthesis by Chemical Vapor Deposition and Their Applications as Sensor, Catalyst and Adsorbent

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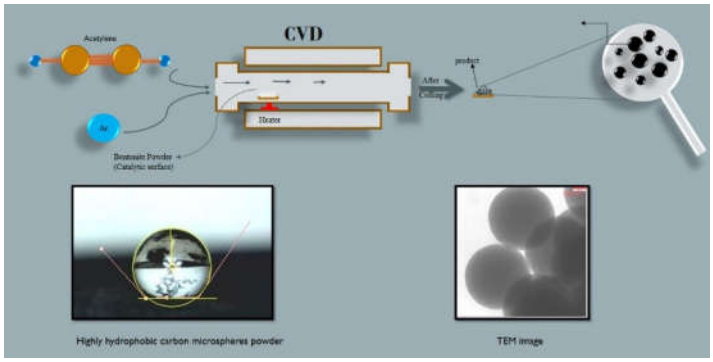
Doped carbon nanostructures (CNTs, graphenes, carbon fibers and fullerenes), have been attracted a worldwide interest as novel nanostructures [1]. Several methods such as spray pyrolysis, laser deposition, chemical vapor deposition (CVD) and hydrothermal have been employed to produce these materials. These materials could be used in electronic devices [2], supercapacitors, electrochemical catalysts, lithium ion batteries, Sensor and as the catalyst for chemical reactions [3]. However, many aspects in the synthesis applications of these compounds, especially in the case of doped materials, are unknown and needs to be investigated. Therefore, during the last 5 years, we have focused to develop efficient and economic methods for the synthesis of simple and doped carbon nanostructures. Moreover, some studies have been performed about the application of these compounds as catalyst in chemical and electrochemical reaction, adsorbent and sensors. It should be considered that because of the high surface/mass ratio of these compounds, they could be suitable nanocatalysts in various transformations. Meanwhile, they can be used as efficient sensors for different molecules such as toxic gases, pollutants and drugs. It is noticeable that when the nanostructures doped with heteroatoms (such as N, B, S and P), their properties will be changed effectively and doping is well-known as an efficient method to obtain the desired properties for each special application.



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Biochemical Synthesis of Ag@AgCl Nanoparticles and its Application in Photodegration of Azo Dyes

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The green synthesis of silver-silver chloride nanoparticles (Ag-AgCl NPs) has been proposed as a simple, easy, eco-friendly and cost effective method. In the present study, the leaf extract for the reduction of silver nitrate into Ag-AgCl NPs and phytochemicals of the leaves act as a reducing, as well as stabilizing agent. The Ag-AgCl NPs thus produced are anisotropic in nature and shows different particle morphology depending on the reaction conditions. The Ag-AgCl NPs synthesis procedure was optimized by varying different reaction parameters including pH, temperature, incubation time, salt concentration, and leaf extract concentration to reaction mixture. The prepared NPs were well characterized using techniques such as FEG-SEM, XRD, TEM, UV−visible spectrometry, and EDS. The Ag-AgCl NPs formation was observed visually by color change and absorbance peak (at around 400 to 450 nm) was observed by UV-visible spectrophotometer. The shape, size, and morphology of synthesized Ag-AgCl NPs were monitored by transmission electron microscopy. The face centered cubic structure of Ag-AgCl NPs was confirmed by X-ray diffraction pattern and element composition by energy dispersive X-ray analysis. The Fourier transform infrared spectroscopy spectrum showed the interaction of the leaf extract with synthesized Ag-AgCl NPs. The Prepared Ag@AgCl nanomaterials exhibited good photocatalytic ability toward degradation of methyl orange and methylene blue azo dyes in aqueous solution in the visible region of light. The catalyst was tested up to four recycles and showed no significant loss of catalytic activity.

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Fabrication of Ultra-Small Ruthenium Nanoparticles on Porous Modified Reduced Graphene Oxide and its Application in Solvent-Free Oxidation of Cyclohexene with Molecular Oxygen

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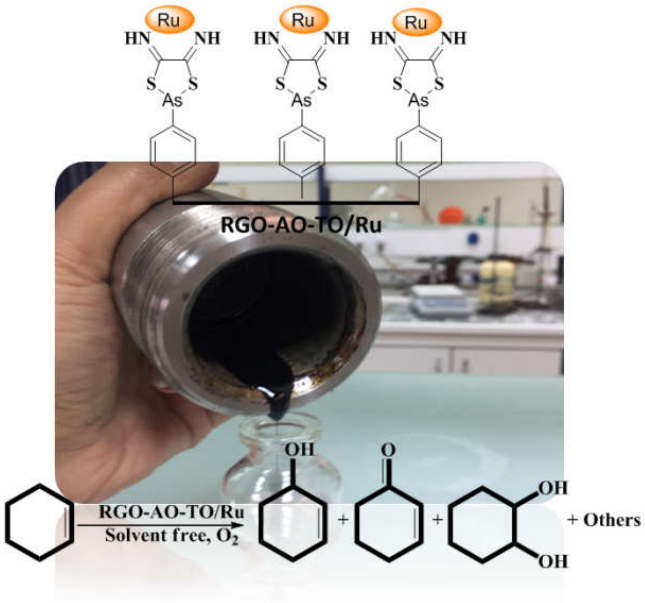
In the present work, Ruthenium nanoparticles were synthesized on functionalized reduced graphene oxide. First, the surface of reduced graphene oxide (rGO) was modified with two para-arsanilic acid and dithiooxamide promoters to create the rGO with scattered hydrophilic positions. The Ruthenium nanoparticles were synthesised and immobilized simultaneously in small hydrophilic micro reactors in a mild condition. Characterization of synthesised nanocatalyst was confirmed with different techniques such as TEM, XRD, FT-IR, and SEM. TEM images of synthesized catalyst show the Ru nanoparticles have diameters less than 6nm. Designed nanonanocatalyst was investigated for the selective liquid phase oxidation of cyclohexene with molecular oxygen in an autoclave under solvent free condition which after optimized conditions a maximum of 91% conversion and 90% selectivity was obtained. The catalytic activity over RGO-AO-TO/Ru recycled catalyst remained at a satisfactory state after at least 5 runs.



Chemistry's Role in the Treatment of Cancer

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Early interactions between chemistry and medicine had been disappointing. Dr. Harvey a 17th century physician, had once called chemist the most ignorant, flatulent, fleshy and vainly boasting sort of mankind. The mutual animosity between chemistry and medicine persisted until 1849, when Dr. Hofmann, acknowledged the chasm between medicine and chemistry. In 1828, a German scientist, Wohler showed that boiling ammonium cyanate, formed urea, a chemical produced by kidney. Organic and inorganic chemical was proved to be interchangeable. Biology is chemistry; a human body was no different from a bag of busily reacting chemicals. Another German scientist, Ehrlich once explained his idea that, it should be possible to find artificial substances that can specifically cure certain diseases. Cancer has been around as long as we have been around. In 400 BC, Hippocrates named the disease Karkinos (carcinos) or crab. For thousands of years we had no drug to treat cancer and physicians around the world including Abu Ali Sina and Razi either removed, burned or treated cancer with natural remedies. Chemotherapy started in 1947 with an antifolate drug, aminopetrin made in the laboratory of a chemist, as well as an Indian physician called, Subbarao. In 1970s, chemotherapy became the battleground of war against cancer. Cancer research was accelerated in 1970s when US government approved an independent budget for National Cancer Institute and the molecular biologist finally discovered the genetic basis of cancer. In two decades, more than 100 oncogenes were discovered and researcher tried to develop targeted drugs for cancers. In 1990s the development of small molecules that interfere with oncogene's activities as well as biological drugs such monoclonal antibodies offered new approaches to combat cancer more efficiently. In 1994, I developed a different strategy to develop safe drugs, using genomic information. The technology was named DNAi and one such drug, an inhibitor of bcl-2 oncogene, was successfully used to treat relapsed non-Hodgkin Lymphoma's patients in USA. We have submitted our IND application to conduct a phase II clinical trial in Isfahan/Iran as soon as we receive the ethic committee approval.

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Design, Synthesis and Biological Evaluation of Novel Ligands as Potential Anti-Alzheimer's Agents

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Memory problems in elderly people could be symptoms of Alzheimer's disease (AD), an irreversible neurodegenerative brain disease causing progressive deterioration of memory, thinking and reasoning skills [1]. AD is a complex multifactor disease that its exact pathogenesis is not fully clear. Neuropathological studies have demonstrated that the low levels of acetylcholine, β-amyloid plaques formation within the brain of AD patients and oxidative damage of neuronal cells are the key factors for the development of AD [2]. Due to the importance of multi-target drugs development for AD therapy and on the basis of above-mentioned findings, we have designed two series of new compounds including benzoheterocycles-based *N*-benzyl pyridinium derivatives and 2,3-dinaminopyridine-coumarin analogs (Fig. 1). The designed compounds were synthesized and evaluated for multifunctional biological activities including anti-cholinesterase, $A\beta_{1\text{-}42}$ protein anti-aggregating, and protective effect against H_2O_2-induced PC12 cell injury, as well as docking study.

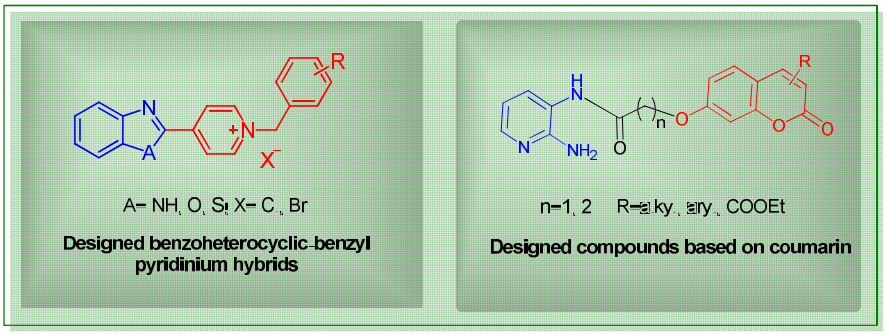

Fig. 1 Structures of newly designed compounds

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Anomeric Based Oxidation

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Classification of basic concepts is one of the major duties of the scientists toward common readers. The origin of the anomeric effect has been a matter of debate, so that there are contradictory approaches for this subject. Very recently, Wiberg *et al.* have published an excellent paper entitled "The anomeric effect: Its complicated" [1]. Nevertheless, further investigations of this important effect are still required [2]. To the best of our knowledge, the origin of the anomeric effect is not a consequence of an effect alone, but it is the result of the several factors, which it is working together. The identifying between stereoelectronic interactions is a major problem (none bonded repulsion and so on), hyperconjugation (negative, positive and neutral) and anomeric effect (endo, exo and reverse) that may be confused by readers. Sharing the electron density from an anion and/or none bonded lone pair(s) electrons into the vacant anti-bonding (σ^*) orbital was known as negative hyperconjugation. Intramolecular negative hyperconjugation is also known as anomeric effect. Each type of stabilizing due to interaction between a sigma bond with donors or acceptors was known as hyperconjugation interactions. Aomeric conjugation (donation from a lone pair to the vicinal sigma* orbital) is an example of hyperconjugation (conjugation that involves a sigma bond). All of the terms of conjugation, hyperconjugation, σ-conjugation and anomeric effect are often recognized as resonance in modern scientific literatures [3-4]. Recently we have introduced a new concept entitled of "anomeric based oxidation" (ABO) which has opened a new synthetic and theoretical insight for the design, synthesis and applying the organic molecules that are important in medicinal and biological activities [5]. The "anomeric based oxidation (ABO)" mechanism is in good agreement with the previous reported "vinylogous anomeric effect" studies [6-8].

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Synthesis of Heterocyclic Compounds Bearing Nitrogen and Oxygen Atoms Using Nano-kaoline/BF_3/Fe_3O_4 Based on Green Chemistry in Different Conditions

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In recent years, using nano-size solid acids in chemical reactions have been known as a principle in development of green chemistry. The efficiency of heterogeneous catalysts can be improved by employing nanosized catalysts because of their extremely small size and large surface to volume ratio and act a bridge between homogeneous and heterogeneous catalysts. On the other side, heterocyclic compounds containing nitrogen or oxygen have received much attention for their biological activities and the wide application in both pharmaceutical and industrial researches. So, the widespread application of solid acids, structural and practical diversity of heterocyclic compounds containing *N*- or *O*- have prompted us to employ the novel and eco-friendly methods for the synthesis of heterocyclic compounds including: 3,4-dihydropyrimidin-2(1*H)*-ones [1], 1,4-dihydropyridines [2], 2,3-dihydro-1*H*-perimidines [3], *N*-arylpyrroles [4], and tetrahydro-4*H*-chromenes [5,6] using nano-kaoline/BF_3/Fe_3O_4 as a green catalyst under different conditions. Initially, nano-kaoline/BF_3/Fe_3O_4 were prepared. Its structure and properties were characterized through the conventional methods of determining materials such as: FESEM, TEM, FT-IR, XRD, EDX, VSM and TGA. Then, this catalyst was used in the synthesis of some heterocyclic compounds bearing *N*- and *O*- atoms. The obtained products have been characterized by FT-IR, ^{1}H NMR and ^{13}C NMR spectroscopy.

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Fabrication of Nitrogen-enriched Graphene Oxide/Cu NPs as a Highly Efficient and Recyclable Heterogeneous Nanocatalyst for the Chan-Lam Cross-Coupling Reaction

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Herein, we demonstrated the direct polymerization of melamine and cyanuric chloride in the surface of graphene oxide (GO) (N-enriched GO) for the development of new nanocatalyst. The supramolecular polymerization of GO not only as a spacer to prevent the restacking of graphene sheets but also as a nitrogen source to generate active centers for Cu NPs attachments. Subsequently, the nitrogen decorated on the surface of the graphene oxide sheets coordinated with copper ions to generate copper nanoparticles (Cu NPs). The prepared nanocatalyst was characterized by Fourier transform infrared (FT-IR), X-ray powder diffraction (XRD), scanning electron microscopy (SEM), energy-dispersive X-ray spectroscopy (EDX), thermogravimetric analysis (TGA) and atomic force microscopy (AFM). This catalyst showed high efficiency and good activity in Chan-Lam cross-coupling reaction of N-heterocycles, aliphatic amines and aniline derivatives with high yields in short reaction times. In addition, nanocatalyst was easily recovered and reused for five consecutive runs without noticeable loss of performance.

Intelligent Chemical Passive Defense

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The life style and humans behave towards one another, due to the advances in knowledge and technology, especially in the chemistry, physics and biology sciences, the increasing of population and the formation of civil society; have changed the environment and nature. Such as human contribution in the destroying of assets, capital and even making of disasters has gradually increased. In the present modern and industrial world, it can be claimed that the main cause of destroying and pollution of most of water resources, air and in general the environment is the consequence of the deliberate or unknowing interference of humankind with the nature. On the other hand, the rapid growth of information technology (IT) and computer science, and the creation of communication channels such as fiber, bluetooth, wifi, WiMAX, and ZigBee, has made it possible simple to manufacture intelligent devices such as sensors, controllers, and so on.

Regarding the concept of chemical defense that is applied for the set of preventive actions, including observation and monitoring, diagnosis and declaration of condition, elimination of pollution, relief and rescue treatment, training, exercise, fitness raising, reduction of vulnerabilities, frame-work protections and facilitation of crisis management against threats and chemical disasters, The use of intelligent tools to monitor accidents involving hazardous materials, as well as application of intelligent equipment during chemical crises can minimize the golden time of coping and responding to emergency situations. These cause to reduction of damaging of people, natural resources and frame-works. For example, due to the occurrence of toxic leaks, fires or explosions, the assets and capitals of a community, including people, agricultural products, natural resources and the environment, are subject to harm, threat, and destruction. Intelligent technology plays an effective role in dealing with chemical accidents and crises before, during and after the incident.

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Perhalopyridine: Synthesis and Synthetic Utility

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Heterocycles represent a larger group of organic compounds and play an important role in all aspects of pure and applied chemistry. The subgroup of this class called perhalogenated heterocyclic compound since the intensive development of the synthetic chemistry of heterocycles started in the last few years [1]. Nowadays halogenated heterocyclic compounds can be found among potent pharmaceuticals, crop protection agents, and products of technical importance. This merging area of organic, heterocyclic, and chlorine organic chemistry is still rapidly growing and in the last decades a large number of halogenated heterocyclic materials have been discovered. Substituted pyridines are important material in organic chemistry, biochemistry, and pharmaceutical chemistry [2]. Preparation of highly substituted pyridine derivatives from pyridine itself is very difficult and only limited progress has been made using such an approach. In contrast, perhalogenated pyridine are potentially excellent scaffolds because they are highly reactive toward nucleophilic attack as a result of their electron-deficient nature, and in principle, all halogen atoms may be displaced by nucleophiles. Mono-, di-, tri- tetra- and penta substituted pyridine, fused heterocyclic compound, macrocyles and other useful organic compounds have been synthesized from the reaction of corresponding C-, N-, S-, P- and O-centered nucleophiles as well as bidentate nucleophiles with perhalogenated pyridine (Fig. 1) [3].

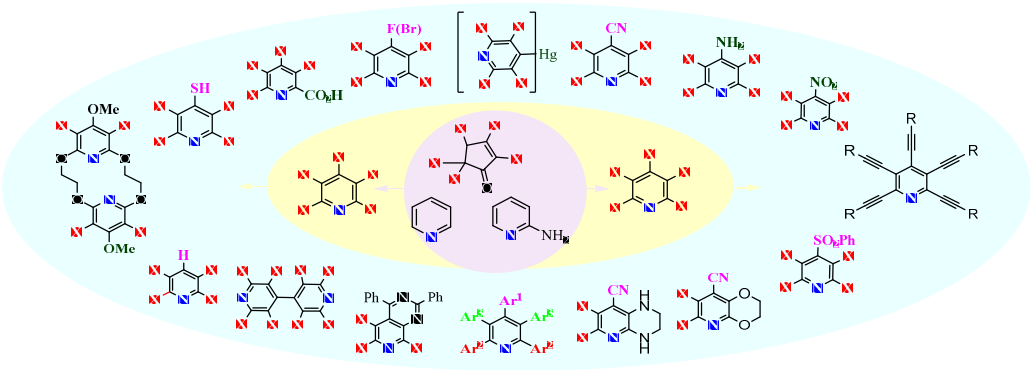

Fig. 1 Synthesis and synthetic utility of perhahlopyridine

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AMHB: Anti(aromaticity) Modulated Hydrogen Bonding

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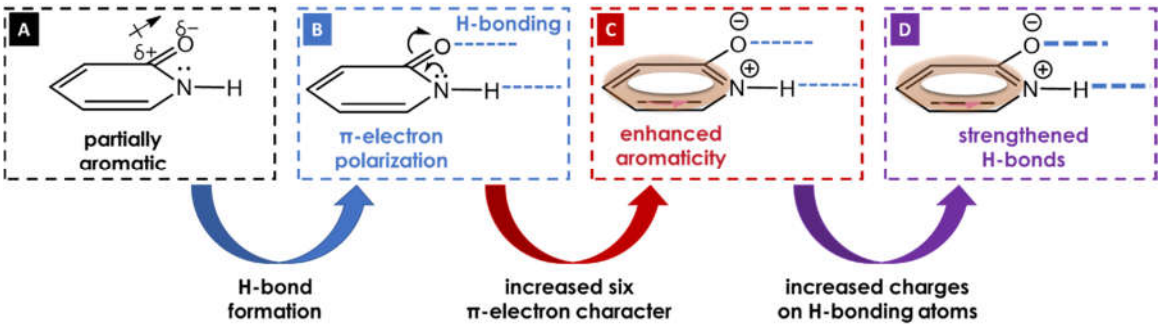
Aromaticity and H-bonding are common features of many heterocycles from DNA base pairs to ligands binding proteins. Despite being known as separate bonding concepts for more than a century, their interplay has been underappreciated. An *in-silico* survey on a wide range of aromatic and antiaromatic heterocycles capable of H-bonding shows a uniform pattern for their interplay: "H-bonding interactions that enhance aromaticity or relieve antiaromaticity are fortified, whereas those that intensify antiaromaticity or disrupt aromaticity are weakened, relative to analogs lacking full π-circuits". Attribution of these energetic to (anti)aromaticity is supported by the calculated changes of dissected nucleus-independent chemical shift ($NICS(1)_{zz}$: a computable index of (anti)aromaticity). Furthermore, experimental measurements show that the effect remains significant in solution phase, and provide energetic, magnetic, and geometric evidence for AMHB.



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Polyethylene Glycol-Bonded Tetraethyl Ammonium *L*-Prolinate: A New Highly Efficient Biodegradable Amino Acid-Based Ionic Liquid for the Synthesis of Some DNA Binders as Anticancer Agents

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As the research on ionic liquids have advanced, numerous problems have been also reported including poor biodegradability, toxicity (some ionic liquids), unsuitable physicochemical properties (large viscosity) and large production costs, which have hindered scaling up ionic liquids for further applications at industrial scale. In order to obtain ‘‘fully green’’ ionic liquids, the starting materials must be at least non-toxic, whilst for a perfect solution and they should be renewable. The bio-renewable natural compounds are ideal materials from the viewpoints of both environmental and economic concerns. A few successful samples have been reported, for example, using lactates [1] and sugar substitutes [2] to prepare anionic constituent and amino acids [3] to prepare cationic constituent of ionic liquids. Amino acid-based ionic liquids have been shown to have a range of useful properties due to the fact that they contain two functional groups, a carboxylic acid and amino group, as well as the fact that a chiral center is present, which can be obtained relatively inexpensively using naturally derived amino acids. Further characteristic of amino acid derived ionic liquids includes the improved biodegradability. Considering these facts, we herein introduced the polyethylene glycol-bonded tetraethyl ammonium *L*-prolinate as a new readily biodegradable amino acid-based ionic liquid for the one-pot *pseudo*-five component synthesis of bis(pyrazolyl)methanes. Moreover, the anticancer activity of synthesized compounds as novel DNA binding agents was successfully evaluated (Figure 1).

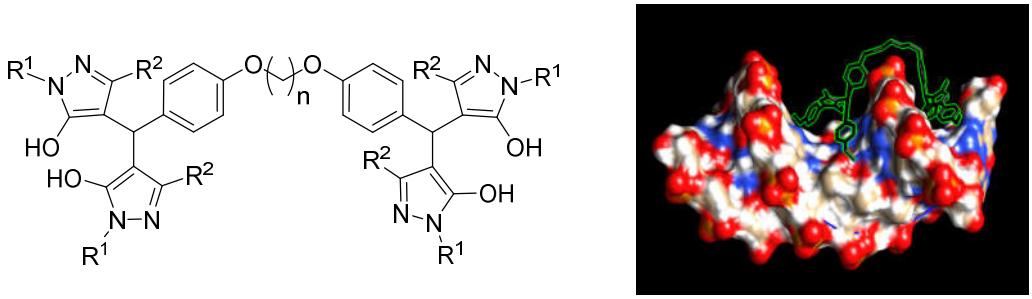

Fig. 1 Bis(pyrazolyl)methanes: Novel DNA binders with anticancer activity

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Green Synthesis of Monocyclic and Fused Nitrogen Heterocycles with Promising Bioactivity Effects

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Pursuing novel synthetic methodologies according to the green chemistry principles has been the active area of research for the past four decades. Heterocyclic building blocks, as an important class of organic compounds, have attracted much attention because of their medicinal, agricultural, and biological applications [1]. Five- and six-membered nitrogen heterocycles have presented broad array biological and medicinal properties. Thus, finding novel synthetic methodologies toward the synthesis of these classes of building blocks would definitely be beneficial for preparation of new products with promising biological and medicinal uses. In the present paper, we have reviewed the attempts toward the green synthesis of some classes of monocyclic and fused nitrogen heterocycles accomplished by us (Fig. 1).

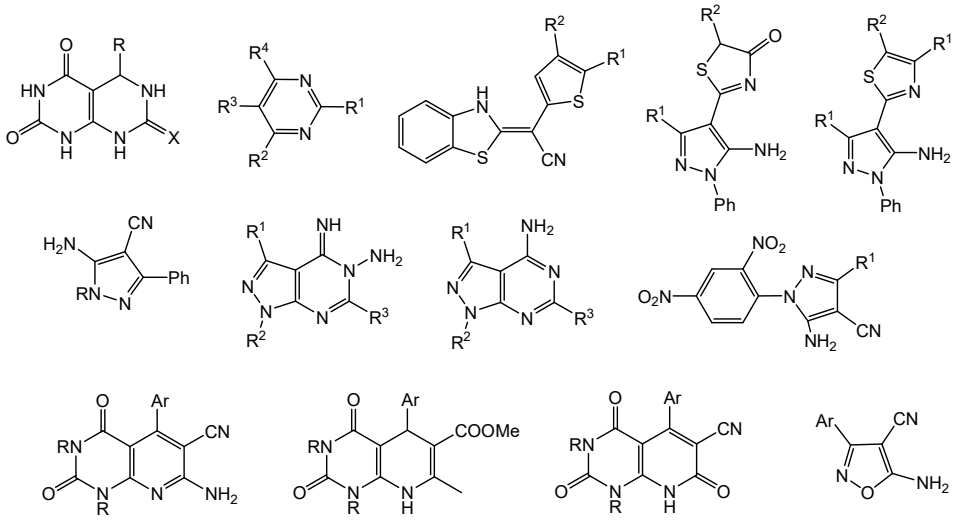

Fig. 1 Monocyclic and fused nitrogen heterocycles with promising bioactivities produced and reported by Aryan and coworkers

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Metal-Organic Frameworks (MOFs) as Heterogeneous (Photo-)Catalysts in Organic Transformation Reactions

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Modern synthetic designs demand the minimization of synthetic steps together with environmentally and chemically more efficient benign processes, which dictate and appeal the further development of such synthetic strategies and tactics. Designing new protocols with emphasis on reducing the use of toxic reaction media, transition metals, oxidants/additives, and precious (rare and expensive) catalysts, remains significantly challenging. Metal–organic frameworks (MOFs), so-called porous coordination polymers (PCPs), are three-dimensionally extended crystalline materials having high porosity, and are composed of metal-ion-containing nodes/secondary building units (SBUs) and organic linkers/struts. By using rationally chosen organic linkers and metal-containing precursors, crystalline solids with uniformly structured cavities, high surface area, high porosity, and tailorable physicochemical properties can be achieved [1,2]. In addition, the possibility of post-synthetic modification (PSM) of MOFs, as an important method to produce new functionalized frameworks, creates new opportunities for their further applications. As a result, MOFs have been recently demonstrated to be highly valuable materials for a wide range of potential applications such as gas storage, separation, sensing, conductivity, light harvesting, drug delivery, deactivation of chemical warfare agents, removing toxic materials from air and water, and catalysis. This emerging class of catalysts exhibits the advantages of both homogeneous and heterogeneous catalysts. Porosity, as a microstructured reactor, can be used both to increase accessible catalytically active sites and to preconcentrate substrates, increasing reaction rates and yields of products. Furthermore, non-covalent interactions, such as van der Waals forces and solvophobic effects may serve to intensify the interaction between substrates and the surface of MOF, resulting in more efficient adsorption and packing, thereby causing the enhancement of the reaction rate. The utilization of MOFs in heterogeneous photocatalysis is currently an emerging field in organic transformations, aiming the use of natural light as renewable energy to minimize the environmental problems. With growing demand for organic chemicals and pharmaceuticals, it is urgent to develop green and effective strategies for selective synthesis of the compounds.

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Introducing the Corresponding Committee on Reference Materials of the Institute of Standards and Industrial Research of Iran (ISIRI/REMCO)

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Committee on reference materials (REMCO) is a part of the international organization for standardization (ISO) with the aim of compilation and presentation of international standards on reference materials. It has members from National Organizations for Standardization of the membership countries, including Iran. ISO has several technical committees, and REMCO is settled in its headquarter in Switzerland. 32 countries are participating (P) members and 40 countries are observer members of REMCO. Iran is a P member with the right of voting [1]. REMCO consisted of a main committee, a consultative group, two special groups and four working groups, targeting preparation of standards in the field of reference materials and communicating with the other technical committees of ISO as well as any other organizations acting in the field of reference materials. So far, 9 international standards have been released by this committee and three standards are in progress [2]. In Iran, secretary of corresponding technical committee of REMCO is in Sistan and Baluchistan which is actively participate in the development of international standards, with over 70 professional members. Currently, a national standard associated with the reference material is being prepared with close contribution of Iran Nanotechnology Innovation Council. Reference materials are referred to those that are sufficiently homogeneous and stable according to specific properties and used to control and trace the results of measurements and also to validate measurement methods, calibrate of equipments, control of the performance of methods and staff and compare with inter laboratory results. They are used in almost all aspects of today's life, since these materials are critical to control the quality of products. In the quality management systems that require laboratory approvals for the issuance of national and international standards such as ISO 9000 and ISO 17025, the use of reference materials is compulsory. All persons and organizations dealing with reference materials, academicians, industries, etc. can participate in the compilation of national and international standards and also in the developing of the international standards dealing with reference materials through ISIRI/REMCO.

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Applications of Phosphonium-Based Ionic Liquids in Chemical Processes

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Among ionic liquids, phosphonium-based ionic liquids (PILs) are quite elegant. This category of ionic liquids represents some merits such as higher thermal and chemical stability compare with other types of ionic liquids. These influential characteristics of PILs, make them as potential materials for various kinds of applications in the laboratory and industrial processes. They can be applied as elegant catalyst and/or solvent for organic functional group interconversion. Also, the diffusivities of gases such as carbon dioxide, in the PILs are much higher than imidazolium-based ionic liquids. PILs have numbers of unique applications in electrochemical systems. PILs are an unprecedented class of electrolytes that can support the electrochemical generation of a stable superoxide ion, unlike of organic solvents. There is also a growing interest for their use in separation processes including metal ions extraction, extractive desulfurization, gas adsorption and dissolution or extraction of biologically relevant compounds. Also, experimental works have also satisfied that the PILs fulfil the necessary requirement of being a good inhibitor of metal corrosion under different media because of their surface active properties. Owning to special physicochemical properties, the PILs are emerging as possible candidates to improve surfactant enhanced oil recovery methods [1-3]. This work will present an excellent puzzle that each of its pieces leads to the rational design, synthesis, and applications of the novel and tasked-specific PILs as multi-purpose materials.

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Preparation and Characterization of New Organocatalysts Supported on Nanomagnetic Particles as Green Nanocatalysts and Their Applications in Organic Synthesis

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Surface functionalization of nano-magnetic nanoparticles is a well-designed way to bridge the gap between heterogeneous and homogeneous catalysis [1-3]. Organocatalysts created a homogenous part which starting materials easily converted to the desired products(s), heterogeneous part of these advanced catalysts separated easily using an external magnet [1-3]. Thus, high conversions in reaction and an easy work-up procedure cause to prepare desired compounds in high pure isolated yields [1-3]. (3-Oxo-[1,2,4]triazolidin-1-yl)bis(butane-1-sulfonic acid) functionalized magnetic γ-Fe_2O_3 (γ-Fe_2O_3@Oxo-triazolidin-sultone) nanoparticles as a novel and heterogeneous nanocatalyst was prepared. The novel nanocatalyst was characterized by X-ray diffraction (XRD), Fourier transform infrared spectroscopy (FT-IR), vibrating sample magnetometry (VSM), Field Emission Scanning Electron Microscopy (FE-SEM), and thermal gravimetric analysis (TGA). The superparamagnetic γ-Fe_2O_3@Oxo-triazolidin-sultone nanoparticles showed enhanced catalytic performance for the preparation of novel spiro[indeno[1,2-*b*]quinoxaline derivatives *via* the four-component condensation of amines, ninhydrin, isatoic anhydride, and *o*-phenylenediamine derivatives. The nanocatalyst can be easily separated from the reaction mixture by an external magnet, recycled, and reused several times without a noticeable decrease in catalytic activity. Glycine-proline-glutamic acid (Gly-Pro-Glu) supported on superparamagnetic silica encapsulated γ-Fe_2O_3 as a novel heterogeneous catalyst was designed and synthesized. The nanocatalyst was characterized by several techniques. MNPs γ-Fe_2O_3@SiO_2-linker- Gly-Pro-Glu as catalyst was used for the facile synthesis of thiazoloquinoline, thiazolopyridine, and thiazolonaphthyridine derivatives.

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Paper code: 1004

The Role of Formaldehyde Coagulation in the Production of Regenerative Fibers from Dairy Products

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It is very important to find a coagulant in a chemical process and, by doing a lot of research, we find the most suitable and the most abundant and cheapest form of aldehyde, therefore, we first mention it. Casein is a protein that exists in large amounts in milk. Protein and peptides are made by a sequence of various amino acids, the most important of which are glycine, cysteine and threonine [1-3]. Glaycine, cistein, teronine. In the present research, initially the cream, which is an important nutrient, is separated from the milk. Then the remaining milk is warmed to 40°C and the protein content is coagulated by acidifying the milk. The coagulated protein is extracted from the aqueous part of the milk, washed to remove the acid and salt and then dried. The collected casein is fully mixed and dissolved in sodium hydroxide solution. after passing through special filters, it is entered into the spinneret fiber making machine. The next stage is the coagulation bath containing sulphuric acid, formaldehyde, and glucose. At the end the spinning operation and casein fibers production is performed.

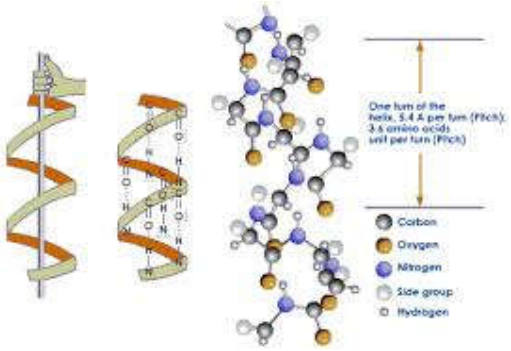

Fig. 1 Pregnancy of the amino acid casein in the presence of potassium carbonate catalyst

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One-Pot Synthesis of 1,4-Dihydropyridines via Hantzsch Reaction Using Nano-kaolin/BF_3/Fe_3O_4 as a Green Catalyst under Solvent-Free Conditions

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1,4-Dihydropyridine derivatives exhibit a large range ofbiological activities. They have been used as anticonvulsant, antidepressive, antianxiety, analgesic, antitumoral, hypnotic, vasodilator, bronchodilator and anti-inflammatoryagents [1]. Some of them, such as amlodipine, felodipine, isradipine, lacidipine and nifedipine are effective drugsas calcium-channel blockers for the treatment ofcardiovascular diseases and hypertension.1,4-dihydropyridinesare also good precursors of the correspondingsubstituted pyridine derivatives and constitute useful reducingagents for imines in the presence of a catalyticamount of lewis acid [2]. Hantzsch first reported in 1882 theone-pot three-component condensation of an aldehydewith ethyl acetoacetate (or 1,3-dicarbonyl compounds) and ammonia (or ammonium acetate) in acetic acid or refluxingalcohol [3]. Yields of the resulting 1,4-dihydropyridinesare usually modest and in recent years, several newefficient methods have been developed including the useof microwaves, ionic liquids, TMSCl–NaI, metal triflates, molecular iodine, SiO_2/$NaHSO_4$, SiO_2/$HClO_4$, ceric ammonium nitrate, Na- and Cs-norit carbons, tetrabutylammonium hydrogen sulfate, fermentingbaker's yeast, and organocatalysts [4].

In this study, we report our results for the synthesis of 1,4-dihydropyridines by a one-pot cyclocondensation of aldehyde with ethyl acetoacetate and ammonium carbonate using nano-kaolin/BF_3/Fe_3O_4 as a magnetic catalyst under solvent-free conditions (Fig.1). The advantages of this study involve in use of solvent-free conditions, an easy experimental work-up system, rapidity, recyclable catalyst and green process.

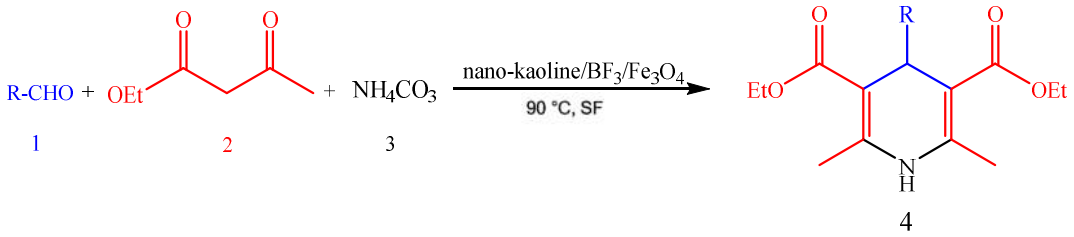

Fig.1 Synthesis of Hantzsch 1,4-dihydropyridines catalyzed by nano-kaoline/BF_3/Fe_3O_4

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Paper code: 1006

The Study and Compartion of Antioxidant Properties of Methanolic Extracts of Portulaca oleracea L. and Colutea buhsei (boiss.) shap from Northern Khorasan Province

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Nowadays, the emergence of allergies, side effects of chemical drugs, antibiotic resistant strains, and the body's need for antioxidant compounds have emphasized the importance of herbal medicine. In this study, antioxidant properties methanol extract of portulaca oleracea L and Colutea buhsei(boiss.) shap, two medical herbs, were investigated. Aerial parts of two plants were collected in June 2017 from Mountains (Govinac around the Raz). The methanolic extracts of the two plants were prepared by maceration technique. After concentration with rotary, their antioxidant activity was assessed by two methods: 2, 2-dipheyil1-picryl hydrazyl (DPPH) [1] and ferric reducing antioxidant power (FRAP) [2,3]. Butylated hydroxy toluene (BHT) was used as a positive control. The IC_{50} value for the portulaca oleracea L. and Colutea buhsei (boiss.) shap and BHT is 1.391, 0.716 and 0.012 mg per ml; respectively, while in the FARP method, the antioxidant activity informs of mmol Fe^{+2}/g of extract for portulaca oleracea L. and for Colutea buhsei (boiss.) shap is calculated 269.27 and 692.79, respectively (The results are presented in Table 1). The results showed that antioxidant activity of two plant extracts of portulaca oleracea L. and Colutea buhsei (boiss.) shap less than BHT, also methanol extract of Colutea buhsei (boiss.) shap has an antioxidant activity higher than portulaca oleracea L.

Table 1. Measuring the antioxidant properties

Sample	Extraction efficiency	DPPH method	FRAP method
		IC_{50} (mg/ml)	mM Fe++ / g extract (1 mg/ml)
Paortulaca olerace L.	32.46	1.391	269.27
Colutea buhsei	20.06	0.716	692.79
BHT	-	0.012	-

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Preparation and Characterization of Ferromagnetic Nanoparticles of La_2O_3 by Thermal Decomposition Approach

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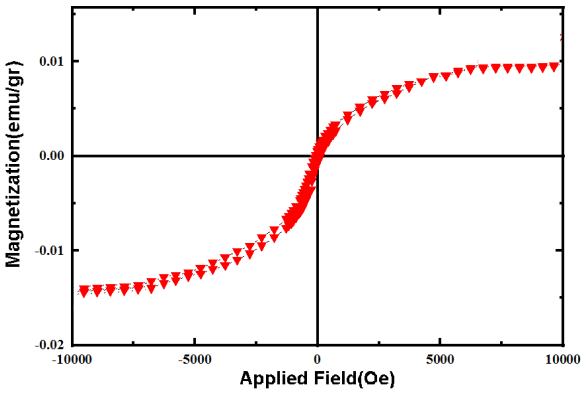
Recently a number of researchers have reported the synthesis of transition metal nanoparticles by thermal decompositionof organometallic complexes as precursors. Nanomaterials have been extensively explored because their properties are different from bulk materials. Nanostructured materials exhibit interesting properties and applications such asin conducting paints, magnetic drug targeting, recording material and catalyst, gas sensor and anti-virus agent, etc [1-3]. In the present work, La_2O_3 nanoparticles were prepared through thermal decomposition of $([La(Pydc)_2(H_2O)_3].4H_2O)_n$. The structural properties of La_2O_3 nanoparticles were studied byFourier transform infrared spectroscopy, X-ray diffraction pattern, scanning electron microscopy and vibrating sample magnetometer. The magnetic properties of La_2O_3 nanoparticles at room temperature through magnetization versus magnetic field is shown in Fig.1 .It is well known that the La_2O_3 nanoparticles display ferromagnetism with a narrow hysteresis loop. The corresponding values of saturation magnetization (M_s), remnant magnetization (M_r) and coercivity (H_c) is 0.01 emu/g, 0.002 emu/g and 282 Oe respectively.



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Paper code: 1008

A di-Nuclear Copper(II) Complex as a Precursor for Octahedron-Like CuO Nanoparticles

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Metal-organic complexes have been extensively studied because of their potential applications in molecular recognition, host–guest chemistry, gas storage, catalysis optical and magnetism [1-3]. In the present work, a new dinuclear copper(II) complex with a formula of $[Cu_2(pydc)_2(inta)_2(H_2O)_2]$ $.3H_2O$ (**1**), that inta is isonicotinic acidhave been synthesized under ultrasound irradiation. Compound **1** was used as an inorganic precursor to prepare CuO nanoparticles through thermal decomposition. Fig. 1 shows the scanning electron microscope image of CuO nanoparticles to understand more structural details and morhological information which clearly shows the octahedron-like morphology for CuO nanoparticles. The SEM image showed that the particles size of CuO crystalsis about to 70–90 nm.

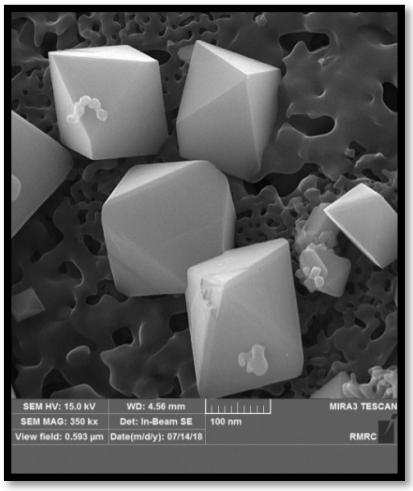

Fig.1 SEM photographs of CuO nanoparticles

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Lactose: A Novel and Green Catalyst for an Environmental Synthesis of Medicinally Important Pyrano[3,2-c]pyrazoles

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Pyrano[2,3-c]pyrazoles are an important class of heterocyclic compounds that are known to be biological agents. they play an essential role such as anti-HIV [1], antibacterial, antifungal [2], anticancer and anti-inflammatory activities [3]. In this study, A simple, high yielding and expeditious one-pot four-component protocol for the synthesis of pyrano[2,3-c]pyrazole derivatives has been investigated using Lactose as a green catalyst (Fig. 1). The influence of reaction parameters like reaction temperature, time, the amount of catalyst, type of solvent and the amount of catalyst were investigated with respect to yield of pyrano[2,3-c]pyrazoles. The reported approach shows significant advantages such as operational simplicity, the use of an inexpensive and non-toxic catalyst, high yields, short reaction time, and ease of product isolation without chromatographic separation.

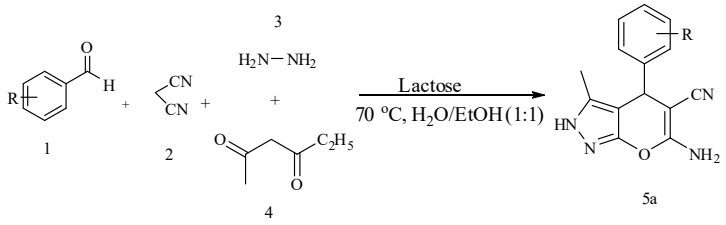

Fig. 1 Lactose-catalyzed four-component synthesis of pyrano[3,2-c]pyrazoles

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Paper code: 1011

Organoselenium-Palladium(II) Complex Supported on Modified Magnetic Nanoparticles as an Efficient Catalyst for Suzuki Reaction

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Among the palladium-catalyzed cross coupling reactions, the Suzuki-Miyaura reaction which is coupling between aryl, vinyl or alkyl halides or pseudohalides and organoboron reagents is one of the most noteworthy and comprehensively protocolsfor the construction of carbon-carbon bonds. The products of this reaction have been widely used for the synthesis of pharmaceuticals compounds, natural products and agrochemicals [1]. The most common catalytic system utilized for C–C coupling reaction is promoted by homogeneous palladium complexes. The accurate selection of the ligand is the key and important factor for the synthesis of these complexes [2]. Chalcogen containing ligands haveattracted considerable attention due to their much less insensitivity to air and moisture, strong electron-donating ability of the chalcogen donor site, solubility in diverse solvents and stability in solution, which make them currently important and suitable for designing Pd-complexes for catalyzing of C–C coupling reactions [3]. In the present study, the Fe_3O_4 magnetic nanoparticlesmodified by SiO_2/aminopropyl triethoxy silane (Fe_3O_4@SiO_2-APTS) utilized for anchoring a moisture- and air-stable organoselenium-palladium complex (Fe_3O_4@SiO_2-Se-T/Pd(II)) and applied as an efficient and retrievable catalyst in Suzuki-Miyaura cross coupling reaction (Fig. 1). The wide substrate scope, high yield, short reaction time, simple separation of the catalysts from reaction mixture and more importantly, the longevity of nanocatalyst for at least four consecutive runs without a discernible decrease in its activity are the main merits of this protocol.

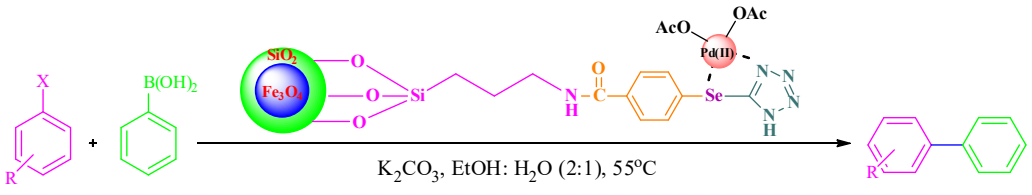

Fig. 1 Synthesis of biaryl derivatives in the presence of Fe_3O_4@SiO_2-Se-T/Pd(II)

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Paper code: 1012

Synthetic Application of Palladium(II) Anchored on a Magnetic Mesoporous Polymelamine-formaldehyde as a Heterogeneous Nanocatalyst with Excellent Regeneracy Performance in Suzuki Coupling Reactions

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Development and design of different mesoporous organic polymers (MOPs) as a type of highly cross-linked amorphous polymers can be done by efficient synthetic strategies including interlinking of miscellaneous chemical group with porous network that present versatile and attractive properties and applications such as gas storage, separation, catalysts and catalyst supports [1]. Particularly, catalysts based on palladium are widely studied due to their well-known applications in the synthesis of organic compounds including Heck, Suzuki, and Negishi coupling reactions [2, 3]. Regeneration of catalyst and designing of a strategy to avoid the risk of gradually decreasing of precious and noble metals is also especially essential issue in the case of economically perspective. In the present work, we develop palladium(II) anchored on magnetic mesoporous poly melamine-formaldehyde "Fe_3O_4-mPMF/Pd(II)" nano-composite as one impressive heterogeneous nanocatalyst with excellent chemical tenability, better durability and desirable porosity. The composite was prepared simply in two steps. This catalyst was applied for Suzuki reaction to create the corresponding coupling product in excellent yields. The influence of reaction time, catalyst amount and temperature was investigated and maximum yield of 98% at optimum conditions was obtained. The synthesized nanocatalyst can be easily separated from the reaction medium and reused without remarkable changes in its catalytic activity.

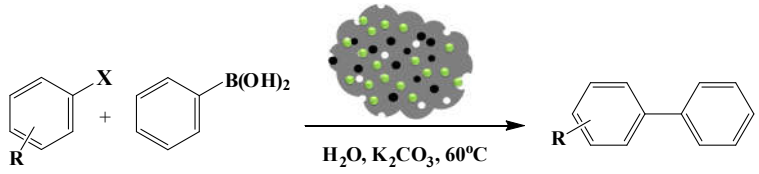

Fig. 1 Suzuki reaction in the presence of Fe_3O_4-mPMF/Pd(II) nanocomposite

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Paper code: 1014

One-Pot Condensation Approach for the Synthesis of Tetrahydrobenzo[b]pyran Derivatives Utilizing Salicylic Acid as an Efficient and Eco-friendly Catalyst

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In recent years, the synthesis of pyran derivatives, especially tetrahydrobenzo[b]pyrans, has received an increasing interest because of attractive pharmacological and biological properties [1]. These compounds are also used in the industry as optical brighteners, laser dyes, pigments, cosmetics and potent biodegradable agrochemicals [1-3]. In a continuation of our endeavors towards the development of new catalytic protocol, we wish to report an efficient one-pot, three-component strategy for the rapid synthesis of dimedone (1 mmol), malononitrile (1 mmol), aldehyde (1 mmol) in the presence of a catalytic amount (20 mol %) of salicylic acid in EtOH/H_2O at 70 °C. The advantages of this protocol are higher product yields in shorter reaction times, easy work-up, and available of the catalyst (Fig .1)

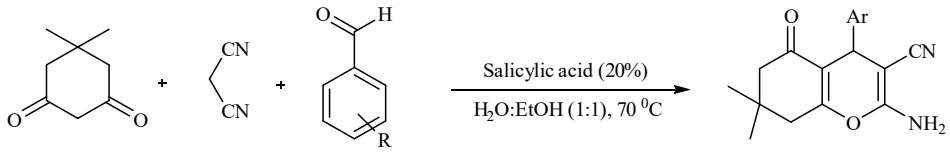

Fig. 1 Multicomponent synthesis of tetrahydrobenzo[*b*]pyran derivatives

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12-14 March, 2019

Paper code: 1016

$Co(NO_3)_2.6H_2O$: A Mild, Efficient and Novel Catalyst for the One-Pot Synthesis of Tetrahydrobenzo[b]pyran Derivatives

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Recently, tetrahydrobenzo[b]pyran derivatives are known as an important class of heterocyclic scaffolds in the field of drugs and pharmaceuticals [1]. These compounds exhibit significant biological properties such as antibacterial, antitumor, anti-allergic, antibiotic, hypolipidemic and immunomodulating activates [1-3]. In this paper, we want to report a one pot reaction for the synthesis of tetrahydrobenzo[b]pyran derivatives using dimedone (1 mmol), malonitrile (1 mmol), aldehyde (1 mmol) in the presence of a catalytic amount (20 mol%) of $Co(NO_3)_2.6H_2O$ in EtOH: H_2O at 70 °C. The advantages of this method are simple work-up, short reaction time, high yields and using eco-friendly metal.

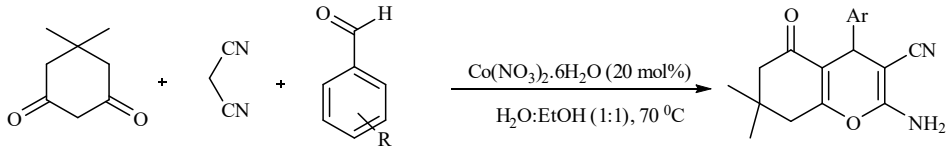

Fig. 1 Three-component synthesis of tetrahydrobenzo[*b*]pyranderivatives in green solvent

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Paper code: 1017

Synthesis of Thiohydantoins with MCM-41-based in Solvent-Free condition and Microwave Irradiation

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2-Thioxoimidazolidine-4-ones are five-membered aromatic heterocycles containing carbonyl, thiocarbonyl and nitrogen atoms. This ring system is found in variety of naturally occurring compounds and biologically active molecules. They are especially useful in medicine, since many antifungal drugs belong to the thiohydantoins class [1]. Various methods were developed for synthesizing these derivatives [2]. In this study, thiohydantoins were prepared *via* a solvent-free and microwave irradiation with nanocatalysts procedure. The best nanocatalyst were MCM-41-$SnSi_4$, MCM-41-$CeSi_3$, MCM-41-$CeSi_4$.
A convenient, environmentally friendly and mild green synthesis of thiohydantoin derivatives was developed by the one-pot reaction of benzils, urea or thiourea derivatives, and nano catalysts at grinding condition. The key advantages are the short reaction times, good yields, simple workup, and easy purification in the solvent-free condition.

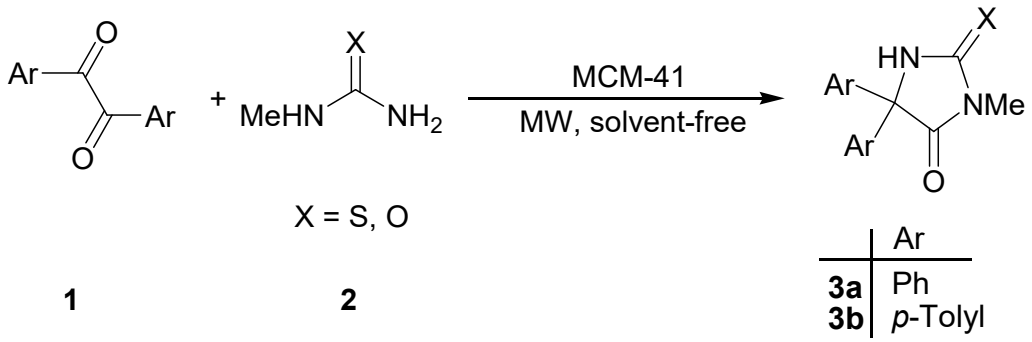

Fig. 1 Green synthesis of hydantoin derivatives

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Study of Antioxidant Activity of Methanolic Extract of (Inula Salicina (L.)) and (Inula Thapsoids (M.B.ex Willd)) With FRAP and DPPH Methods

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Antioxidant compounds are very important in human life. Antioxidants are the main factors for neutralizing the free radicals which are active and harmful for human. Preparing antioxidation resources to reduce the effects of oxidation stress is important [1,2]. Thus, this research was carried out to study the antioxidation properties of metanolic extracts of *Inula salicina* (L.) and *Inula thopsoides* (M.B. ex Willd). In this laboratory study, the plants were collected from North Khorasan Province of Iran, in spring of 2017 and the metanolic extract from aerial parts of plants was prepared by maceration extraction method. the antioxidant activities of the samples were determined by two different test systems, namely, DPPH free radical scavenging and iron deficiency reduction (FRAP) methods; and the results were compared with synthetic antioxidant BHT. In this study, IC_{50} value of the metanolic extracts were obtained 3.217 and 4.489 $mg.mL^{-1}$ of *Inula salicina* (L.) and *Inula thopspides*(M.B.ex Willd) respectively, whiles this value was 0.116 $mg\ mL^{-1}$ for synthetic antioxidant (BHT). Also, the reducing power of extracts reported 1199.68 and 945.33 (mmol of Fe^{+2}/ mg extract) for *Inula salicina* (L.) and *Inula thopsoides* (M.B. ex Willd) respectively.
The results show that the *Inula Salicina* L. plant has an antioxidant effect on *the Inula Thapsoids* (M.B. ex Willd) but the methanolic extract both significantly less antioxidant than the BHT positive control. The results of extraction efficiency and antioxidant properties of the extracts are presented in the table below.

Table 1. The extraction efficiency and antioxidant properties

Name	*Extraction efficiency*	*Fe^{2+} (mmol /mg)*	*$IC_{50(mg/ml)}$*
Inula Salicina	0.0963	1199.68	3.2177
Inula Thapsoids	0.0665	945.33	4.4891
BHT	-	-	0.1162

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Paper code: 1020

Influences of Decor Raw Paper and Type of Thermosetting Resins on the Quality of Laminated Wood Panel

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Paper impregnated and coated with thermosetting resins is usually used as a decorative and protective laminate for wood panel [1]. In the present study, Melamine Formaldehyde (MF) and Urea Formaldehyde (UF) and three raw papers from different suppliers (Wenge, Olive ash& Gruen) were used for impregnation process in lab scale to see the influence of some important manufacturing variables on the products quality. The resin picks up, weight of raw paper, percentage of UF and MF blending were investigated by some quality tests such as scratch resistance (SR), abrasion resistance (AR) and resistance to steam according to Europe EN438-2 standard test method [2]. As the UF resin pick up in impregnation process was increased, the scratch and abrasion properties decreased. The raw paper weight (RPW) didn't affect the properties of the panel same as SR and AR, but these parameters were significantly improved by increasing the MF resin pick-up (Table. 1) and is showed that MF resin is more resistance to mentioned tests than UF resin

Table 1. The quality properties of MF/UF impregnated papers with different samples and different ratios

Type	MF pick up (%)	UF pick up (%)	RPW (gr/m2)	SR (N)	AR (Rpm)	Resistance to steam	Impregnation Process
1	33.8	24.2	75	4.2	490	+	2-step
2	28	28	85	3.7	465.6	+	2-step
3	62	-	85	6.5	707.3	+	1-step

+ ,resistance

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Paper code: 1021

Investigation of Melamine Formaldehyde (MF) and Rubber Blending on Some Quality Effect of Composite Product

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Melamine formaldehyde (MF) is one of the hardest thermosetting polymers, which provides good properties and performance. It is an amino resin and has various material advantages, such as thermal stability, excellent boil resistance, moisture resistance and surface smoothness, which lead MF to large industrial application [1]. The copolymerization reaction in thermosetting resin in the coating industry, an understanding the viscosity of the resin is very important because it controls other factors such as flow rate, thermal and mechanical properties and dry rate [2]. The reactive blending of MF resin with rubber as a way of developing the paint binder for emulsion paint formulation has been investigated. By increasing some parameters of MF resin such as viscosity and total solid content (TSC), other properties in compound same as melting point, density, reactive index and free formaldehyde emission were increased which shown in figure1, while other parameters such as moisture content and dry time were decreased. Also, the solubility of MF- rubber compound has been studied in different viscosity. Solubility of MF blending resin decreases with increasing the viscosity. This result is due to difference in molecular weight and crosslink density.

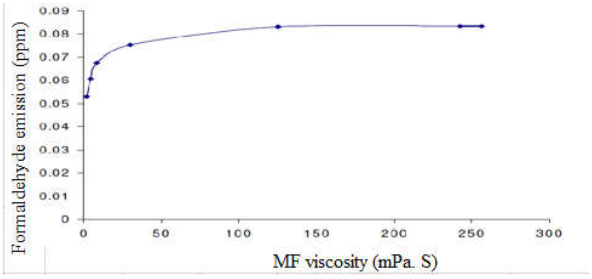

Fig. 1 Effect of MF viscosity on the formaldehyde emission on MF-Rubber blending

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12-14 March, 2019

Paper code: 1023

Purgation of the Environment Using Natural Materials from the Environment: Study of the Recent Development in Isotherms, kinetics, and Thermodynamics of the Adsorption

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Due to the increasing growth rate of the population, the attention has been centered around the water remediation. Thus, several methods are used in this regard which the adsorption process has been found to be the most favorite manner [1]. Hydrogels have met the expectations in the adsorption, hence, preparation of an appropriate hydrogel nanocomposite (HNC) was aimed using natural materials, tragacanth gum (TG) and calcite nanoparticles (CC NPs). CC NPs were modified using ethylenediaminetetraacetic acid (EDTA). Preparation of HNC (TG/CC@EDTA HNC) was carried out through the previous work [2]. Characterization and properties of the obtained HNC were done using several techniques. The HNC was used as an adsorbent of methylene blue dye (MBD). Results indicated that for either of isotherm and kinetic models, linear approaches are more accurate. Based on the linear equations, Langmuir and pseudo-first-order were suitable models for the adsorption which suggest monolayer and physical adsorption, respectively. The maximum adsorption capacity was found to be 469 mg/g. Thermodynamic calculations proved an endothermic and spontaneous process along with physiochemical adsorption. Fig. 1 shows possible interactions between MBD and TG/CC@EDTA HNC.

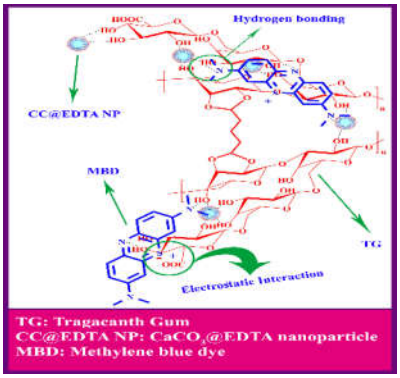

Fig. 1 Schematic probable interactions between TG/CC@EDTA HNC 5 wt% and MBD

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Paper code: 1026

Influence of ZnO-Folic Acid Nanoparticles on the Bioactivity Property of Polycaprolactone in the Simulated Body Fluid

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Among of biopolymers, polycaprolactone (PCL) is a good candidate for bone tissue engineering and substitution of damage tissues due to its biodegradability, biocompatibility, low-cost, and accessibility [1]. In order to prevent the agglomeration of ZnO nanoparticles (NPs) in the polymer matrix, in this study an attempt has been done to modify the surface of ZnO NPs with folic acid (FA) as a biosafe and biodegradable molecule. In the next step, ZnO-FA NPs (2, 5, and 8 wt %) were embedded in PCL. Fig. 1 shows the probable interactions between filler and matrix. The sonochemical process as a safe, fast, and green method [2], was used for the preparation of ZnO-FA NPs and PCL/ZnO-FA nanocomposite (NC) films. For characterization of NC films, different methods like field emission scanning electron microscopy, thermogravimetric analysis, UV-Visible spectroscopy, water contact angle, and transmission electron microscopy (TEM) were applied. TEM images showed good dispersion of NPs in the PCL matrix (Fig. 1). By increasing the amount of ZnO-FA NPs in the PCL matrix, the intensity of absorption peaks in the UV-Vis spectra was increased. Also, the *in-vitro* bioactivity evaluation of NCs showed the formation of the hydroxyapatite layers on the surface of these compounds in the simulated body fluid after 28 days.

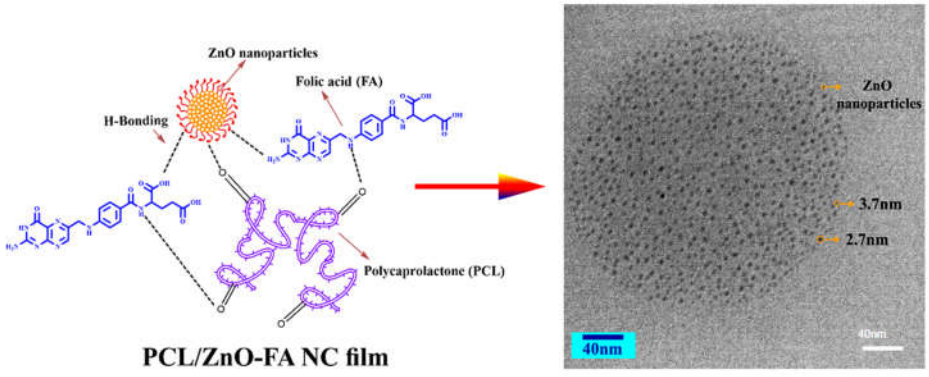

Fig. 1 Possible interactions inside the PCL/ZnO-FA NC and TEM image of PCL/ZnO-FA NC film

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Paper code: 1027

Poly(vinyl alcohol)/TiO_2@Folic Acid Nanocomposite Films: Survey of Optical, Thermal and Antibacterial Properties

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The surface modification of the nano-metal oxide has been introduced as an effective method to improve the dispersion of nanoparticles (NPs) and reduce agglomeration into the polymeric matrix [1]. In this project, the surface of TiO_2 NP was modified with folic acid (FA) as a safe and biodegradable molecule. Then, the modified TiO_2 NPs were added as a suitable nanofiller into the matrix of poly(vinyl alcohol) (PVA) with different percentages. The process was done by ultrasonic irradiation as a fast, cheap and green method [2]. The TiO_2-FA NPs and PVA/TiO_2-FA NC films were characterized by different methods. Thermogravimetric analysis and UV-Visible spectroscopy showed the better thermal stability and higher absorption of NC films in comparison with the pure PVA, respectively. Also, the prepared NC films showed the antibacterial activity under UV irradiation against*Escherichia coli (E. coli*) as gram-negative and *Staphylococcus aureus (S. aureus*) as gram-positive bacteria (Fig. 1). This property is related to the photo-catalytic property of TiO_2 NPs. In fact, in the presence of UV irradiation, the TiO_2 NPs can produce the reactive species like hydrogen peroxide, hydroxyl radical, and superoxide which can kill the microorganisms [3]. At last, it seems that the prepared PVA/TiO_2-FA NC films can be a suitable choice for the packaging system due to antibacterial properties and high absorption of UV-Vis radiation.

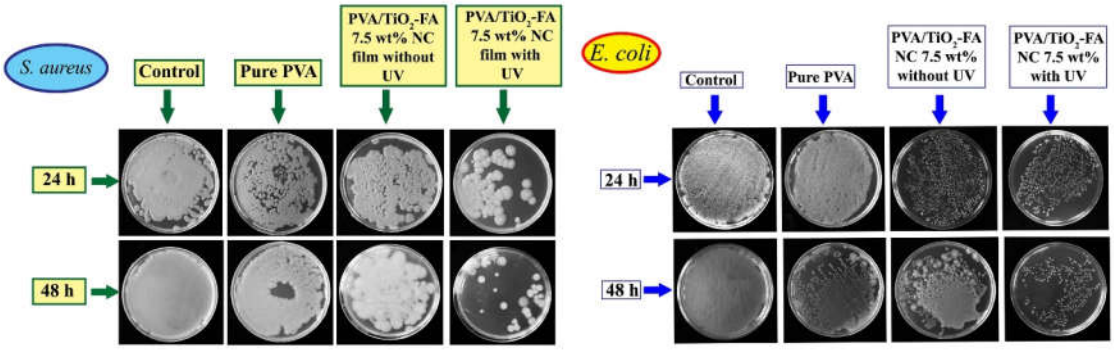

Fig. 1 Pictures of growth of viable *S. aureus* and *E. coli* on samples

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University of Zabol
12-14 March, 2019

Paper code: 1028

A Benign Route for the Production of Polymer Nanocomposite Films Based on Poly(vinyl alcohol) and SiO_2–Folic Acid Nanoparticles

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The synthesis of polymer/inorganic nanocomposites (NCs) has attracted much attention. This comes from the combination of the advantageous properties of inorganic nanoparticles (NPs) and polymers. SiO_2 NPs are used widely due to their properties such as high refractive index, high thermal stability, non-toxicity, environmental compatibility, and relatively inexpensive prices [1]. To solve the problem of agglomeration of SiO_2 NPs, surface modification is the best method [1]. Poly(vinyl alcohol) (PVA) is a water-soluble polymer which has been studied as a host matrix for a large number of nano-fillers, due to its excellent properties. It is biodegradable, biocompatible and nontoxic [2]. In this paper, to prevent the agglomeration of SiO_2 NPs, their surface was modified by folic acid (FA). Then, modified NPs was placed in a PVA matrix and SiO_2-FA/PVA NC films with 2, 5, and 8 wt% were produced by casting method under ultrasonic radiation as a green and low-cost method (Fig. 1A). Transmission electron microscopy (TEM) showed that the size of SiO_2-FA NPs in the PVA matrix was between 12-18 nm (Fig. 1B). With the insertion of SiO_2-FA in PVA matrix, the thermal resistance, flexibility, and wettability properties were increased.

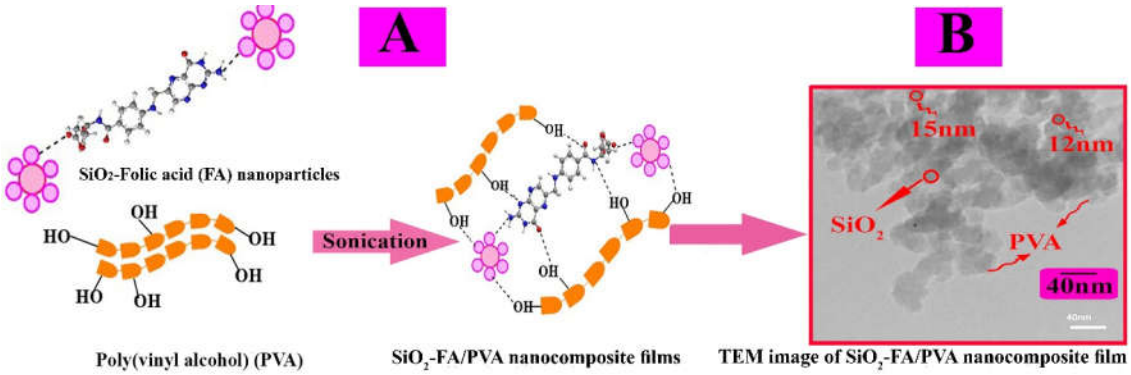

Fig. 1 (A) The schematic preparation of SiO_2-FA/PVA NC films, and (B) TEM image of SiO_2-FA/PVA 5 wt% NC films

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Paper code: 1030

Efficient Elimination of Methyl Orange Dye from Wastewater through Recyclable Bio-intercalate LDH-Fe_3O_4/PVA Nanocomposite

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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]. Layered double hydroxides (LDHs), also known as hydrotalcite like compounds, have attracted attention, which has led to a variety of applications [2, 3]. In this study intercalated LDH (I-LDH) with biosafe and anionic organic diacid was produced with the coprecipitation method. An effective intercalation of the examined diacid in the LDH layers was confirmed with variety of spectroscopic analysis. Fig.1(a) shows the increasing in the basal spacing of I-LDH in compared to the pure LDH. Then, I-LDH samples were composited with the pre-synthesized Fe_3O_4 nanoparticles (I-LDH@Fe_3O_4) through ultrasonic irradiation. LDH@Fe_3O_4 composite was dispersed in the matrix of poly(vinyl alcohol) (PVA) through ultrasonic irradiation and the physiochemical properties of prepared nanocomposites (NCs) were studied. Finally, the performance of NC 6 wt% as an efficient magnetic adsorbent was studied for removal of poisonous methyl orange from aqueous solution. The maximum adsorption capacity of NC 6 wt% was about 97 % (Fig. 1(b)).

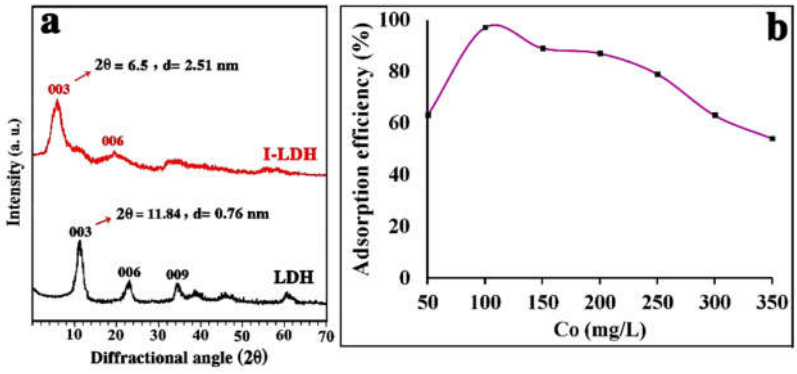

Fig. 1 (a) XRD patterns of pure LDH and I-LDH and (b) adsorption efficiency of NC 6 wt%

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Paper code: 1031

Selective and Efficient Oxidation of Benzyl alcohols to Benzaldehydes by Polydoxirane in the Presence of Molecular Oxygen at Room Temperature

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Oxidation of alcohols that lead to the preparation of carbonyl compounds are an important class in organic synthesis due to their applications in production of various pharmaceutical and chemical materials [1]. Various protocols and attempts to oxidation of alcohols (primary and secondary) in order to form carbonyl compounds show the importance of this basic reaction in organic synthesis [2]. However, there is a continuous demand to develop synthetic methods for discriminating efficiently various functional groups, because most of the reported methods suffer from lack of selectivity, using toxic solvents and oxidant, tedious work-up and harsh condition. In this point of view, chemoselective methods allow the oxidation of primary alcohols without the exhorting of competitive secondary alcohols. Salicylaldehyde is one of the safe, readily available organic compounds in health and reactivity point of view, which can be extracted from natural sources such as buckwheat [3]. In this work, we used an efficient and selective method for oxidation of a variety of benzyl alcohols to the corresponding benzaldehydes in the presence of polydioxirane (PDOX) by molecular oxygen at room temperature (Fig. 1). PDOX was prepared by polycondensation reaction of 5-chloromethyl salicylaldehyde followed by decoration of dioxirane groups of the framework of PDOX. In our previous work we have demonstrated the ability of the PDOX over selective epoxidation of olefins at room temperature as efficient alternative to dimethyldioxirane.

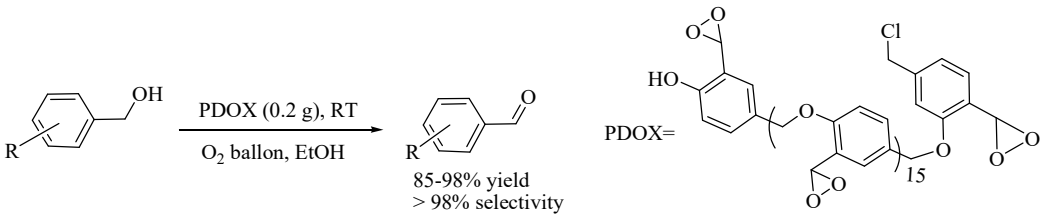

Fig. 1 Selective oxidation of benzyl alcohols using PDOX in the presence of molecular oxygen

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The 26th Iranian Seminar of Organic Chemistry
University of Zabol
12-14 March, 2019

Paper code: 1034

One-Pot Three Component Synthesis of 2,3-Dihydro-1*H*-1,5-benzodiazepines by a Magnetically Recyclable Nanocatalyst Fe_3O_4@SiO_2-Cu-salen

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Benzodiazepines and their polycyclic derivatives are an important class of bioactive compounds. Many functionalized benzodiazepines are widely used as anti-convulsant, anti-anxiety, analgesic, sedative, anti-depressive and hypnotic agents. These compounds also, finding applications as dyes for acrylic fibers and anti-inflammatory agents. 1,5-Benzodiazepines are key intermediates for the synthesis of various fused ring compounds such as triazolo-, oxadiazolo- and oxizino-diazepines [1]. Due to their broad spectrum of biological activity, these compounds received a lot of attention towards their synthesis. The general method for the synthesis of 1,5-benzodiazepines involves an acid-catalyzed condensation of *o*-phenylenediamines with *α,β*-unsaturated carbonyl compounds or β-halo ketones or ketones. Many reagents have been utilized for this reaction including polyphosphoric acid-SiO_2, $BF_3{\cdot}OEt_2$, $NaBH_4$, $Yb(OTf)_3$, MgO-$POCl_3$, and more recently acetic acid under microwave conditions [2]. In continuation of our research towards the synthesis of biologically important molecules in this study various 1,5-benzodiazepine derivatives were synthesized by the condensation reaction of o-phenylenediamine with various ketones using the Fe_3O_4@SiO_2-Cu-salen [3] as an efficient, heterogeneous magnetically recyclable catalyst (Fig. 1).

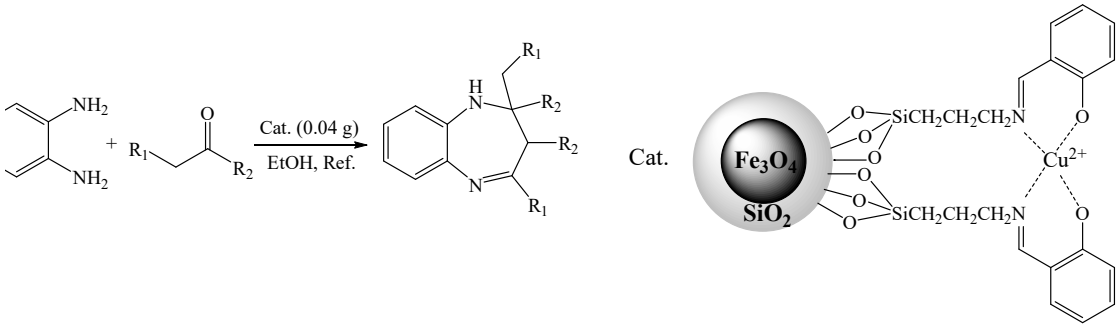

Fig. 1 Synthesis of 2,3-dihydro-1*H*-1,5-benzodiazepines by Fe_3O_4@SiO_2-Cu-salen

References

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The 26th Iranian Seminar of Organic Chemistry
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12-14 March, 2019

Paper code: 1035

An Efficient Synthesis of Benzimidazole Derivatives Using a New Binuclear Cu-Bis-Salen Complex at Room Temperature

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Benzimidazole derivatives have attracted a significant attention in recent years because of their medicinal applications as antiviral, antiulcer, antifungal, antihypertensive, anticancer, and antihistamine compounds [1]. Apart from therapeutic applications, benzimidazoles also play an important role as intermediates in different organic reactions. Two general methods are reported for the synthesis of 2-substituted benzimidazoles; (1) coupling of phenylenediamines and carboxylic acids or their derivatives (nitriles, imidates, or orthoesters) as well as (2) a two-step procedure that consists of the oxidative cyclodehydrogenation of aniline Schiff's bases, which are often generated in situ from the condensation of phenylenediamines with aldehydes [2]. However, most of these methods involve drastic reaction conditions, tedious work-up procedures and low yields [3]. The additional serious drawbacks relate to the use of homogeneous catalysts that are somewhat modified in the work-up procedure and cannot be recovered. In continuation of our work on the development of low loaded, environmentally sound, affordable, stable and selective catalysts for greener organic reactions, herein we report the use homogeneous effective catalytic system based on bis-Cu(II)-salen complex for the synthesis of benzimidazole compounds under mild reaction conditions. This homogeneous catalytic system possesses inherent advantages for benzimidazole synthesis including high activity, low metal loading in the catalyst as well as the use of a relatively inexpensive transition metal (Cu) system that prepared by accessible and cheap starting materials.

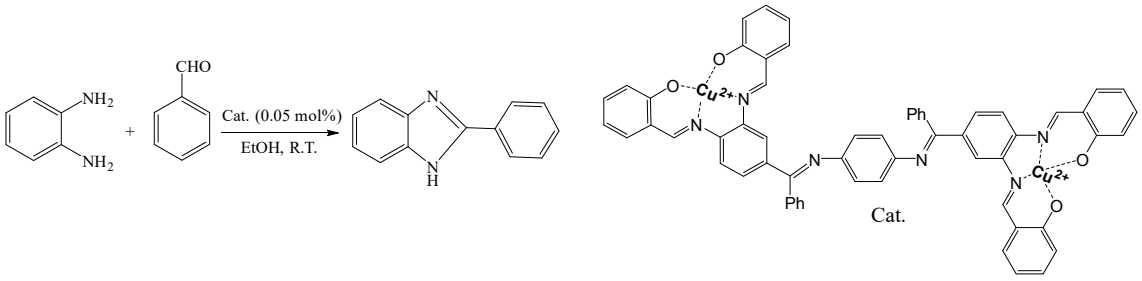

Fig. 1 Synthesis of 2,3-dihydro-1*H*-1,5-benzodiazepines by Fe_3O_4@SiO_2-Cu-salen

References

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12-14 March, 2019

Paper code: 1036

One-Step, Three-Component Synthesis of Highly Substituted Pyridines Using $CuFe_2O_4@SO_3H$ as Reusable Catalyst

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The synthesis of 'privileged medicinal scaffolds' is highly important as these compounds often act as ligands for a number of functionally and structurally diverse biological receptors, and consequently, serve as a platform for developing pharmaceutical agents for diverse applications. Among them, 2-amino-3,5-dicarbonitrile-6-sulfanylpyridines exhibit various pharmacological activities and are useful as antihepatitis B virus, antiprion, antibacterial, and anticancer agents, and as potassium channel openers for treatment of urinary incontinence. Moreover, some of these compounds were found to be highly selective ligands for adenosine receptors, implicated Parkinson's disease, hypoxia/ischemia, asthma, kidney disease, and epilepsy. These vast applications have inspired the development of a number of methods for the preparation of pyridine derivatives. however, literature studies reveal that most of the methods involve multistep sequences and low isolated yields, use of toxic and expensive catalysts, and lack generality. The synthesis of pyridines a through multicomponent reaction (MCR) of aldehydes, malononitrile, and thiols has recently attracted much attention owing to excellent synthetic efficiency, intrinsic atom economy, high selectivity, procedural simplicity, and environmental friendliness [1-3]. In conclusion, we have demonstrated an efficient and general procedure for the synthesis of 2-amino-3,5-dicarbonitrile-6-sulfanylpyridines via multicomponent reaction of aldehydes, malononitrile, and thiols using of $CuFe_2O_4@SO_3H$ as a very mild, effective, environmentally benign, and reusable catalyst.

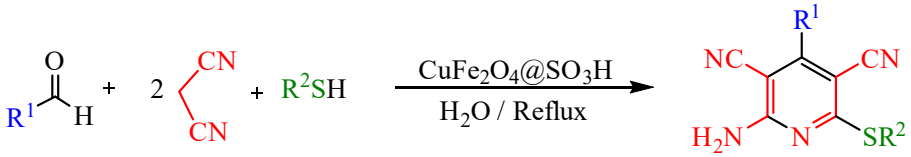

Fig. 1 Synthesis of 2-amino-3,5-dicarbonitrile-6-sulfanylpyridines

References

[1] G. Shanthi, P.T. Perumal, *Tetrahedron Letters,* **2009**, 50:3959-3962.
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The 26th Iranian Seminar of Organic Chemistry
University of Zabol
12-14 March, 2019

Paper code: 1037

$CuFe_2O_4@SO_3H$: A Mild, Efficient and Reusable Heterogeneous Catalyst for the Synthesis of Highly Functionalized Piperidines

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Multi-component reactions (MCRs) are special types of synthetically useful organic reactions in which three or more different starting materials react to give a final product in a one-pot procedure. MCRs are becoming powerful tools in the modern synthesis chemistry due to their efficiency, atom economy, and convenience in the construction of multiple new bonds in one-pot processes, which played powerful roles in approaching complex structures and promoting the 'green chemistry' [1, 2]. The piperidines and its analogues are important heterocycles that are present in many naturally occurring alkaloids, biologically active synthetic molecules and organic fine chemicals. Some of them also act as pharmaceutical agents. Compounds containing piperidine structural motif exhibit anti-hypertensive, antibacterial, antimalarial, anticonvulsant and anti-inflammatory activities. Thus, the synthesis of highly substituted piperidines has gained considerable attention, and number of procedures have been developed using several approaches such as tandem cyclopropane ring-opening/Conia-ene cyclization, imino Diels-Alder reactions, aza-Prins-cyclizations, intramolecular Michael reactions and intramolecular Mannich reaction onto iminium ions. The functionalized piperidines have been reported using MCRs strategy by employing bromodimethylsulfonium bromide (BDMS), $InCl_3$ and LProline/TFA. However, use of expensive and excess amount of catalysts are some of the disadvantages of the above mentioned methods. Therefore, there is a need for highly efficient, versatile and eco-friendly synthetic protocol to obtain these valuable compounds in good yields [3]. We report herein full details of a novel, convenient, and simple procedure to realize a one-pot pseudo five-component reaction of aldehydes, amines, and 1,3-dicarbonyl compounds, catalyzed by $CuFe_2O_4@SO_3H$, for the preparation of piperidinecompounds in EtOH with high yields (72-95%) and short times.

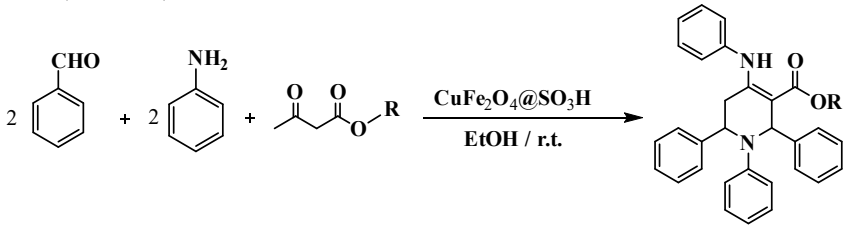

Fig. 1 Synthesis of piperidine compounds using $CuFe_2O_4@SO_3H$ as catalyst

References

[1] G. Shanthi, P.T. Perumal, *Tetrahedron Letters*, **2009**, 50:3959-3962.
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The 26th Iranian Seminar of Organic Chemistry
University of Zabol
12-14 March, 2019

Paper code: 1038

Synthesis of a 3D-Network Polymer Based on a Calix[4]resorcinarene Containing N_3Anion: A Green and Reactive Solid Supported Reagent

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In this work, a cationic polymer containing pendant pyrazine groups was synthesized via two post-functionalization steps. Initially, the active homogeneous moiety was chemically immobilized onto a polymeric support based on calix[4]resorcinarene by silylation of the hydroxyl groups to form a cationic polymer that contains pyrazine moieties [1,2]. The formation of this cationic polymer was confirmed by CHN, SEM, TGA and DTG analysis. Subsequently, N_3 anion was incorporated into the polymer along the pyrazine pendant groups via a well-known ion exchange reaction. Elemental analysis data revealed that the cationic polymer was conveniently loaded with the desired N_3 anion, therefore, it provides a novel polymer supported reagent for achieving synthetic goals.

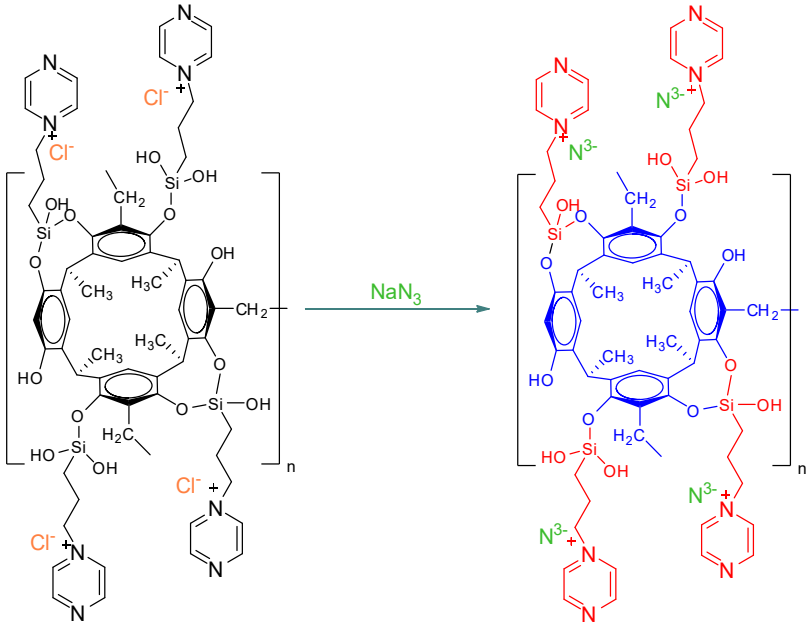

Fig. 1 Synthesis of polymer supported reagent

References

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The 26th Iranian Seminar of Organic Chemistry
University of Zabol
12-14 March, 2019

Paper code: 1039

Comparison the Effects of ZnO Nanoparticles and ZnO/Chitosan Nanocomposites on Diabetes-Induced Memory Impairment in Rats

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Among different nanomaterials, ZnO nanoparticles and ZnO/Chitosan nanocomposites possess a special status due to their own merits such as high specific surface area, optical transparency, bio-compatibility, non-toxicity, chemical and photochemical stability, convenient fabrication, high-electron communication features and electrochemical activities [1]. Meanwhile ZnO nanoparticles have biological activity [2]. Chitosan a polysaccharide biopolymer [3], derived from naturally occurring chitin, is extensively being investigated in field of biomedical material and drug delivery [4]. In this project, ZnO nanoparticles and ZnO/Chitosan nanocomposites were synthesized, and their effectiveness in preventing diabetes-induced memory loss and lipid peroxidation was evaluated. ZnO nanoparticles and ZnO/Chitosan nanocomposites reversed diabetes-induced cognition insufficiency in passive avoidance learning and memory task ($P < 0.05$). The brain lipid peroxidation ($P < 0.001$) was lower in both groups compared to the untreated rats. Moreover, treatment with both nanoparticles prohibited learning and memory deficits of diabetic groups; however, there was no significant difference between the groups treated with ZnO/Chitosan nanocomposites or of ZnO nanoparticles. In conclusion, both ZnO nanoparticles and ZnO/Chitosan nanocomposites were effective in preventing diabetes-induced memory loss and lipid peroxidation.

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The 26th Iranian Seminar of Organic Chemistry
University of Zabol
12-14 March, 2019

Paper code: 1040

Synthesis of the 2,4,6-Triarylpyridines and 2,5,7-Triaryl-1,3-thiazepine Derivatives by Using a Green and Reactive Polymer Supported Reagent Based on Calix[4]resorcinarene

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A cationic polymer containing pendant pyrazine groups was synthesized via post-functionalization of the polymeric backbone based on a calix [4]resorcinarene [1], and characterized by AFM, TEM, analytical CHN, TGA, and DTG techniques. The functionalized polymer is conveniently loaded with desired anion thereby providing green and recyclable polymer-supported reagent for achieving synthetic goals. The thermal stability of this cationic polymer (up to 250 °C by TGA) allows thermally demanding ring transformation and expansion of 2,4,6-triarylthiopyrylium salts [2] on its side chains and polymeric backbone without decomposition and leaching of active species in the reaction media. The unique features of this polymeric reagent, such as superior thermal stability, recyclability, excellent activity in terms of yield and reaction time are potentially important for the applications of this reagent in green synthesis of various compounds.

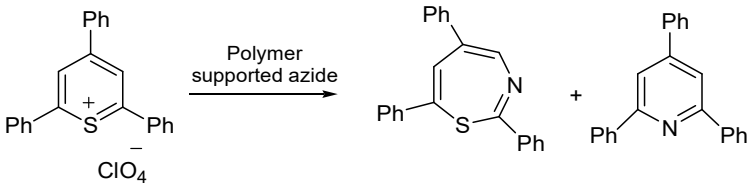

Fig. 1 Synthesis of 2,4,6-triarylpyridines and 2,5,7-triaryl-1,3-thiazepine derivatives

References

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The 26th Iranian Seminar of Organic Chemistry
University of Zabol
12-14 March, 2019

Paper code: 1041

One-Pot Three Component Synthesis of 2,3-Dihydroquinazolin-4(*1H*)-ones by a Heterogeneous and Reusable Polyvinyl Alcohol Immobilized Cu(II) Schiff base Complex

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One of the most frequently encountered heterocycles in medicinal chemistry is quinazolinone derivatives with wide applications including anticancer, antihypertensive, antidiuretic, anti-convulsant, antibacterial, antihistaminic, antidiabetic, and anti-inflammatory activities [1,2]. 2,3-Dihydroquinazoline derivatives are a class of heterocycles which exhibit biological and pharmaceutical activity and herbicidal agents, as well as plant growth regulators [2]. Also, recently a number of classical -methods for the synthesis of 2,3-dihydroquinazolin-4(1*H*) one have been reported in literature involving homogeneous, heterogeneous, solid acid and transition metal complexes [3]. However, most of the reported methods have certain limitations such as the use of organic solvents, long reaction times, tedious processes, harsh reaction conditions and low yields of product. Thus, developing versatile approaches to synthesize quinazolinone derivatives still remains a highly desired goal in organic synthesis. For sake of notable property of quinazolinone derivatives, herein, we have developed a recoverable and reusable heterogeneous catalyst to overcome some of the above-mentioned impediments by working under mild and green conditions to perform efficiently preparation of 5-substituted quinazolinone derivatives (Fig. 1). In our previous work we have demonstrated the ability of the PVA@Cu(II)-Schiff base complex over efficient preparation of 5-substituent-1*H*-tetrazoles at room temperature.

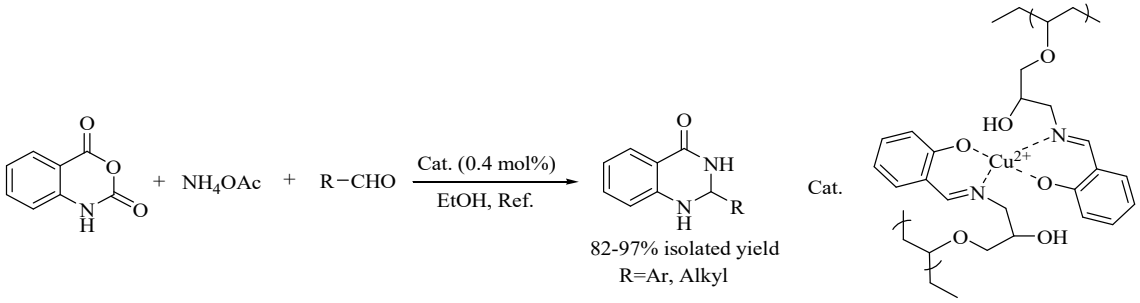

Fig. 1 Synthesis of 2,3-dihydroquinazolin-4(1*H*)-ones by PVA@Cu(II)-Schiff base complex

References

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Paper code: 1042

Green Synthesis of Novel 1,2,4-Triazole-3-thione Derivatives in Natural Deep Eutectic Solvent

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1,2,4-Triazoles are biologically active compounds which prepared *via* a variety of synthetic methods [1]. Some multicomponent and one-pot procedures were also developed for their preparation. Deep eutectic solvents (DESs) as environmentally friendly solvents were widely applied in different chemical processes [2, 3]. As part of our current studies on the development of new routes in organic synthesis, we report an efficient and green procedure for the synthesis of functionalized 1,2,4-triazoles-3-thione derivatives under optimized conditions *via* reaction of aryl hydrazides and alkyl or aryl isothiocyanates (fig. 1). Glycerol/potassium carbonate was used as catalyst and reaction media. 1,2,4-Triazoles-3-thione derivatives were obtained in very good yields without the need for additional purification steps.

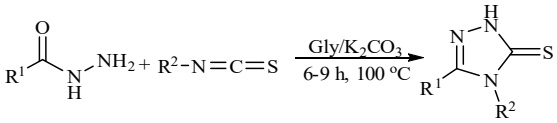

Fig. 1 Synthesis of 1,2,4-triazole-3-thione derivatives

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12-14 March, 2019

Paper code: 1043

A Green One-pot Synthesis of 3-Substituted 1,2,4-Triazol-5-Amines as Potential Antimicrobial Agents

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*Correspondence e-mail: *hbeyzaei@yahoo.com*

Heterocyclic compounds occupy an important place in medicinal chemistry. Triazole ring is present in many natural products and biologically active compounds [1, 2]. An efficient procedure was proposed for the synthesis of 3-substituted 1,2,4-triazol-5-amines *via* one-pot reaction of thiourea, dimethyl sulfate and various hydrazides. 1,2,4-Triazoles were prepared in aqueos media under mild conditions while adhering to some principles of green chemistry (Fig. 1). Inhibitory activities of all compounds were evaluated against some pathogenic bacteria and fungi. The best antibacterial effects were observed with 3-phenyl-1*H*-1,2,4-triazol-5-amine according to its MIC values (4-8 μg ml^{-1}). All derivatives could block the growth of fungi. Acceptable antioxidant properties were recorded only in 3-(4-nitrophenyl)-1*H*-1,2,4-triazol-5-amine.

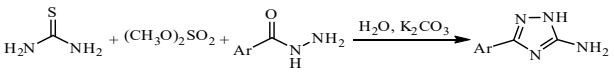

Fig. 1 Multi-component synthesis of 3-substituted 1,2,4-triazol-5-amines

References

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The 26th Iranian Seminar of Organic Chemistry
University of Zabol
12-14 March, 2019

Paper code: 1044

Triphenylphosphane: 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 tiphenylphosphane as the efficient catalyst. Here, 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 separation of pure products with high yields, simplicity experimental procedure, operationally simple, and eco-friendly.

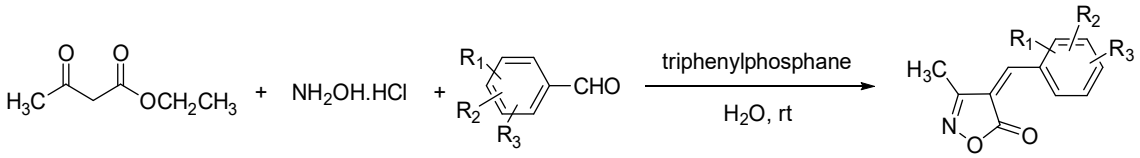

Fig. 1 Three-component synthesis of arylmethylidene-isoxazole-5(4*H*)-ones in green solvent

References

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The 26th Iranian Seminar of Organic Chemistry
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12-14 March, 2019

Paper code: 1045

Electrochemical Synthesis of 4-Aryl-2-styryl-1*H*-benzo[b][1,4]diazepines from *o*-Phenylenediamine and 1,5-Diarylpenta-2,4-dien-1-ones

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Diazepine is a seven-membered heterocyclic compound with two nitrogen atoms. Some of diazepine derivatives are psychoactive drugswhose core chemical structure is the diazepine ring system. The first such drug, chlordiazepoxide (Librium), was discovered accidentally in 1955, and they are usually useful for insomnia [1]. The common procedure for the synthesis of these compounds is a one pot condensation between *o*-phenylenediamines and *α,β*-unsaturated carbonyl compounds in the presence of catalysts[2, 3]. In this study, we report a synthesis of 1,4-diazepine derivatives under mild conditions*via* a metal and oxidant-free anodic oxidation in an undivided cell at room temperature. This environmentally benign approach afforded 4-aryl-2-styryl-1*H*-benzo[b][1,4]diazepines in satisfactory yields by using a cheap pencil graphite and a Nickel electrode. The structure of products was characterized by NMR, IR, and mass spectral data.

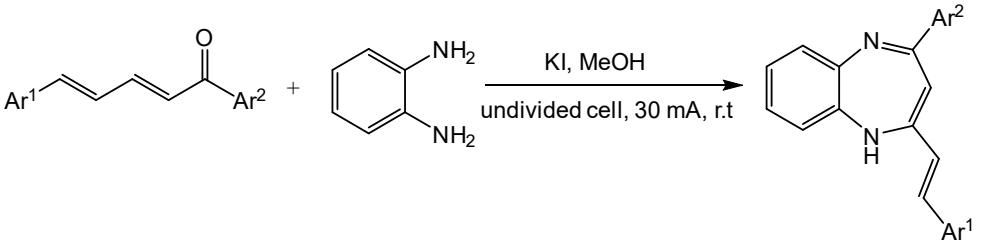

Fig. 1 Synthesis of 4-aryl-2-styryl-1*H*-benzo[b][1,4]diazepines

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12-14 March, 2019

Paper code: 1046

Green Synthesis of Silver Nanoparticles Supported on Magnetic Functionalized Graphene oxide and its Application as Recoverable Catalyst for Reduction of the Dye Pollutants in Water

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Recently, graphene oxide (GO) has been extensively investigated as a new class of promising support or catalysts due to their high stability and high specific surface area [1]. Despite the high catalytic activities of GO or (RGO), their separation techniques are consuming a very energy and a long time. Fortunately, this technical limitation can be overcome by introducing Fe_3O_4 magnetic nanoparticles onto the surface of the GO [2,3]. This kind of supporting allows catalyst to be easily separated from the reaction mixture by an extra magnet and reused several times. There is a drastic need to develop a newer eco-friendly method for the synthesis of metal/GO nanocomposites under a mild condition. In this article, GO and $SOCl_2$ were added to generate GO-Cl and then melamine was added to GO-Cl under nitrogen atmosphere for 8 h at 60°C.The obtained product was treated with methyl methacrylate and ethylenediamine. Then $AgNO_3$ was added into the catalyst and nanocatalyst was prepared by plant extract (Fig.1). At the end, magnetic nanocomposite was fabricated by Fe_3O_4 nanoparticles. The results show that the nanocomposite can be employed as a magnetically recycled catalyst for the reduction of organic dyes such as methylene blue, methyl orange, rhodamine 6G and 4-nitrophenol in water at room temperature.

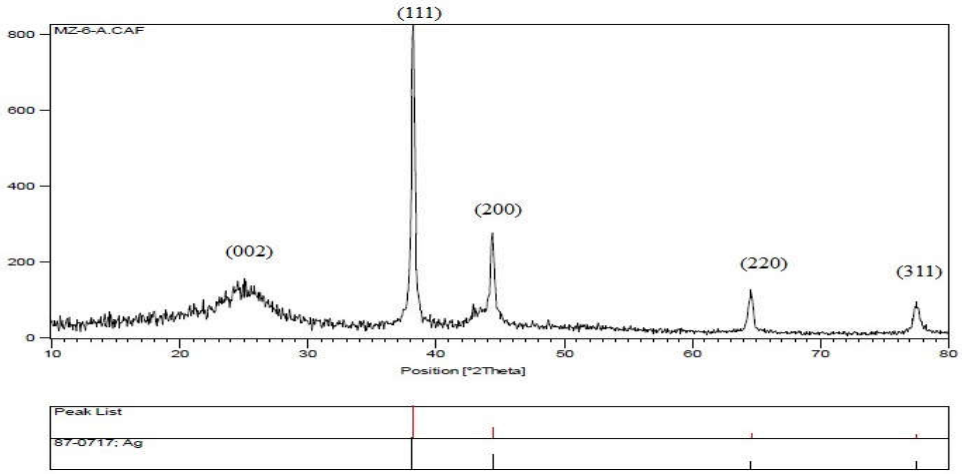

Fig.1 XRD pattern of silver nanocatalyst

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The 26th Iranian Seminar of Organic Chemistry
University of Zabol
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Paper code: 1047

Preparation of Functionalized Graphene Oxide Loaded with Silver Nanoparticles and Investigation of its Antibacterial Activities

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Metal nanoparticles are a particular class of nanomaterials that have garnered huge interest in the field of scientific research, and in many other technical disciplines, due to their chemical and physical properties and the numerous effective applications [1]. Silver nanoparticles has been proved to be the most effective antimicrobial agent. Ag NPs has antibacterial activity against gram negative and gram positive bacteria. Some of the most problematic multi drug resistant (MDR) microorganisms that are encountered currently include *Pseudomonas aeruginosa* and *Staphylococcus aureus* [2]. In this article, the antibacterial activity of nanocatalyst was evaluated by agar well diffusion method against to two bacteria, *Staphylococcus aureus (*ATCC29737) as Gram-positive and also *Escherichia coli* (ATCC25922) as Gram-negative bacteria. Firstly, GO and $SOCl_2$ were added to generate GO-Cl and then melamine was added to GO-Cl under nitrogen atmosphere. The obtained product was treated with methyl methacrylate and ethylenediamine, then $AgNO_3$ was added into the catalyst and nanocatalyst was prepared by plant extract. The result has been shown that these nanocomposites have good effect on both gram negative and gram positive bacteria. The nanocatalysts have been shown more antibacterial activity against *Staphylococcusa aureus* bacteria (Fig. 1).

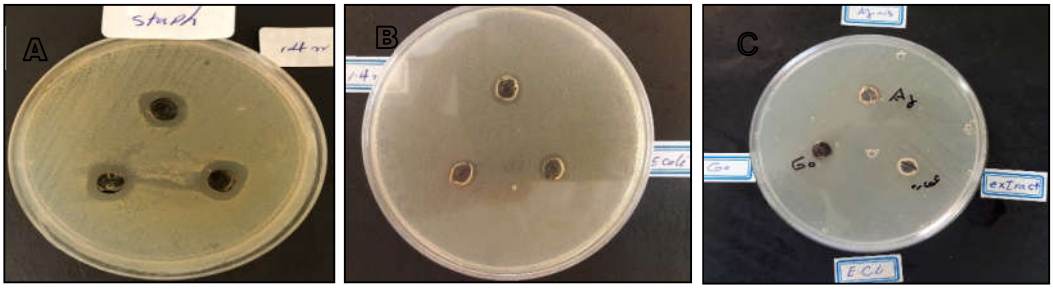

Fig. 1 a) *Staphylococcus aureus*, b) *Escherichia coli*, and c) Inhibitory zone pattern of GO, AgNPs and extract

References

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The 26th Iranian Seminar of Organic Chemistry
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Paper code: 1048

A Green Protocol for Direct Esterification of TMS and THP Ethers with Aldehydes Using KCN and Air as the Simplest Available and Free of Cost Oxidant

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Esterification reaction is an important and very useful reaction in organic synthesis. The chemical structure of many pharmaceutical compounds, fragrances, essences and oils involves the ester moiety. In addition, this reaction is applied for protection of hydroxyl groups. The reaction between a carboxylic acid and alcohol is a known route for ester synthesis. However, these compounds are also produced from other sources such as aldehydes. Various oxidative methods have been reported for the synthesis of esters from alcohols and aldehydes directly using an oxidant such as ^{t}BuOOH in the presence of Co^{II}/CF_3COOH as a catalyst [1] and urea hydrogen peroxide and *p*-toluenesulfonyl chloride [2]. However, many of these methods suffer from some disadvantages such as restriction to narrow choice of alcohols with relatively low boiling point such as methanol, ethanol and isopropanol, the use of external oxidant and expensive and unavailable catalyst, the use of alcohols in excess amounts (as solvent), low yields and operation in acidic conditions. Herein, in continuation of our previous work [3] and for first time, a green protocol is reported for direct esterification of trimethylsilyl (TMS) and tetrahydropyranyl (THP) ethers with aldehydes using KCN and air as the simplest available and free of cost oxidant (Fig. 1).

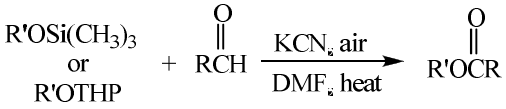

Fig. 1. Direct esterification of TMS and THP ethers with aldehydes using KCN and air.

This method is not restricted to only some these ethers, but also different kinds of them are used in nearly equal molar amount to aldehyde. In addition, the present green protocol does not need to an external oxidant and also indicates a version of transprotection of hydroxyl group which can be used in organic synthesis.

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12-14 March, 2019

Paper code: 1049

Solid-State Synthesis of Nanocopolymer of Aniline and 3-Aminobenzenesulfonic acid in the Presence of *p*-Toluene sulfonic acid and its Application in Solar Cell

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In this paper, synthesis of nanocopolymer [nano-poly (*m*-aminobenzene sulfonic acid-co-aniline)] using aniline and *m*-aminobenzene sulfonic acid as monomer and *p*-toluene sulfonic acid was performed to create acidic conditions at ambient temperature and solid state (Fig. 1). Copolymer synthesis was confirmed using FT-IR spectroscopy and UV-Vis spectroscopy. Using elemental analysis (CHNS), it has been proven that both monomers have been introduced into the polymer chains and are composed of copolymers. Also, using SEM microscopy, the copolymer morphology was determined and its nano was confirmed. Then, using a copolymer, the solar cell was constructed using Dr Blade's method. From the solar cell, the I-V test was taken and the solar cell efficiency was reported in the paper.

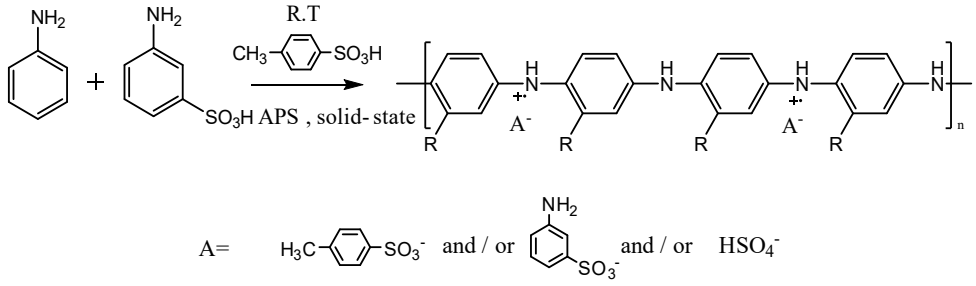

Fig. 1 The general scheme of copolymerization, R= H and / or SO_3H

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12-14 March, 2019

Paper code: 1050

Solid-State Synthesis of Nanocopolymer [poly(*m*-AminoBenzenesulfonic Acid-*co*-aniline] in the Presence of Methanesulfonic Acid and its Application in Solar Cells

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In this article, First, the nano copolymer [poly *m*-amino-benzene sulfonic acid-*co*- aniline] was synthesized under solid state (Solvent-free) condition and in the presence of methane sulfonic acid. All materials were high purity and there was no need of purifying. After polymer synthesis, analyzes were performed to detect the synthesized polymer. In FT-IR spectroscopy, the presence of an important peak 1500 (cm^{-1}) associated with benzenoid rings and peak 1600 (cm^{-1}) associated with quinone rings was the reason for the formation of a polymer [1,2]. In UV-Vis spectroscopy, the existence of peaks of 300 nm and 600 nm are the reason for synthesis of the polymer formation emeraldine form [3]. The elemental analysis of CHNS indicates the proportions of the elements in the chain, where the presence of sulfur in chains is a reason for the creation of nanoparticles. Using SEM images and investigating them, it was found that the synthesized nanoparticles were based on copolymer. After detecting and proving the synthesized copolymer were used in the manufacture of solar cell. After building the solar cell, the analysis of I-V was taken and the efficiency and power of the solar cell were obtained.

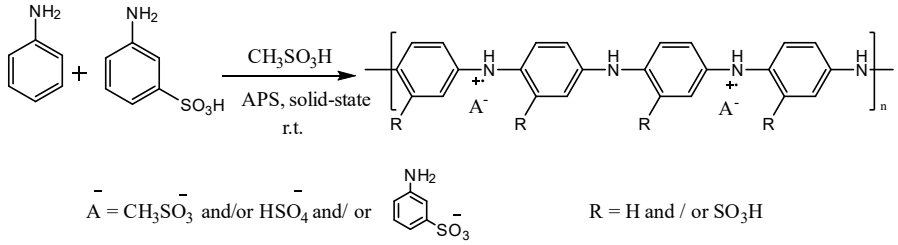

Fig. 1 The general scheme of copolymerization

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12-14 March, 2019

Paper code: 1051

Three-Component Process for the Synthesis of 4H-Pyrans Using a Recyclable Ionic Liquid in Aqueous Media

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In the past decade, because of various therapeutic applications of 4H-pyrans in the pharmaceutical industry, the different synthetic protocols for their preparation have been reported [1-3]. In this study, the 4H-pyran derivatives were synthesized *via* three-component reaction of dimedone or 4-hydroxycoumarin or ethyl acetoacetate with malononitrile and various aldehyde using a basic ionic liquid in aqueous media (Fig. 1). 4H-Pyrans were produced in excellent yields and short times. From the viewpoint of greener chemical processes, combination of recyclable ionic liquid and water as a green co-solvent for the synthesis of 4H-pyrans makes this ionic liquid an attractive and eco-friendly alternative solvent and catalyst.

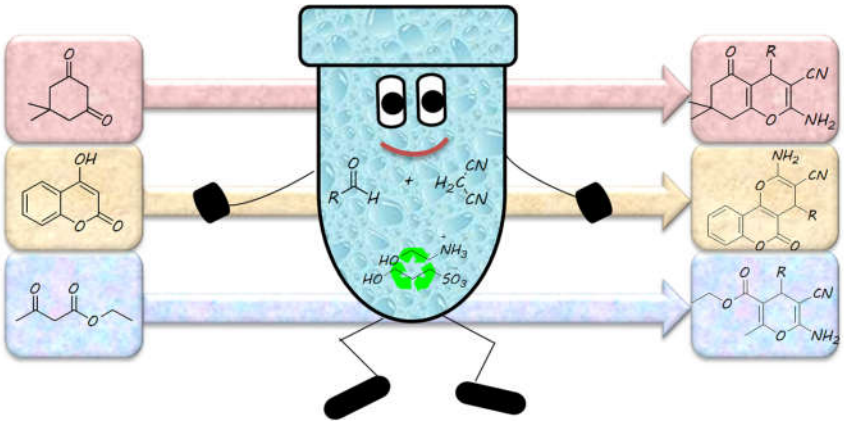

Fig. 1 Three-component synthesis of 4H-pyran derivatives

References

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The 26th Iranian Seminar of Organic Chemistry
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Paper code: 1052

Synthesis and Characterization of 3-Aminopropylammonium Hydrogensulfate as a Nano Aliphatic Quaternary Ammonium Salt

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Aliphatic quaternary ammonium (AQA) salts have received significant interest because of their special properties. They have wide applications in various fields such as electrochemical technologies, catalysis and chemical separations [1,2]. Nanotechnology is emerging as a cutting edge technology interdisciplinary with biology, chemistry and material science [3].
In this work, we have synthesized 3-aminopropylammonium hydrogensulphate [(APA)(HS)] as a novel nano organosalt from readily available starting materials and characterized by various techniques (Fig. 1). The results of ^{1}H NMR, FT-IR and elemental analysis was indicated that [(APA)(HS)] was successfully synthesized. The TG analysis of [(APA)(HS)] was showed that the synthesized organosalt have high thermal stability up to 294 ºC. According to the results of SEM and TEM were found that [(APA)(HS)] has a unique spherical morphology with good monodispersity. The particle size distribution of [(APA)(HS)] was evaluated using XRD (11.1-19.3 nm), TEM (6-20 nm) and AFM (15> nm).

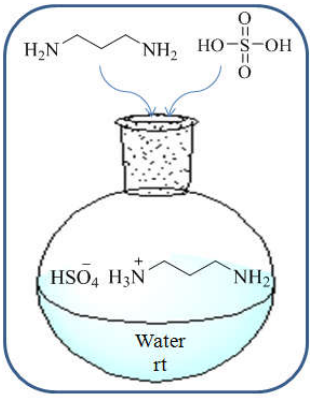

Fig. 1 The synthesis of 3-aminopropylammonium hydrogensulphate [(APA)(HS)]

References

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12-14 March, 2019

Paper code: 1053

A Convenient Synthesis of Functionalized 2,3-Diazaspiro[4.4]nona-1,6,8-trienes

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Among pyrazolone derivatives, spirocyclic pyrazolone systems [1] have attracted extensive interest because of their remarkable bioactivities. Despite many efforts devoted to the development of new preparative methods for these heterocyclic systems, the development of synthetically effective protocols for such compounds is still a challenge [2]. In view of our interest in the synthesis of spiroheterocycles [3], we now report a convenient Michael addition/cyclization sequence of alkyl isocyanide–acetylenic ester adducts with various pyrazolones, leading to the formation of diazaspiro[4.4]nona-1,6,8-trienes in moderate to good yields. The structures of all molecules were confirmed by NMR spectroscopic data.

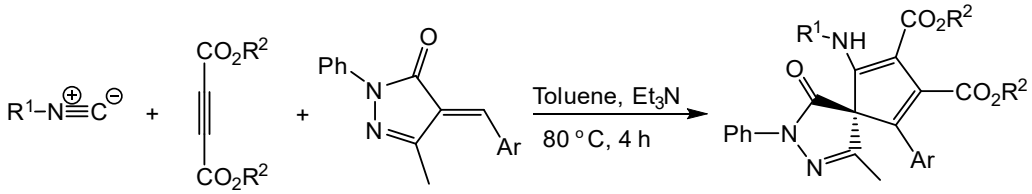

Fig. 1 The synthesis of functionalized diazaspiro[4.4]nona-1,6,8-trienes

References

[1] P. Chauhan, S. Mahajan, D. Enders. *Chemical Communication*, **2015**, 51:12890-12907.
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Paper code: 1054

Synthesis and Characterization of Iron Oxide Superparamagnetic Nanoparticles (Magnetite) by co-Precipitation Method Coated with Biocompatible (Polymeric, Organic and Inorganic) Compounds and Evaluation of *In vitro* Toxicity of Synthesized Nanoparticles

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Recent advances in the use of magnetite nanoparticles for biomedical applications have led to special attention to magnetite nanoparticles. The unique properties of iron oxide nanoparticles such as superparamagnetism, low toxicity and the ability to bond with biological molecules are suitable for drug delivery, diagnostic methods and therapeutic approaches. This article examines various coatings of magnetite (iron oxide) nanoparticles for toxicity assessment and compares them in terms of structure and characteristics. Of course, cytotoxicity of these magnetic nanoparticles was investigated with HepG2 cell line was probed using MTT assay. Treated cells, did not showed evident cell cycle arrest. The results from the Fourier Transform Infrared (FTIR) spectroscopy, Powder X-ray diffraction (XRD), Transmission Electron Microscopy (TEM) showed that the well coating of magnetite nanoparticles by organic, inorganic and polymer coatings.

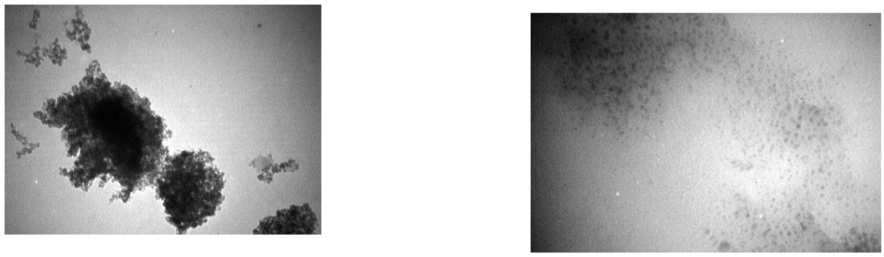

Fig. 1 TEM images of the a) IO@PEG@SiO_2 and b) IO@OA nanoparticles

References

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12-14 March, 2019

Paper code: 1055

A Convenient Synthesis of Functionalized Pyrazolones Bearing a Highly Twisted 1,3-Butadiene Moiety with Skew Geometry

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Pyrazolones are important heterocycles, which have been used in many fields, since they exhibit biological and pharmacological properties [1]. In recent years, much effort has devoted to designing new isocyanide-based multicomponent reactions toward the synthesis of various compounds [2]. The four-component reaction among arylhydrazine, alkyl acetoacetatederivatives, alkyl isocyanides, and dialkyl acetylenedicarboxylates, leading to the formation of dialkyl 2-[(*Z*)-(alkylamino) (3-alkyl-5-oxo-1-phenyl-1,5-dihydro-4*H*-pyrazol-4-ylidene) methyl] fumarates isdescribed. The structure of target compounds was confirmed usingX-ray diffraction study. These pyrazolone derivatives contain a highlytwisted exocyclic 1,3-butadiene moiety with highly twisted skew (ϕ=87º) geometry. Various features of these reactions will be presented and discussed.

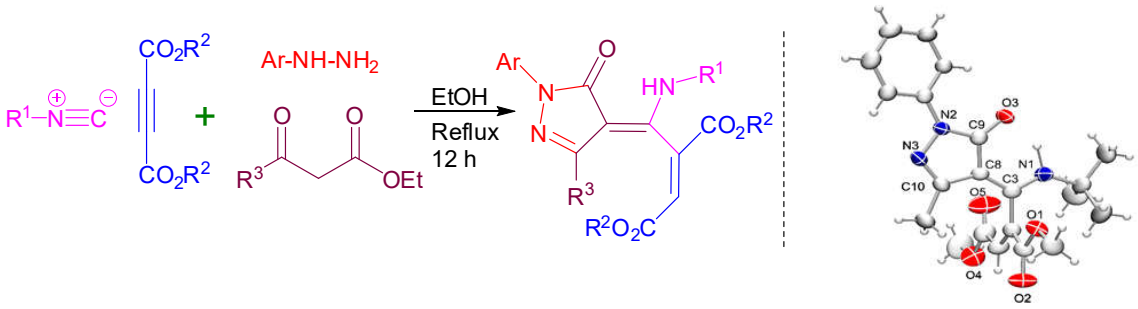

Fig. 1 Multicomponent synthesis and X-ray crystal structure ofdialkyl 2-[(*Z*)-(alkylamino) (3-alkyl-5- oxo-1-phenyl-1,5-dihydro-4*H*-pyrazol-4-ylidene) methyl] fumarates

References

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University of Zabol
12-14 March, 2019

Paper code: 1056

Formation of Trichloromethylated-1,3,5-triazines from Guanidine, Trichloroacetonitrile, and Isothiocyanates

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Triazines have been defined as six-membered heterocyclic aromatic compounds of considerable interest having three nitrogen atoms that are well known for a long time. The most important member of this group is 1,3,5-triazines that exist in the structure of many pesticides and pigments and have widespread applications in the textile, plastic, and rubber industries. Most triazine derivatives are important medicinal compounds; some of them can act as antitumor [1]. Several synthetic methods for the preparation of these compounds have been reported [2], nevertheless, the preparation of polyfunctional and trichloromethylated 1,3,5-triazines is still a challenge. In this work, we describe a method based on the use of trichloroacetamidine resulting from trichloroacetonitrile and guanidine, as bidentate nucleophile and isothiocyanate as electrophile, to afford tricholoromethylated-1,3,5-triazine system [3]. As shown in Scheme 1, the reaction of guanidine (**1**) and trichloroacetonitrile (**2**) in the presence of isothiocyanates (**3**) at room temperature leads to production of **4**.

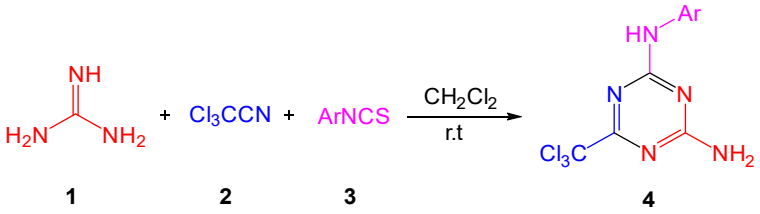

Fig. 1 Synthesis of trichloromethylated-1,3,5-triazines

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The 26th Iranian Seminar of Organic Chemistry
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12-14 March, 2019

Paper code: 1057

Application of the Immobilized Sulfonic Acid on the Magnetic Cobalt Ferrite Nanocatalyst ($CoFe_2O_4/SiO_2/SO_3H$) in the Synthesis of Organic Materials

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Sulfuric acid as a homogeneous Bronsted acid catalyst is widely applied for the synthesis of chemical compounds, but some drawbacks such as tedious workup, equipment corrosion, and contamination of products restricted the use of this catalyst [1]. The heterogenization of Bronsted acids can solve these drawbacks and many solid supports such as magnetic nanoparticles are good nominate for this purpose [2]. On the other hand, spirooxindoles are common structures in alkaloids skeleton which have privileged chemotypes for antiviral drug development [3]. In this study, chlorosulfonic acid was supported onto the $CoFe_2O_4/SiO_2$ and the heterogeneous magnetic solid acid ($CoFe_2O_4/SiO_2/SO_3H$) was characterized and used for the synthesis of spirooxindoles derivatives (Fig. 1). The results showed that the catalyst has excellent efficiency and the reusability and the products were synthesized at a short time (4 min) in green media (Water/EtOH 1:1) with high yield.

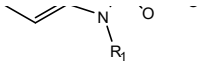

Fig. 1 Multicomponent synthesis of spirooxindole catalyzed by $CoFe_2O_4/SiO_2/SO_3H$ MNPs

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Paper code: 1058

Fe_3O_4-Supported Macroacyclic Schiff-Base Copper Complex: A valuable Heterogeneous Nanocatalyst for One-Pot Synthesis of New Pyrano[2,3-*b*]pyridine-3-carboxamide Derivatives

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Over the following few decades, environmental problems and green chemistry have become increasingly important issues and much effort has been directed towards the development of sustainably enhanced and environmentally benign synthetic procedures for organic chemistry [1]. In this context, a growing field of research in green chemistry has been devoted to the development of a wide variety of recyclable, eco-friendly, selective, easily accessible, and economically viable catalysts, and their application in chemical transformations and industrial fields [2, 3]. A novel macroacyclic Cu(II) Schiff-base complex immobilized on core-shell magnetic Fe_3O_4 nanoparticles [Fe_3O_4@SiO_2-4N-Cu(II)] was successfully designed and synthesized. The structural features of these nanoparticles were studied and confirmed by using various techniques including FT-IR, SEM, TEM, EDS, VSM, XRD, WDX and ICP. These synthesized nanoparticles have been used as an efficient heterogeneous nanocatalytic system for the one-pot multicomponent synthesis of new pyrano[2,3-*b*]pyridine-3-carboxamide derivatives (Fig. 1). Notably, the catalyst could be easily separated from the reaction mixture by using an external magnet and reused for several successive reaction runs with no significant loss of activity or copper leaching. The present protocol benefits from a hitherto unreported MNPs-immobilized macroacyclic Cu(II) Schiff-base complex as an efficient nanocatalyst for the synthesis of newly reported derivatives of pyrano[2,3-*b*]pyridine-3-carboxamide.

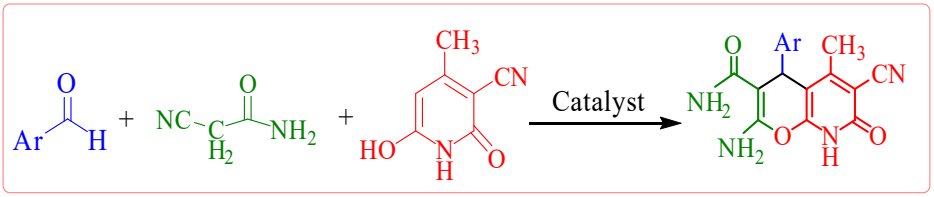

Fig. 1 Fe_3O_4@SiO_2-4N-Cu(II) catalyzed the synthesis of pyrano[2,3-*b*]pyridine-3-carboxamide derivatives

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Paper code: 1059

Synthesis and Characterization of Iron Oxide Nanoparticles *via* co-Precipitation and Reverse Micelles Methods in the Biological Applications

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In recent years, the wide applications of iron oxide nanoparticles in the field of medicine, imaging and drug delivery increase the usage of this product in the medicine and pharmacy. Due to the significance of this issue, the synthesis of these nanoparticles is vitally important. Among the synthetic methods of nanoparticles, the simplest procedure is co-precipitation in which in the presence of an alkali, divalent and trivalent iron salts react with each other [1-3]. However, based upon the control of size in the clinical applications, the reverse micelles method seems valuable. In this procedure, using surfactant produces the iron oxide nanoparticles with desired sizes. This can be due to the control of surfactant amounts and its proportion with starting materials, divalent iron salts. It should be mentioned that this method cannot be applicable about the pH procedure and trivalent iron salts. In this research, some characterization spectrum of nanoparticles has been compared to result in the best condition of co-precipitation method with the control and investigation of nanoparticles production procedures.

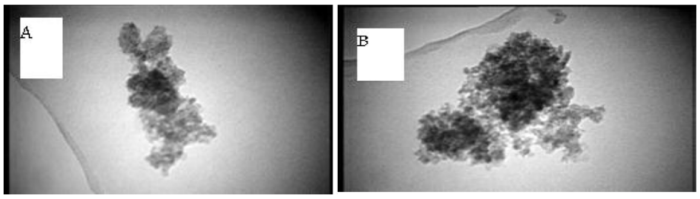

Fig. 1 The TEM of iron oxide nanoparticles synthesized by A) Co-precipitation and B) Reverse micelle

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12-14 March, 2019

Paper code: 1060

Survey Reaction of Benzoimidazolo/Benzooxazolo/Benzothiazolo 2-thioacetophenone Derivatives Using TiO_2-Nanoparticles

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2-((Benzimidazol-2-yl)thio)-1-arylethan-1-ones, 2-((benzothiazol-2-yl)thio)-1-arylethan-1-ones and 2-((benzoxazol-2-yl)thio)-1-arylethan-1-ones have various biological properties. There are various methods for synthesis of this heterocyclic compounds [1-3]. In this investigation benzothiazolo-2-thioacetophenone, benzooxazolo-2-thioacetophenone and benzoimidazolo- 2-thioacetophenone derivatives were synthesized in the presence of TiO_2 nanoparticles as catalyst in high yield. Firstly, 2- mercaptobenzoimidazole has been synthesis from reaction of the orthophenylendiamine with amoniumisothiocyanide in the presence of amoniumchloride as a catalyst by heating under solvent free conditions. Then this derivative, 2-mercaptobenzooxazole and 2-mercaptobenzothiazole have been reacted with phenacyl bromide/ 2-bromo 4′-methoxyacetophenone/2-bromo 4′-phenyl acetophenone using TiO_2 nanoparticles as catalyst by ball-miling and under solvent free conditions for synthesize of benzothiazole-2-thioacetophenone, benzooxazole-2-thioacetophenone and benzoimidazole-2-thioacetophenone.

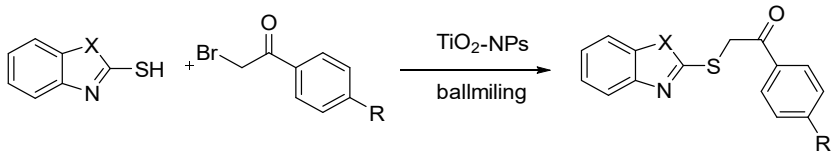

Fig. 1 Synthesis of benzoimidazolo/benzooxazolo/benzothiazolo 2-thioacetophenone derivatives under solvent free condition

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The 26th Iranian Seminar of Organic Chemistry
University of Zabol
12-14 March, 2019

Paper code: 1061

Application of Cobalt Phthalocyanine as a Nanostructured Catalyst for Synthesis of Biological Henna-Based Compounds

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Henna-based compounds such as benzo[*a*]pyrano[2,3-*c*]phenazines, 2-amino-3-cyano-4-aryl-5,10-dioxo-5,10-dihydro-4*H*-benzo[*g*]chromenes, hydroxyl naphthalene-1,4-diones, pyrazolyl naphthoquinones, benzo[*b*]xanthene-triones and their derivatives are of substantial interest as they possess a broad range of biological properties, such as anti-cancer, spasmolytic, diuretic, anti-coagulant and anti-anaphylactic activity [1]. In continuation of our efforts to synthesize of novel catalysts and MCRs, we wish to report the synthesis of novel nano molten salt tetra-2,3-pyridiniumporphyrazinato cobalt tribromomethanide [Co(TPPABr)]CBr_3 as an efficient catalyst for the synthesis of henna-based compounds under various conditions [2].

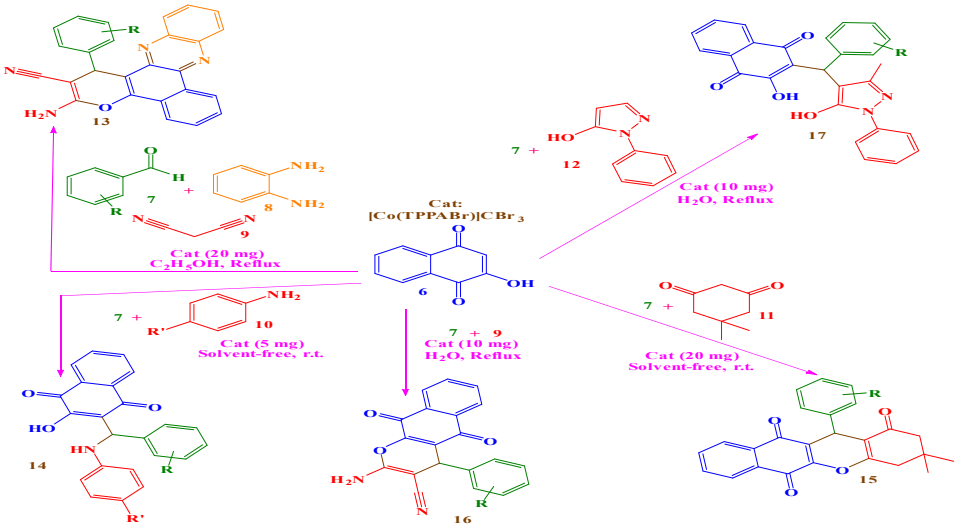

Fig. 1 Synthesis of henna-based compounds using novel nano molten salt [Co(TPPABr)]CBr_3

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12-14 March, 2019

Paper code: 1062

One-Pot Synthesis of *β*-Amino Ketones *via* Direct Mannich-type Reaction Catalyzed with $CuFe_2O_4@SO_3H$

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Mannich reactions are among the most important carbon–carbon bond forming reactions in organic synthesis. They provide *β*-amino carbonyl compounds, which are important synthetic intermediates for various pharmaceuticals and natural products [1]. Therefore, the development of new synthetic methods leading to *β*-amino carbonyl compounds or their derivatives has attracted much attention. However, the classic Mannich reaction has limited applications. Attempts have been made in the past to improve methodologies based on two-component reactions, where the imine as electrophile is formed and then reacted with nucleophiles such as enolates, enol ethers, and enamines [2]. However, in most cases these protocols use hazardous organic solvents, costly and non-recoverable catalysts, and requirement of special effort for catalyst preparation, and suffer from long reaction time with low yields [3]. Therefore, the development of modern versions of the reaction that work under mild conditions is of great importance. $CuFe_2O_4@SO_3H$ is an excellent acidic catalyst, which is frequently used to promote some important reactions. We report herein full details of a novel, convenient, and simple procedure to realize a one-pot three-component reaction of aldehydes, amines, and ketones, catalyzed by $CuFe_2O_4@SO_3H$, for the preparation of *β*-amino carbonyl compounds in EtOH.

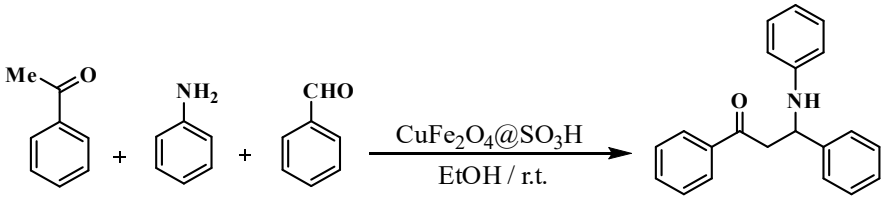

Fig.1 The preparation of *β*-amino carbonyl compounds

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University of Zabol
12-14 March, 2019

Paper code: 1063

A Green Procedure for One-Pot Synthesis of Quinazolinone Derivatives Using $CuFe_2O_4@SO_3H$ as an Efficient and Reusable Catalyst under Solvent-Free Conditions

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Multicomponent reactions (MCRs) are special types of synthetically useful organic reactions in which three or more different starting materials react to give a final product in a one-pot procedure [1,2].2,3-Dihydroquinazolin-4(1*H*)-ones are important class of heterocycles with a wide range of pharmacological and biological activities [3]. A number of synthetic methods to prepare these compounds have been described in the past few years. Developments of magnetic nanoparticles (MNPs) for use as supports and investigations of their catalytic applications indicate an important branch of green nanotechnology as they enable environmentally friendly and sustainable catalytic processes. By easy recoverable MNPs from reaction media, various protocols by surface modification, binding and self-assembly offer a broad scope of approaches for preparing magnetically recyclable catalysts. Copper/iron oxide-based catalysts are environmentally compatible, air and moisture insensitive and separation of the reaction mixture is very easy by using an external magnetic field. Surface modified copper/iron oxide MNPs are a kind of new functional materials which have been widely used in biotechnology and analysis. In this research, we report a new, simple, mild, and effective procedure for the one-pot synthesis of 2,3-dihydroquinazolin-4(1*H*)-one derivatives *via* a multi-component condensation reaction between aryl aldehydes, isatoic anhydridesand ammonium acetate or amines in the presence of $CuFe_2O_4@SO_3H$ as catalyst with high yields (72-95%) and short time. In conclusion we have developed a facile, convenient and environment-friendly multi-component protocol for the synthesis of 2,3-dihydroquinazolin-4(1*H*)-ones under green condition.

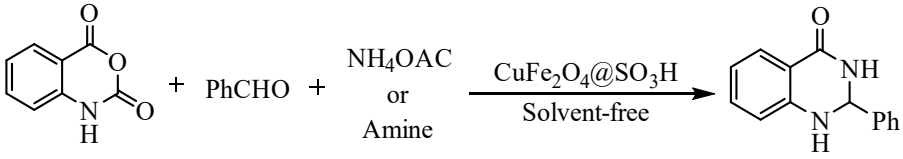

Fig. 1 Synthesis of 2,3-dihydroquinazolin-4(1*H*)-ones

References

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The 26th Iranian Seminar of Organic Chemistry
University of Zabol
12-14 March, 2019

Paper code: 1065

Self-Assembly of Surfactant Mixtures on GrapheneNanosheets: Insights from Molecular Dynamic Simulation

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Because of two-dimensional structure, large surface area and unique mechanical, thermal, optical and electrical properties of graphene, it has attracted much attention for promising applications, such as in energy, composites, biotechnology and electronics [1]. However, these applications rely on the mass production of high-quality and low-cost graphene. Owing to the hydrophobic nature of graphene nanosheets, their non-covalent functionalization with surfactants is an effective method for the production of graphene stable aqueous suspensions [2]. Computer simulation has been a powerful tool for gathering information at molecular-level about the process of adsorption and assembly of different molecules on nanomaterials [3]. In this study, large-scale and all-atomistic molecular dynamic simulations were used to study the effect of mixing two surfactants on micelle assemblies structure formed on graphene. For examination of the structural assemblies' characteristics formed from surfactants on graphene, the density profiles of the head and tail groups of surfactant were plotted as a function of the z distance perpendicular to graphene (Fig. 1). The simulations showed thatthe random adsorption model first changes to the monolayer model and then the hemispherical model with an increased surfactant concentration.

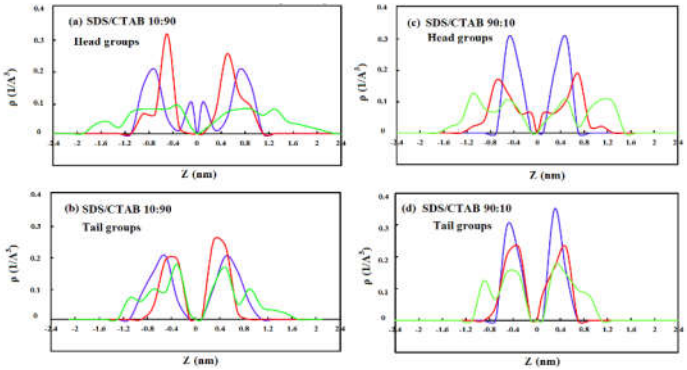

Fig. 1 The simulated density profiles of the head groups (a and c) and the tail groups (b and d) as a function of the distance from the z-axis of the graphene for two cationic-rich and anionic-rich mixtures with three different surface coverages including low surface coverage (blue line), medium surface coverage (red line) and high surface coverage (green line).

References

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12-14 March, 2019

Paper code: 1066

Conjugate Addition of Indoles to Electron-Deficient Olefins Catalyzed by $CuFe_2O_4@SO_3H$ under Mild Conditions

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Over the past few years a variety of methods has been reported for the preparation of 3-substituted indoles. Addition reactions of indoles to electron deficient olefins have received much interest because a number of their derivatives occur in nature and possess a variety of biological activities. Since the 3-position of indole is the preferred site for electrophilic substitution reactions, 3-alkyl indoles are versatile intermediates for the synthesis of a wide range of indole derivatives. A simple and direct method for the synthesis of 3-alkylated indoles involves the conjugate addition of indoles to *α,β*-unsaturated compounds in the presence of either protic or Lewis acids. However, the acid-catalyzed conjugate addition of indoles requires careful control of acidity to prevent side reactions such as dimerization or polymerization [1-3]. In continuation of our work on the development of useful synthetic methodologies we recently observed that $CuFe_2O_4@SO_3H$ catalyzes the conjugate addition of indoles to electron-deficient olefins to form the corresponding Michael adducts under mild conditions. Initial research was focused on the reaction of indole with chalcone, and different solvents and different amounts of the catalyst were tested to find the optimized conditions.

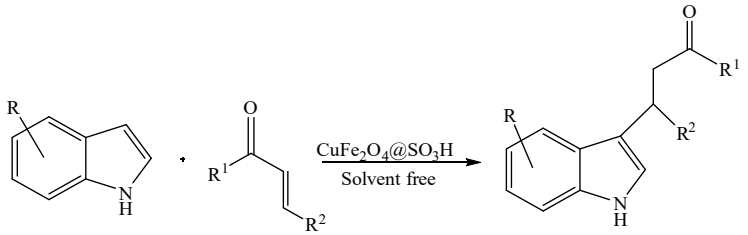

Fig. 1 $CuFe_2O_4@SO_3H$ catalyzes the conjugate addition of indoles to olefins

References

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12-14 March, 2019

Paper code: 1067

An Efficient, High Yielding Protocol for the Synthesis of Functionalized Quinolines *via* the Tandem Addition/Annulation Reaction of *O*-Aminoaryl Ketones with *α*-Methylene Ketones

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Quinolines are well known for a wide range of medicinal properties being used as antimalarial, antiasthmatic, antihypertensive, antibacterial and tyrosine kinase inhibiting agents [1]. They are also applied for the preparation of nano and meso structures having enhanced electronic and photonic properties [2]. Thus, the synthesis of quinolines is an important and useful task in organic chemistry. The Friedlander annulation is a straight forward synthesis of these compounds [3]. This method involves the acid or base catalyzed or thermal condensation between *α*-2-aminoaryl ketone and another carbonyl compound possessing a reactive α-methylene group followed by cyclodehydration.

We recently observed that $CaFe_2O_4@SiO_2@SO_3H$ catalyzes the synthesis of quinolines under mild conditions (Fig. 1). Initial research was focused on the reaction between *α*-2-aminoaryl ketone and another carbonyl compound possessing a reactive *α*-methylene group followed by cyclodehydration and different solvents and different amounts of the catalyst were tested to find the optimized conditions. The easy removal of the catalyst makes this method a suitable choice for the synthesis of new biologically active compounds. A simple process, short reaction time, green condition, availability and use of inexpensive reagents make the procedure novel and unique. High yields (75-96%) are other advantages of our method.

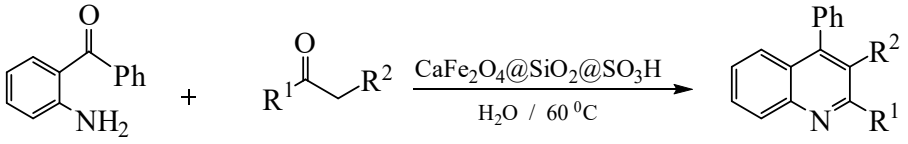

Fig. 1 $CaFe_2O_4@SiO_2@SO_3H$ catalyzes the synthesis of quinolones

References

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The 26th Iranian Seminar of Organic Chemistry
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12-14 March, 2019

Paper code: 1069

A One-Pot Procedure for the Synthesis of Highly Functionalized Derivatives of a Novel Five-Cyclic Scaffold: Pyrazolo[5'',1'':2',3']pyrimido[4',5':5,6][1,4]thiazino[2,3-*b*]quinoxaline

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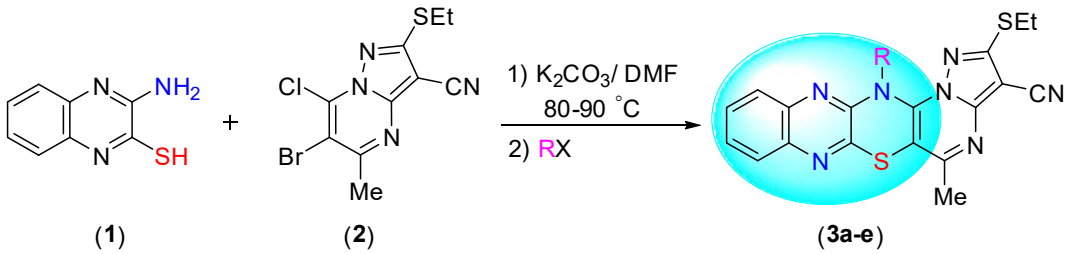
Quinoxalines display a broad spectrum of biological and pharmacological activities such as insecticides, fungicides, herbicides, antibacterial, antimycobacterial, antiprotozoal and anticancer properties [1]. Furthermore, quinoxaline units are present in the structure of various antibiotics such as echinomycin, levomycin and actinoleutin, which are known to inhibit the growth of gram positive bacteria and are active against various transplantable tumours [2]. In addition, quinoxaline derivatives have found applications in dyes, electron luminescent materials and chemically controllable switches, as building blocks for the synthesis of anion receptors, cavitands, dehydroannulenes, organic semiconductors and as electron transport materials in multilayer OLEDs [3]. Although great attempts have been performed for the synthesis of quioxaline-fused heterocyclic derivatives, the development of new strategies for the preparation of structurally diverse five-cyclic pyrazolo-pyrimido-thiazino-quinoxaline still remains as an important and challenging goal for the organic chemists, due to its synthesis involving several reaction steps. We now wish to report a straightforward approach to the synthesis of various derivatives of pyrazolo[5'',1'':2',3']pyrimido[4',5':5,6][1,4]thiazino[2,3-*b*]quinoxaline as a novel heterocyclic system. These potential pharmacologically active and fluorescent derivatives (**3a-e**) were synthesized via domino reaction of 3-aminoquinoxaline-2-thiol (**1**) with pyrazolo[1,5-*a*]pyrimidine (**2**) and *N*-alkylation with some alkyl halides in K_2CO_3/*N,N*-dimethylformamide.



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The 26th Iranian Seminar of Organic Chemistry
University of Zabol
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Paper code: 1070

One-Pot Three-Component Synthesis of 1-Amidoalkyl-2-naphthols Derivtives by using Sulfamic Acid-Supported Piperidine-4-carboxylic Acid (PPCA) Functionalized Fe_3O_4 Nanoparticles as Highly Efficient and Rec clable Catalyst

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1-Amidoalkyl-2-naphthol derivatives are important class of compounds as they can be easily converted to biologically active compounds, 1-aminoalkyl-2-naphthols, by amide hydrolysis reaction [1]. The synthesis of 1-amidoalkyl-2-naphthols can be carried out by multicomponent condensation of aldehydes, 2-naphthol and amide in the presence of various catalysts such as $SnCl_4.5H_2O$, Nano-sulfated zirconia, dodecylphosphonic acid, and $Bi(NO_3)_3.5H_2O$ [2-4]. However, some of these methods are not environmentally friendly and suffer from one or more disadvantages, such as prolonged reaction times, low yields, toxicity and recovery and reusability of the catalyst. The demand for environmentally benign procedure with heterogeneous and reusable catalyst, promoted us to develop a safe alternate method for the preparation of amidoalkylnaphthols. In this study, we describe the catalytic activity of sulfonic acid supported piperidine-4-carboxylic acid functionalized Fe_3O_4 (Fe_3O_4–SAPCA) as a novel catalyst for one-pot synthesis of 1-amidoalkyl-2-naphthols by one-pot three-component coupling of β-naphthol, aromatic and aliphatic aldehydes and urea or amides under solvent free (Fig. 1).

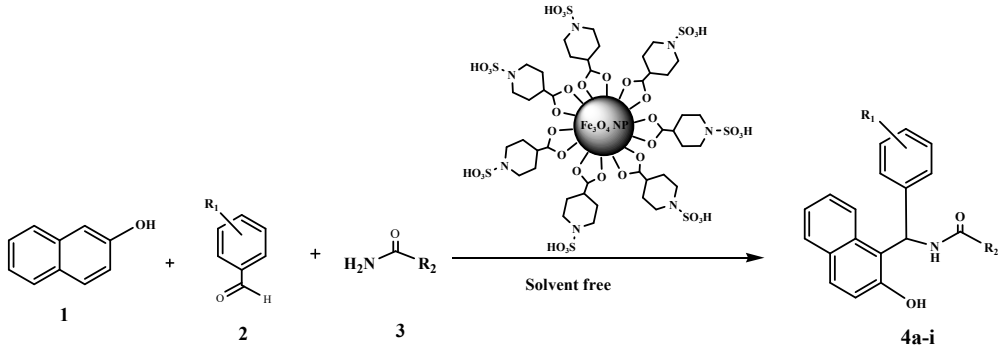

Fig. 1 General reaction scheme for the synthesis of 1-amidoalkyl-2-naphthols

This method offers several advantages including short reaction time, excellent yield, simple work-up, ease of separation, and recyclability of the magnetic catalyst, as well as the ability to tolerate a wide variety of substitutions in the reagents.

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12-14 March, 2019

Paper code: 1071

Synthesis of Bi(cyclopropane) *β*-Amino Tricarboxylic Acids from Fulvalene

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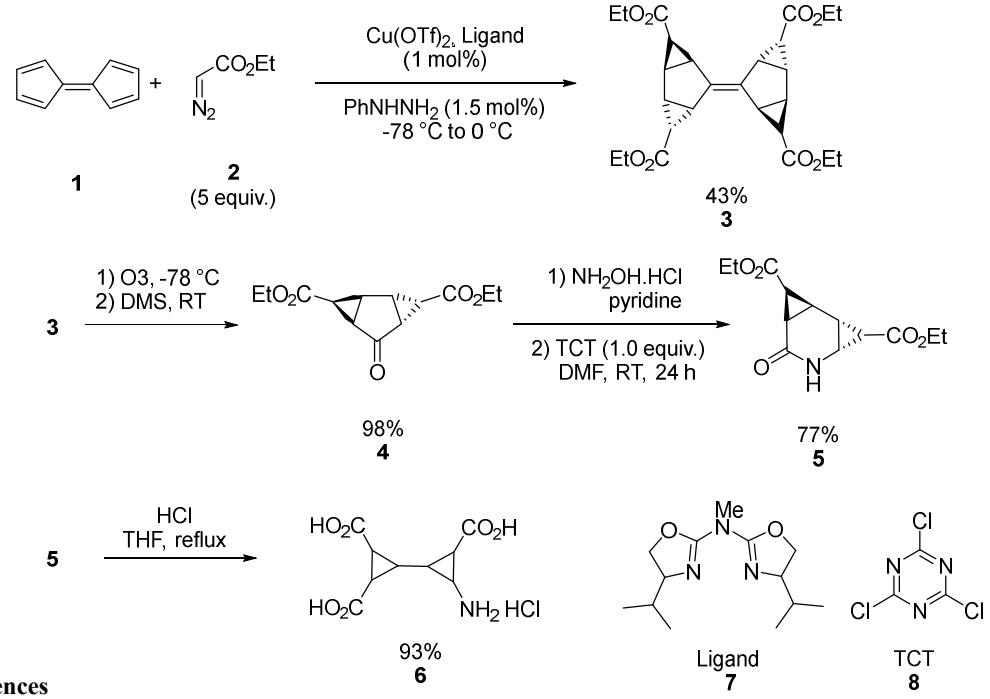
The synthesis of cyclopropane amino acids is an important process due to the occurrence of this moiety in natural products [1]and in several bioactive unnatural analogues [2]. Hereby we report synthesis of bi(cyclopropane) β-amino tricarboxylic acid **6** via cyclopropanation [3] of fulvalene **1** [4]followed by ozonolysis of the C-C double bond of bi(cyclopropanated) cycloadduct **3** to give tricyclic ketone **4** in high yield. This ketone **4** undergoes a Beckmann rearrangement to give rise to δ-valreolactam **5** which yields bi(cyclopropane) β-amino tricarboxylic acid **6** via hydrolysis of the amide and ester bonds. Stereoselective synthesis of the bi(cyclopropane) β-amino tricarboxylic acid **6** using enantiomerically pure bisoxazoline ligand **7** is being investigated in our research group.



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12-14 March, 2019

Paper code: 1072

Synthesis of Various Derivatives of a Novel Heterocyclic System of Tetrazolo[1,5-*a*][1,2,3]triazolo[4,5-*d*]pyrimidine

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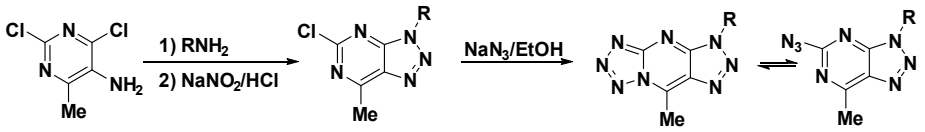
1,2,3-Triazole has become one of the most important heterocycles in current chemistry research, due to its important industrial, agrochemical and pharmaceutical applications, especially in biological science, material chemistry, and medicinal chemistry [1]. Additionally, the chemistry of the tetrazole ring is gaining increasing attention due to its importance in a variety of synthetic and industrial processes and excellent properties as a metabolically stable isosteric replacement for the carboxylic acid moiety and as a cis-peptide bond mimetic [2]. Tetrazoles have also been used as precursors to other heterocycles and in high energy compounds [3]. In the present work, initially the reaction of 2,4-dichloro-6-methylpyrimidin-5-amine **(1)** with different primary amines in refluxing *i*-PrOH gave the corresponding *sec*-amino derivatives which were consequently treated with $NaNO_2$/HCl solution to yield quantitatively the corresponding diazo derivatives of 5-chloro-3-alkyl-7-methyl-3*H*-[1,2,3]triazolo[4,5-*d*]pyrimidine **(2a-e).** Further reaction of compounds **(2a-e)** with NaN_3 in EtOH was resulted in various derivatives of novel heterocyclic system of tetrazolo[1,5-*a*][1,2,3]triazolo[4,5-*d*]pyrimidine **(3a-e)** that are in equilibrium with azide forms.



(1) (2a-e) (3a-e)

R: Et, *i*-Pr, *i*-Bu, *n*-Bu, *cyclo*-Hex

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Paper code: 1073

Synthesis, Spectral Characterization and Antimicrobial Activity of Schiff Base Ligands Derived from 4-Amino-2,3-dimethyl-1-phenyl-3-pyrazolin-5-one

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The Schiff bases of 4-amino-2,3-dimethyl-1-phenyl-3-pyrazolin-5-one have attracted the attention of the researchers because of their biological and analytical activities. These compounds and its complexes provide a great variety of biological activity ranging from anti-tumor, fungicide, bactericide, anti-inflammatory, and antiviral activities [1-3]. In this research, we report the synthesis and crystal structures of Schiff base ligands derived from 4-amino-2,3-dimethyl-1-phenyl-3-pyrazolin-5-one and substituted salicylaldehyde. These compounds obtained through the condensation of substituted salicylaldehyde with 4-aminoantipyrine in ethanol at room temperature. These ligands were characterized by ^{1}H NMR, ^{13}C NMR, FT-IR and single crystal X-ray diffraction. The antibacterial activities of the Schiff base ligands were tested against the bacterial species *Escherichia coli* ATCC 25922 (gram negativebacteria) and *Staphylococcus aureus*ATCC 25923 (gram positive bacteria) by the disc diffusion method. The experiments were performed in triplicates. The MIC of the chemically synthesized compounds was tested against bacterial strains through a broth dilutions method.

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Paper code: 1074

Mixed Metal Oxides Modified Mesoporous Silica with Magnetic Core: A Reusable Catalyst for the Synthesis of 2-Substituted Pramipexole Dihydrochloride

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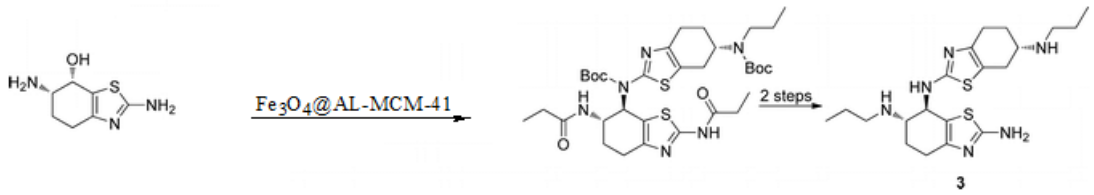
The use of magnetically recoverable catalysts has received considerable importance in organic synthesis because of their ease of handling, simple work-up and recoverability. Among the various heterogeneous catalysts, particularly, mesoporuos supported catalysts have advantages of high surface area and thermal stability. Metal modified mesoporous silica and also magnetically recoverable mesoporous silica have been applied in many organic transformations [1]. In this work, we wish to report an efficient method for the synthesis of 2-substituted pramipexole dihydrochloride from the reaction of alkylating and (*S*)-(-)-2,6-diamino-4,5,6,7-tetrahydrobenzothiazole with an alkylating agent, in the presence of catalytic amount of mesoporous silica containing AL metal oxides with magnetic core (Fe_3O_4@AL-MCM) [2].



Various types of (*S*)-(-)-2,6-diamino-4,5,6,7-tetrahydrobenzothiazole were reacted with *an* alkylating agent, in the presence of catalytic amount of Fe_3O_4@AL-MCM-41 at reflux condition and corresponding 2-sudstiuted pramipexole dihydrochloride were produced in high yields. Recovery and reusability of the catalysts was studied and results indicate that the catalyst can be reused many times with moderate change in its activity. In conclusion, we introduced a Fe_3O_4@AL-MCM-41 as simple, efficient and eco-friendly catalyst for the synthesis of 2-substituted pramipexole dihydrochloride. Simple workup and reusability of catalysts are other advantages of this method.

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Paper code: 1079

A Novel Method for the One-Pot Synthesis of Imidazole Derivatives in the Presence of Potassium Persulfate (KPS) as a Free Radical Initiator

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Imidazoles are one of the most important five-membered ring heteroaromatic nitrogen-bearing compounds that show a broad range of pharmaceutical, industrial and various biological activity [1-2]. Organic peroxides each have a peroxide bond (-O-O-), which is readily cleaved to give two oxygen centered radicals. Among these, one of the strongest known radical initiator agents is potassium persulfate (KPS). KPS is widely used as a free radical initiator in industrial processes such as polymer synthesis and chemical oxidant and also used as a chemical reagent for Minisci reaction [3]. However, until now, the synthesis of heterocycle cmpounds using thermally activated potassium persulfate is not reported. We have successfully developed a novel and efficient method to prepare a variety of 2,4,5 trisubstituted and 1,2,4,5-tetrasubstituted imidazole derivatives in the presence of potassium persulphate as a free radical initiator for the first time. Low cost of the starting materials, solvent free conditions, short reaction times, simple performance, easy work-up and good to excellent yields are some of the advantages of this procedure.

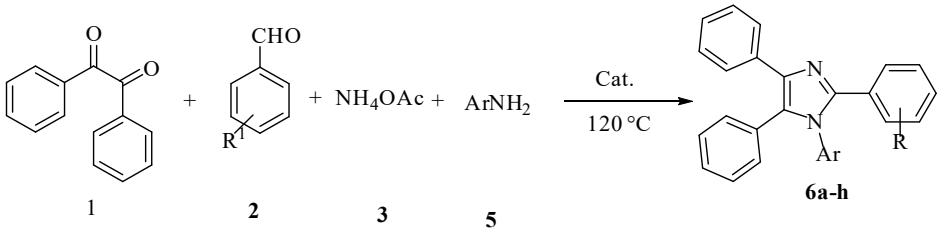

Fig. 1 Multicomponent synthesis of imidazole derivatives

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12-14 March, 2019

Paper code: 1080

Tannic Acid-Functionalized Fe_3O_4/SiO_2 Magnetite Nanoparticles as an Efficient, Reusable and Magnetically Separable Catalyst for the Synthesis of Acridinone Derivatives under Solvent-Free Conditions

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In recent years, magnetic nanoparticles (MNPs) have emerged as attractive solid supports for the immobilization of homogeneous catalysts [1]. This is because MNPs can be well dispersed in reaction mixtures without a magnetic field, providing a large surface that is readily accessible to substrate molecules. More importantly, after completing the reactions, the MNPs-supported catalysts can be isolated efficiently from the product solution through simple magnetic separation, eliminating the need for catalyst filtration and centrifugation [2]. Among various MNPs, magnetite (Fe_3O_4) is the material most widely used for catalyst supports [3]. Acridinones and their derivatives are well-known heterocycles in which two carbonyl groups are attached to the structure. Generally, 1,8-dioxodecahydroacridines are generally synthesized by one-pot MCRs in the presence of various catalysts. Herein, we report the synthesis of new silica-coated Fe_3O_4 nanoparticle-supported tannic acid (MNPs@TA) and its application as a magnetically recoverable catalyst, for the synthesis of acridinone derivatives via the one-pot multi-component reaction under solvent-free classical heating conditions. The nanomagnetic catalyst could be readily separated from the solution via application of an external magnet, allowing straightforward recovery and reuse at least five times without noticeably reducing catalytic activity.

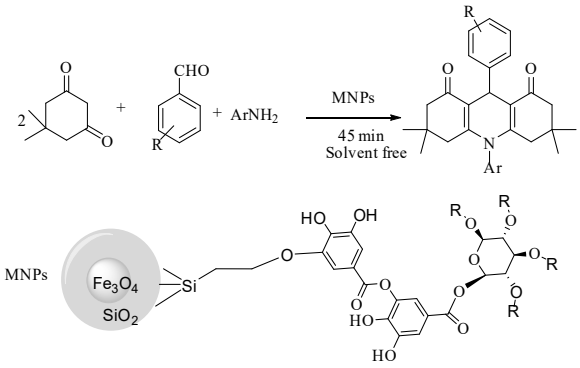

Fig. 1 Synthesis of 1,8-dioxodecahydroacridines

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12-14 March, 2019

Paper code: 1081

MoO_2(ONO) Schiff Base Complex: A Homogeneous Catalyst for the Synthesis of Benzimidazoles Under Various Reaction Conditions

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The benzimidazole ring is an important pharmacophore in modern drug discovery. Benzimidazole derivatives exhibit significant activity against several viruses such as HIV, HSV-1 and HCMV [1-2]. Benzimidazoles are very important intermediates in organic reactions. Therefore, the preparation of benzimidazoles has gained considerable attention in recent years. Recently, triaryl benzimidazoles as a new class of antibacterial agents against resistant pathogenic microorganisms have been synthesized [3]. In this study, benzimidazoles were prepared under various reaction conditions by taking a 1:1.1 mol ratio mixture of *o*-phenylenediamine and the arylaldehydes in the presence of 7 mol % MoO_2(ONO) Schiff base complex to give the desired products in excellent yield (Fig. 1). Efficient preparation of benzimidazoles by reaction of *o*-phenylenediamine with arylaldehydes in the presence of catalytic amounts of MoO_2(ONO) Schiff base complex as a homogeneous catalyst under reflux conditions is reported. Sonication of this system enhanced the catalytic activity of the catalyst and this was led to higher product yields and shorter reaction times. Another advantage of the systems, under ultrasonic irradiation, is the ability to carry out large-scale reactions.

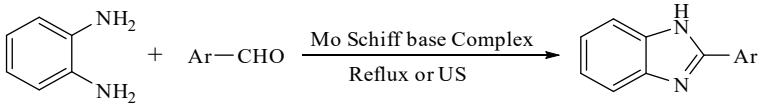

Fig. 1 synthesis of benzimidazoles under various reaction conditions

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12-14 March, 2019

Paper code: 1082

Gold Nanoparticles: Synthesis and Interaction Studies with Calf Thymus DNA

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Au-nanoparticles have unique physical and chemical properties, such as high electrical conductivity, small size, high surface area-to-volume ratio, adjustable measurements and high environmental compatibility [1]. Typically, Au-nanoparticles ranging from 13 to 60 nm can be easily made by a simple reduction of the gold salts in water [2, 3]. In this study, we synthesized Au-nanoparticles using microwave, sonochemical and organic reducing agents and their anticancer effects were investigated. The resulting Au-nanoparticles were characterized using UV-Vis and FT-IR spectroscopy, scanning electron microscopy (SEM), transmission electron microscopy (TEM), X-ray diffraction (XRD) techniques. The interaction of calf thymus DNA with Au-nanoparticles has been investigated following UV-Vis spectroscopic studies at 300 and 310 K. $[L]_{1/2}$, ΔG^0, ΔS^0, ΔH^0 values were obtained at 300 K, 0.2874415 mM, 27.641 (KJ/mol), 0.8501 (KJ/mol.k), 282.671 (KJ/mol) respectively and at 310 K, 0.3208555 mM, 19.14 (KJ/mol), 0.8501 (KJ/mol.k), 282.671 (KJ/mol) respectively.

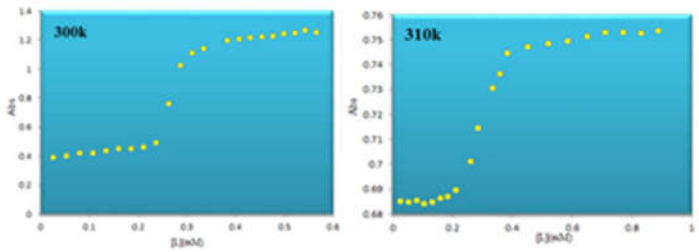

Fig. 1 Diagram of denaturation CT-DNA with gold nanoparticles at 300 and 310 K.

References

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University of Zabol
12-14 March, 2019

Paper code: 1084

Theoretical Study on Some Substituted Hydrazones as Anti-Depressant Agents

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Monoamine oxidase (MAO) is a mitochondrial enzyme that takes part in the oxidative deamination of various monoamines. This enzyme consists of two isoforms that identified as MAO-A and MAO-B [1]. The MAO-A inhibitors are preferred as controlling anti-depressant agents [2,3]. Thus, some substituted hydrazones was examined using computational quantum chemistry and molecular docking studies to evaluate their MAO-A inhibitor activities in this work. Results indicate that affinities of the mentioned hydrazones are in the range of -6.80 − -8.90 kcal mol^{-1}. Also, CF_3 is the best substituent that has the best affinity toward amino acids of enzyme among other ones. Molecular docking studies reveal that substituted hydrazones interplay with amino acids of enzyme via various interactions. However, hydrazone with CF_3 substituent interacts with amino acids preferably through π-π stacking interactions (Fig. 1). This result highlights the role of non-covalent interactions in better orientation and affinity of CF_3-hydrazone toward amino acids.

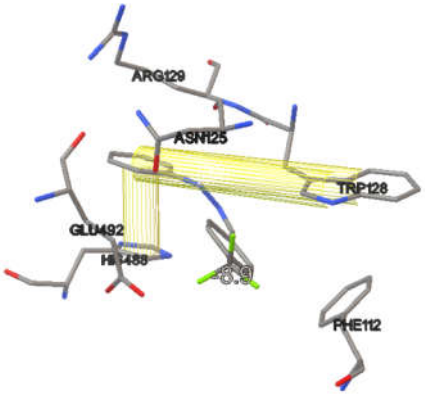

Fig. 1 Presentation of π-π stacking interactions between CF_3-hydrazone and amino acids of MAO-A

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Paper code: 1085

Computational Study Regards Inhibitory Effects of Some Pyrimidine Based Drugs against Kinase Protein for Treatment of Cardiovascular Disease

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The targeting of protein kinases [1] has enormous potential for the design of new drugs against cardiovascular diseases [2,3]. Thus, some substituted pyrimidine based drugs was explored using computational quantum chemistry and molecular docking studies to evaluate their inhibitory activities against kinase protein in the present study. Results indicate that CF3 is the best substituent for the mentioned drugs that leads to the best affinity toward kinase enzyme (PDBID: 3V8S) among other ones. Molecular docking studies reveal that pyrimidine based drugs interplay with amino acids of enzyme via hydrogen bonding and π-π stacking interactions that draw attention to the role of these interactions in inhibitory effect of these drugs against kinase enzyme for treatment of cardiovascular disease.

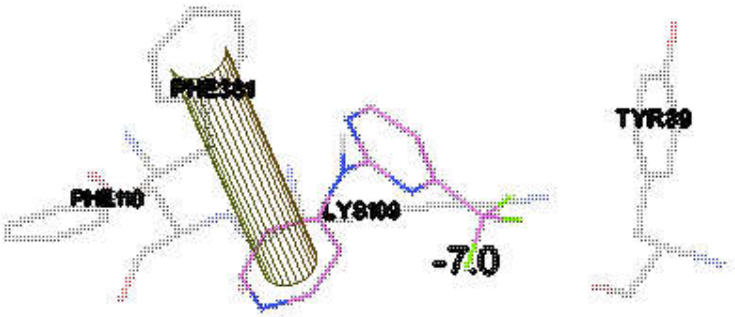

Fig. 1 Manifestation of interactions between the best substituted pyrimidine based drug and amino acids of kinase enzyme

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Paper code: 1087

One-Pot, Four-Component Synthesis of Pyrano[2,3-c]pyrazoles Catalyzed by Vanadium Oxo Pyridinoporphyrazine

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Tetrapyridinoporphyrazines are derivatives of phthalocyanines which have pyridine rings instead of outerbenzene rings [1]. Porphyrazines containing metal ions such as Zn(II), Ni(II), Cu(II) are strongly stabile. This situation is very important for the application this macrocyclic complexes as a stable catalyst in organic reactions. Pyrazole derivetives are the significant kind of heterocyclic compounds that feature in several pharmaceutical targets and natural products of medicinal interest. Dihydropyrano[2,3-c]pyrazole derivatives have showed a wide variety of biological activities counting anticancer, antimicrobial, anti-inflammatory, insecticidal, and molluscicidal activities. In continuation of our efforts to synthesize of novel catalysts [2] and multicomponent reactions we wish to report the synthesis of vanadium-oxo tetrapyridinoporphyrazine [VO(TPPA)] as an efficient catalyst for the synthesis of dihydropyrano[2,3-c]pyrazole through the condensation reaction of aryl aldehydes, ethyl acetoacetate, malononitrile, and phenyl hydrazine under solvent free condition at 60 °C (Fig. 1).

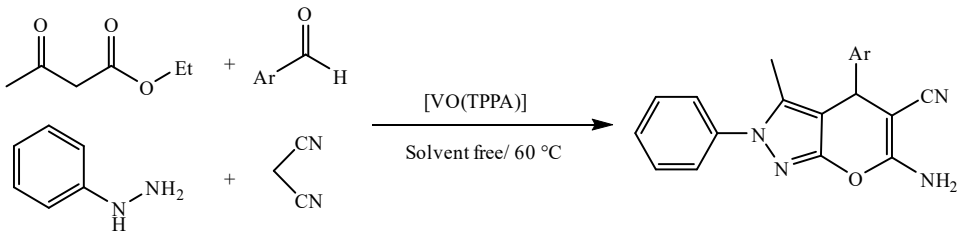

Fig. 1 Multicomponent synthesis of pyrano[2,3-c] pyrazoles

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The 26th Iranian Seminar of Organic Chemistry
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12-14 March, 2019

Paper code: 1088

Biopolymeric Alginic acid: an Efficient Recyclable Green Catalyst for One-Pot, Four-Component Synthesis of Pyrano [2,3-c]pyrazoles

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One of the main challenges in medicinal chemistry is the design and synthesis of biologically active molecules. Dihydropyrano[2,3-c]pyrazoles play an essential role as biologically active compounds and represent an interesting template for medicinal chemistry. Many of these compounds are known for their antimicrobial, insecticidal and anti-inflammatory activities. Furthermore, dihydropyrano[2,3-c] pyrazoles show molluscicidal activity, and are identified as a screening kit for Chk1 kinase inhibitor. They also find applications as pharmaceutical ingredients and biodegradable agrochemicals [1, 2]. Recently, a very cheap, naturally available (from cell wall of brownalgae), nontoxic, biodegradable and recyclable alginic acidhas been found as an efficient heterogeneous biopolymericBrønsted acid catalyst for organic transformation [3]. In continuation of our interest in the application of heterogeneous catalyst in organic transformation, we report the simple and efficient procedure for one pot synthesis of pyrano[2,3-c]pyrazole derivatives using aryl aldehydes, ethyl acetoacetate, malononitrile, and phenyl hydrazinein presence ofalginic acid as catalyst under solvent free at 60° C condition (Fig. 1).

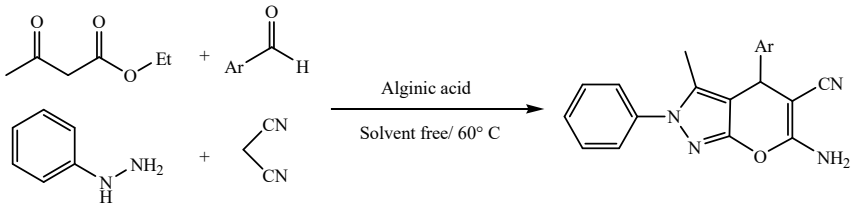

Fig. 1 Multicomponent synthesis of pyrano[2,3-c] pyrazoles

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Paper code: 1089

Synthesis and Characterization of Crosslinked Cellulose Schiff base as a Novel Bio Based Polymer Ligand

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Cellulose is recognized as the most abundant biopolymer in nature offer wide chance to be used for superior applications such as water purification [1,2]. It is natural, renewable, environmentally friendly, efficient and cost-effective, sustainable, bio–degradable and derived also easily from plant sources [3]. In this context, fully biobased and crosslinked adsorbent polymer Schiff base was prepared by using oxidation reaction of extracted cellulose biopolymer. A safe crosslinked cellulose dialdehyde (CCDA) was synthesized through epichlorohydrin and sodium metaperiodate ($NaIO_4$) followed by Schiff base formation with p-phenylenediamine [Fig. 1]. Crosslinking, oxidation and Schiff base formation of the extracted cellulose was confirmed by using FTIR spectrum. The index bonds of crosslinked cellulose (CC), CCDA and the crosslinked cellulose Schiff base (CCSch) were appeared at about 3419, 1727 and 1607 cm^{-1} respectively. The prepared imine bands and microstructure of the synthesized product was investigated from EDS and SEM analyses.

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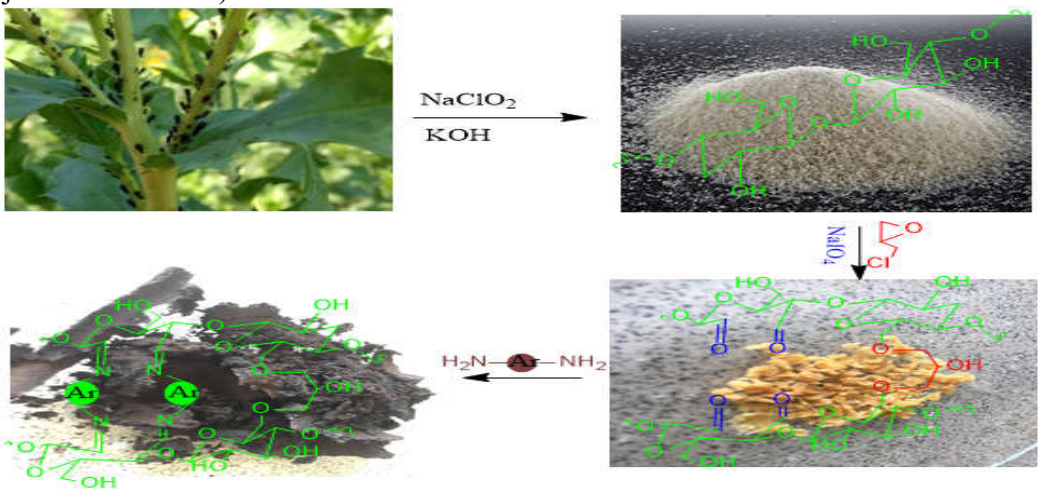

Fig. 1 Scheme of green polymer Schiff base preparation process

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Paper code: 1090

Synthesis of Reduced Graphene oxide/Silicate from Industrial Grade Graphite Flakes

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Graphene oxide (GO) is a chemical oxidized of graphite carbon material, including hydroxyl, carboxyl, carbonyls or epoxides functional groups [1, 2]. The presence of these groups on the GO surface provides reactive sites for the immobilization of electrical insulating materials (e.g./ SiO_2, Al_2O_3, SiC, $Al(OH)_3$ or nitrides) [3]. Herein, we report a simple synthesis procedure of GO from industrial grade graphite at room temperature. SiO_2 decorated with reduced GO (SiO_2@rGO) as thermally conductive electrically insulating composite was synthesized (Fig. 1). The prepared composite can act as a base material for the future various applications like electronic packaging, thermal management and the perfect functional additive for polymer composite preparation. The FTIR spectrum index bands of prepared GO and SiO_2@rGO were appeared at about 1725 and 1064 cm^{-1} respectively. SEM images and EDS analyses were employed to verification of surface morphology of product and chemical fluctuations of SiO_2 respectively.

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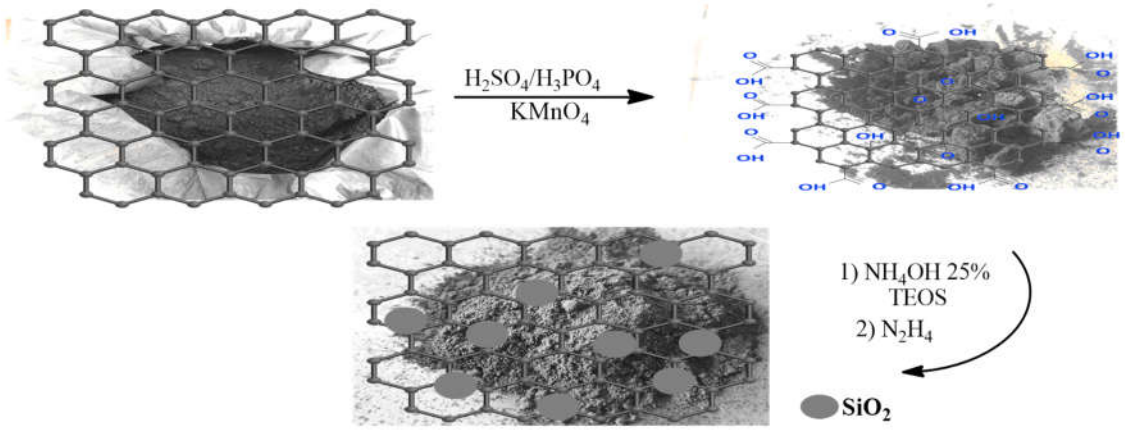

Fig. 1 Schematic pathway of SiO_2@rGO preparation

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Paper code: 1091

Preparation and Characterization of Chitosan/Poly(vinyl alcohol) Injectable Hydrogel as Drug Carrier

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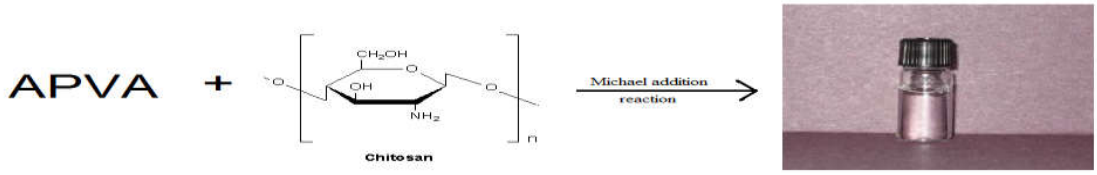
Hydrogels are a unique three-dimensional cross-linked network of natural polymers, which have the ability to absorbe large amounts of water. These materials are stable upon swelling in water and are capable of imbibing a major value of water, varying from10% to thousands of times of its own volume [1]. The most important properties of hydrogels can be pointed to low toxicity, similarity to body tissue and their biologically compatible in order to performing chemical reactions without any side effects. In addition, injectable hydrogels can be used as drug delivery systems in different fields including cell/drug delivery andtissue engineering applications due to its good biocompatibility feature, renewability, controllable physical and suitable chemical properties [2]. In this research, the injectable biodegradable hydrogel has been successfully synthesized based on Michael addition reaction between natural monomer of Chitosan (CS) and synthesis monomer of polyvinyl alcohol (PVA). APVA was prepared by functionalized polyvinyl alcohol at 80 °C for 24 hours and then chitosan solution was added. Chitosan hydrogel followed by stirring and heating for 20 hours at 70 °Cand pH=4. The swelling studies of a product were carried out as a function of time, temperature and pH. An anti-cancer drug was loaded into this hydrogel and the loading amount of the desired substances amount were evaluated. Also, the effect of this drug release was studied in a simulated biological environment and a cancerous cell (acidic medium). The synthesized hydrogelproperty was determined using different characterization techniques such as FT-IR, TGA, XRD and melting point.



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12-14 March, 2019

Paper code: 1092

Design and Synthesis a Self-Healing Polymeric Coating Formed through Diels-Alder Reaction between Bismaleimide and Furan-Modified Polyethyleneglycol

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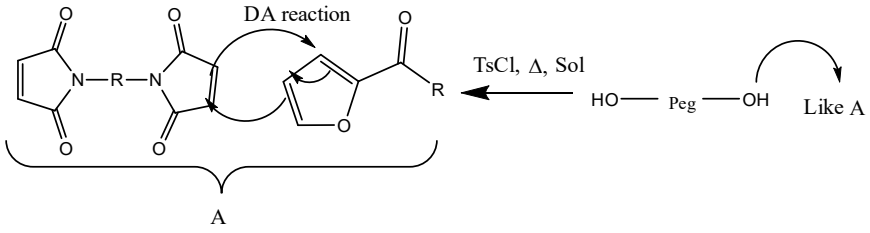
Self-healing material is a new generation of smart polymers which has the ability to repair damage and small cracks by itself and recover mechanical properties upon the external stimulus [1]. These materials lead to increased useful life, a durability of structures, reduces maintenance costs, restore their structure and prevents waste of materials. Self-healing based on heat is performed in the reversibility of reactions and bonds through the Diels-Alder (DA) reaction as an external stimulus [2]. The DA reaction has been widely used as one of the most well-known chemical reactions for designing self-healing polymers, which belongs to the family of "click chemistry" defined by high selectivity, high efficiency without byproducts [3]. In this study, poly (ethylene glycol) polymer was chosen as the alcoholic polymer that plays an important role for the enhancement of self-healing property. The flexible polymer chains of poly (ethylene glycol) (PEG) are functionalized by the derivatives of diene and dienophile in order to carry out the Diels-Alder reaction. The Diels-Alder product shows good thermal and mechanical properties due to the use of hydroxyl matrices. The self–healing property of the synthesized compound evaluated and observed at different times and temperatures by the use of an optical microscope. Identification of products is done by using techniques such as FT-IR, ^{1}H, ^{13}C NMR, TGA-DSC and melting point.



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Paper code: 1093

One-Pot Synthesis of Succinimide-3-Carboxamide Derivatives Using Microwave and Mechanistic Insights and Kinetics Analysis by Computational Method

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In the present work, one-pot, four-component condensation of meldrum's acid and acetone with tert-butyl isocyanides in the presence of primary amines under microwave irradiation which provided 1-tert-butyl-4,4-dimethyl-2,5-dioxopyrrolidine-3-carboxamides in short time with high yields have been investigated. Also, multiple mechanisms have been studied theoretically for comparing formation of the amidosuccinimide with triamide products using ab initio molecular orbital theory in gas phase. The potential energy profile was constructed at the HF/6-311G (d, p) level of theory. Among four speculative proposed path only the pathway A (intramolecular reaction to formation amidosuccinimide product) was recognized as a desirable mechanism. Theoretical kinetics data involving k and activation parametres (Ea, ΔG‡, ΔS‡ and ΔH‡) were calculated for each step of the paths. In order to determine the possible nucleophilic sites for the N17, N33 local reactivity has been evaluated through Fukui indices.

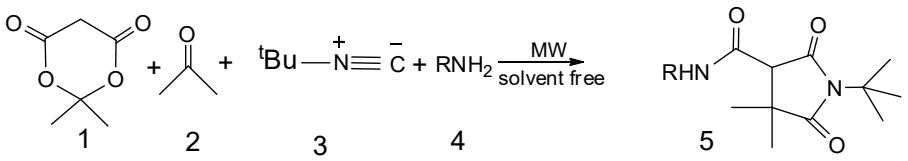

Fig. 1 Reaction between *tert*-butyl isocyanide with meldrum acid and acetone in the presence of primary amines for the generation of amidosuccinimide derivatives.

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Paper code: 1094

Theoretical Studies to Examine the Inhibition of Two New Thiourea Derivatives

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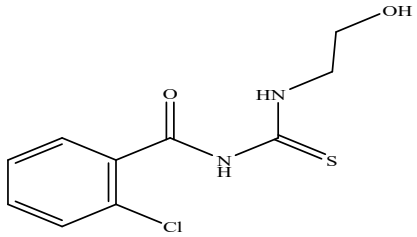
Organic compounds containing heteroatoms such as N, O and S have been reported efficient corrosion inhibitors for metals and alloys [1]. Quantum chemical calculations were performed for two organic derivatives of thiourea as corrosion inhibitors using the density functional theory (DFT) method at the hybrid functional B3LYP level of theory with 6-31+G** basis set [2]. The optimized molecular structures and some electronic properties such as energy of the highest occupied molecular orbital (E_{HOMO}), energy of the lowest unoccupied molecular orbital (E_{LUMO}), hardness (η), dipole moment (μ), polarizability (α), electronegativity(χ), global electrophilicity index (ω) and the fraction of the transferred electron (ΔN)were calculated and discussed [3]. The calculated parameters for inhibitors showed that thiourea 2 has well possible for inhibition of corrosion.



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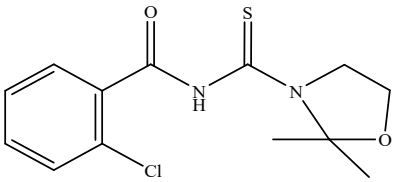

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A DFT Study of the Cheletropic Reaction between Diacetyl and Trimethylphosphite

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The mechanism of the cheletropic reaction between diacetyl and trimethylphosphite has been studied by density functional-based hybrid functional M062x with 6-31+G(d,p) basis set [1, 2]. The ground and transition states were confirmed by the frequency calculations. The rate constants and activation energies of this reaction is 12.71×10^{-11} $M^{-1}s^{-1}$ and 22.26 $kcalmol^{-1}$. The global reactivity index analysis was performed for the related reactants. The frontier molecular orbital (FMO) analysis allowed us to understand the nature of these [4 + 2] cycloaddition. An analysis of the FMO for diacetyl and trimethylphosphite indicated that the most favorable interaction along the cycloaddition process takes place between HOMO trimethylphosphite and LUMO diacetyl, the energy gap was 7.22 eV. A good electrophile was characterized by a low value of chemical potential (μ) and hardness (η) and high value of ω. The μ, η and ω for diacetyl (-4.86, 8.77, 1.56) and trimethylphosphite (-3.90, 7.59, 0.87) is shown that diactyl is electrophile. The trimethylphosphite and diactylewas classified as marginal and moderate electrophile within the electrophilicity scale [3]. The Δω for the reaction had a low value (0.68 eV), thus indicating that the corresponding cycloaddition will have a low polar character.

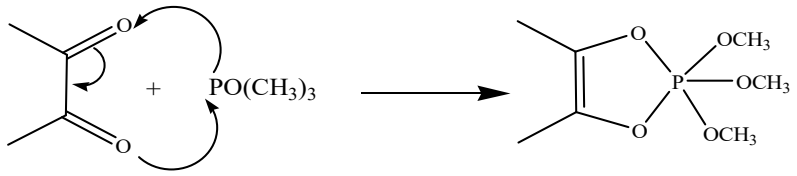

Fig. 1 Chelotropic Reaction of diacetyl and trimethylphosphite

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12-14 March, 2019

Paper code: 1096

Iron(III) Chloride Hexahydrate as an Efficient Heterogeneous Recyclable Catalyst for the Synthesis of 2-Substituted Quinazolinones

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The quinazolinone ring system as an important structural unit has been widely found in more than 100 naturally occurring alkaloids and biological and pharmacological activities and extensive applications on pharmaceutical active molecules [1]. Its derivatives has never faded since the first report of 4(3*H*)-quinazolinone compound in 1869 [2].

Quinazolinones are commonly prepared by the condensation of o-aminobenzamides with aldehydes using oxidants or carboxylic acid derivatives under harsh conditions. Recently, oxidative condensations of the alcohol, methylarene, or amines with o-aminobenzamides have also been developed. In spide of these notable advances they generally suffer from one or more drawbacks such as requirement of stoichiometric or excess amounts of strong oxidants, high temperatures, and transition metal catalysts [3, 4].

Herein, we report that iron(III) chloride hexahydrate can be used as an effective catalyst for the synthesis of quinazolinone derivatives by the condensation of *o*-aminobenzamides with aldehydes using with DDQ as an efficient and easily recyclable oxidant.

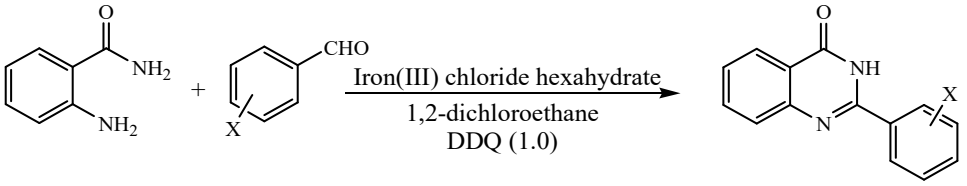

Fig. 1 Synthesis of 2-Substituted Quinazolinones

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Paper code: 1097

Design and Synthesis of Acidic Deep Eutectic Solvents Based on Choline Chloride and Discovery of a Highly Efficient Catalyst for the Synthesis of Benzoazepinones

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Benzodiazepines are biaryl lactams which have attracted the attention of scientist as these are the privileged core, discovered in many alkaloids and pharmaceutically relevant organic molecules. This moiety is also very important due to being a core intermediate for LY411575, an γ-secretase inhibitor, a clinical candidate for Alzheimer's disease [1].They are anti-inflammatory, antidepressive, anticonvulsant, antiviral, antimicrobial, anti-HIV, antianxiety, anti-ulcerative, antitumor, analgesic, antihistaminic, anti-allergic, hypnotic and antipyretic [2]. Benzodiazepines are generally synthesized by the reaction of *β*-haloketones with o-phenylenediamine, condensation of *α,β*-unsaturated compounds with o-phenylenediamines and condensation of ketones with o-phenylenediamine in the presence of ytterbium trichloride. The disadvantages of previously reported procedures for the synthesis of benzodiazepines are their multistep reactions, anhydrous conditions, tedious work-up, long reaction times and generation of undesirable by-products [3].

Herein, we report the acidic deep eutectic solvents based on choline chloride which can be used as an effective catalyst for the synthesis of benzoazepinones derivatives by the condensation of *o*-phenylenediamines, dimedone and various benzaldehydes derivative.

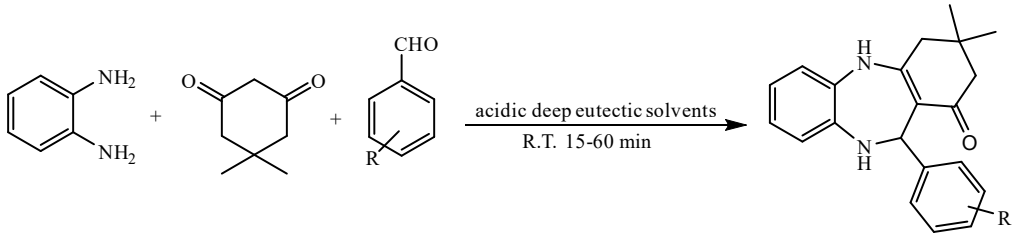

Fig. 1 Synthesis of benzoazepinones

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Paper code: 1098

Polyphenols in Pistachio Hulls

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Pistachio (Iranian type) is one of the principal agriculture plants in Iran. Regarding to the presence of the phenolics in Pistachio hulls very few studies have been reported in general, particularly considering Iran's pistachio hulls. In the present study, polyphenols in the hulls of the two most important Iran's pistachio varieties (Kerman and Damghan) were extracted using methanol and ethanol solvent and various dilutions of these solvents with water. Folin method as one the most reliable procedure for the phenolics measurement was used in this study, to determine the concentration [1-3]. Among the solvents used for Damghan variety the yield of the ethanolic extract at the level of the 50:50 (H_2O) was higher (28.8 mg Polyphenols per g the denied pistachio hulls). While the yield of the ethanolic extract at the ratio of 75:25 (H_2O) from Kerman's pistachio hulls was higher among the yield obtained from other solvents used for this variety (19.8 mg Polyphenols per g the denied pistachio hulls). The relationship between plant phenolics and antioxidant activities is well documented in the literature. In order to determine the antioxidant activities of the ethanolic extracts from the Pistachio hulls according to the defined procedures, detailed experiments are being under taken in our laboratory.

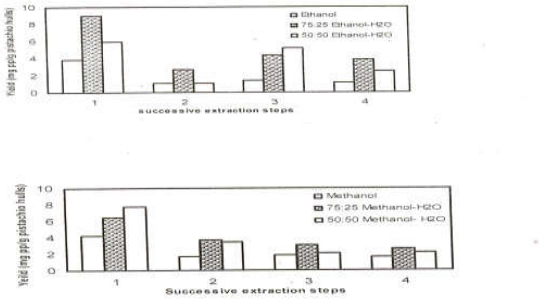

Fig. 1 Yield of polyphenols pistachio hulls extracted four times using different solvents (A: Damghan variety, B: Kerman variety).

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The 26th Iranian Seminar of Organic Chemistry
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12-14 March, 2019

Paper code: 1099

Uniform Copper Nanoparticles on Tunable Porous N-Doped Carbon Nanospheres for Esterification of Various Aryl Aldehydes with Alcohols

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Synthesis of esters as an important intermediate from carboxylic acids or aldehydes is one of the popular transformations in organic chemistry [1]. Traditionally base/acid homogeneous catalysts were applied for the direct esterification of carboxylic acids. In the recent years, heterogeneous catalysts had also been reported which most of these catalytic systems are present acidic nature. Metal oxides such as Al_2O_3, Fe_3O_4, SnO, ZnO, CaO, ZnO–La_2O_3, sulfated zirconia, and sulfated carbon were used for catalytic synthesis of esters from carboxylic acids and alcohols. In the last years, carbon with attractive properties such as porous structure, excellent electrical conductivity, and high stability find widespread applications as support in catalysts [2]. It is well known that structural modifications on the surface of carbon can effectively change the nature of the catalysts. Heteroatom doping strategy can control the intrinsic reactivity of the active metallic sites [3]. Among different dopants, nitrogen is the most intensively investigated. In this paper, we have prepared highly monodispersed, nitrogen-doped porous carbon nanospheres as a solid ligand for generation of Cu nanoparticles for esterification of various aryl aldehydes with primary, secondary and *tertiary* alcohols (Fig. 1). Generally, nitrogen doping provides basic properties, which can enhance the interaction between substrates and carbon surfaces. Also, nitrogen doping was able to increase the hydrophilicity of catalyst which led to the high dispersion ability of catalytic system in aqueous media.

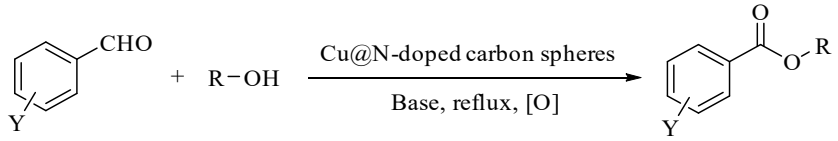

Fig. 1 Cu@N-doped Cs catalyzed esterification reaction of various carboxylic acids with alcohols

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Paper code: 1100

N-Sulfopiperidine-4-Carboxylic Acid Functionalized Fe_3O_4 Nanoparticles as Catalyst for One-Pot Synthesis of Dipyrromethanes under Solvent-Free Condition

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In recent years, dipyrromethanes and its derivatives have aroused a strong interest due to their useful physiological properties and biological activities as important building blocks for the synthesis of porphyrins, calixpyrrols and corroles [1]. As a consequence, the synthesis and the applications of dipyrromethane derivatives still attract the attention of organic chemists. The most common strategy involved in the synthesis of dipyrromethanes is the mixture of pyrrole (2 mmol) and ketone (1 mmol) or aldehyde (1 mmol) compounds. Of the various other methods, syntheses involving transition-metal salts or lewis acid have recently been described for the preparation of substituted dipyrromethane derivatives [2-4]. In connection with our ongoing studies, we wish, herein, to report on the use of Chlorosulfonic acid supported Piperidine-4-carboxylic acid (PPCA) functionalized Fe_3O_4 nanoparticles (Fe_3O_4-PPCA) as a more robust and efficient catalyst in the one-pot synthesis of dipyrromethane derivatives (**3**a-j) by the reaction of pyrrole (**1**) and ketone or aldehyde (**2**a-j) under solvent free conditions (Fig. 1).

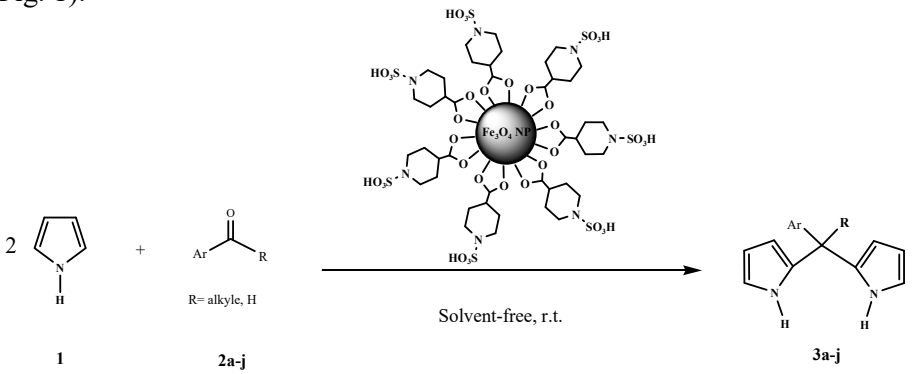

Fig. 1 General reaction scheme for the synthesis of dipyrromethane

The main advantages of the presented protocol are mild, clean and environmentally benign reaction conditions, as well as the high yields, simple work-up, ease of separation, and recyclability of the magnetic catalyst.

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Paper code: 1101

Nanosized Vanadium Oxide (V_2O_5/NPs): A Hetrogenous Catalyst for Direct Epoxidation of Some Alkenes Compounds

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In recent year, the catalytic epoxidation of alkens are a very important area in chemistry and chemical engineering. The simplest epoxide, is ethylene epoxides, is produced by vapor-phase oxidation of ethylene with air or oxygen over a silver catalyst, promoted by alkali metals and supported on a non-porous form of α-alumina. This process was introduced by Union Carbide in 1937 and by Shell in 1958 to replace the practice of ethylene oxide production via the chlorohydrin process. However, this silver catalyzed process can only by applied to olefins which do not process C-H allylic bonds, such as ethylene, 1,3-butadiene and styrene. For all the other olefins, such as propane, low yields of the desired product are obtained, due to the competing oxidation of allylic C-H bonds, which leads to numerous by-products [1,2]. In this study V_2O_5/NPs were prepared by a green sol-gel method according to our past project [2] and tert-butylehydroperoxid (TBHP) (1 mmol) was added to a solution of different alkenes (0.5 mmol) and V_2O_5 /NPs (0.005 mmol) in MeOH (7 ml). The mixture was stirred at 85 °C under air condition. The reaction progress was monitored using gas chromatography and the yield of products was determined by GC analysis. Assignments of products were made by comparison with starting materials or were identified by their IR, ^{1}HNMR and GC-Mass spectral data. Influence of the solvent, temperature, catalyst concentration and influence of different TBHP were studied by monitoring their reaction by GC-Mass technique see Figure 1. In general the high efficiency and selectivity obtained by using this catalyst.

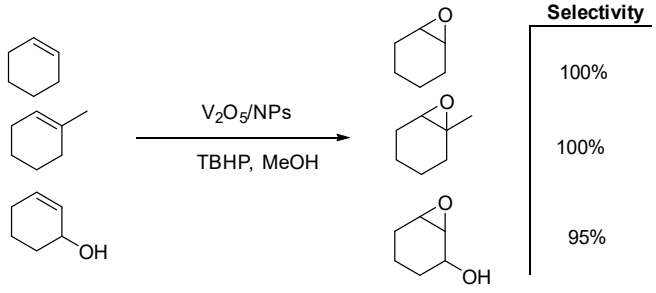

Fig. 1 Epoxidation of alkens using TBHP catalysed by V_2O5/NPs

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The 26th Iranian Seminar of Organic Chemistry
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12-14 March, 2019

Paper code: 1102

Synthesis, Characterization and Theoretical Study on the Structural Properties of a Tetradentate Schiff Base Compound

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Imine derivatives or Schiff bases exhibit wide application in biological systems, dyes, coordination chemistry and catalytic reactions and as nonlinear optical materials in some dye lasers. Many organic compounds are especially interesting for study of NLO property. In the other hand theoretical studies are important part of computational chemistry, that used in study and predicting of molecular properties and chemical behaviors of new compounds. In this work bis-(2-hydroxyl-4-azophenyl) salicylaldimine)-*N*-(2,2-dimethyl-1,3-propandiamine) was prepared by refluxing of its precursor ligand with 2,2-dimethyl-1,3- propandiamine (1:1) in ethanol as solvent for 4h. The prepared compound was recrystallized from ethanol: hexane (1:1), and the reaction product was studied by spectroscopic methods like: FT-IR, UV-Vis, ^{1}HNMR, ^{13}CNMR, GC mass and C, H, N analyses. In the other part of this work the electronic properties of this compound was studied with DFT calculations by using G03 program package and the correlation between the molecular structure and some calculated electronic properties have been investigated by using DFT-B3LYP with suitable basis sets, and the effect of structural properties on chemical activity for this imino compound has been studied. The highest occupied molecular orbital (HOMO), lowest unoccupied molecular orbital (LUMO), energy level, energy gap, charge density for all atoms and the NLO property have been calculated, and then the relations between the inhibition efficiency and all quantum chemical parameters have been discussed.

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Paper code: 1103

Synthesis and Characterization of Two Transition Metal Ionic Schiff Base Complexes and Investigate the Anticancer Activity

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Metal complexes of Schiff bases have occupied a central role in the development of coordination chemistry[1]. This situation is manifested by the huge number of publications ranging from the purely synthetic to modern physicochemical to biochemically relevant studies of these complexes[2]. Large numbers of Schiff bases have also been shown to exhibit a broad range of biological activities, including antitumor, anti-bacterial, fungicidal and anti-carcinogenic properties [2]. In this study the solphonium salophen Schiff base complex of Cu(II),$(A\text{-}Cu)^-$ and imidazolium salophen chloride Schiff base complex of Fe(II),$(B\text{-}Fe)^+$ was synthesized and after characterization, the anticancer activity of them was investigated. Moreover, the anticancer activity of the ionic complex of these two cationic and anionic complex, $(A\text{-}Cu)^-(B\text{-}Fe)^+$ was investigated. The IC50 results show that the anticancer activity of the ionic complex, $(A\text{-}Cu)^-(B\text{-}Fe)^+$ is better than the anionic and cationic complexes in compare with cisplatin.

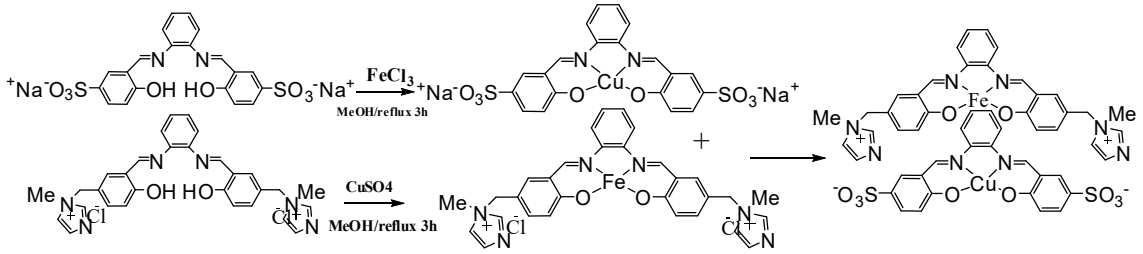

Fig. 1 Synthesis of the ionic Schiff base complex

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The 26th Iranian Seminar of Organic Chemistry
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12-14 March, 2019

Paper code: 1104

Polyoxyethylene-Based Epoxy/Graphene Oxide Thermosetting Materials with Enhanced Storage Moduli

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Epoxy resins have so many applications such as adhesives, coatings and castings [1]. However, in all these applications, they are brittle and rigid in nature, so its many end use applications are limited [2]. Therefore, many investigations have been performed with the aim of toughening of epoxy polymers. A common method for preparing epoxy resins with high toughness is based upon the participation of polyoxyalkylenes units into the network [3].
In this work, along with two conventional monomers, i.e., diglycidyl ether of bisphenol A (DGEBA) and isophorone diamine (IPD) two polyoxyethylene-based macromonomers including epoxy-terminated polyoxyethylene (ETPOE) and amine-terminated polyoxyethylene (ATPOE) are use to prepare the the corresponding epoxy networks. This maromonomers are initially synthesized from polyethylene glycol. To reinforce the storage modulus (E' values) the networks obtained, an aminated graphene oxide (AGO) with 0.1 wt.% is used for loading into the epoxy matrix. The resulting nanocomposites are fully charecterized by thermogravimetric analysis (TGA) and dynamic mechanical analysis (DMA) techniques.

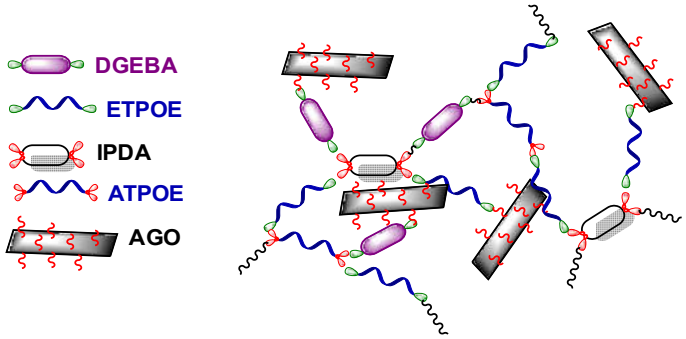

Fig. 1 Fabrication of epoxy networks using a combination of DGEBA and DGEPEG cured by a combination of IPD and APEG.

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Paper code: 1105

Fabrication and Investigation of Poly[*St-Co-CMS*] Loaded by Modified SiO_2 as Initiator via ATRP Method

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Poly[*St-co-CMS*] is unique functionalized copolymer, which has been used in the field of polymeric materials [1]. The pendant chloromethyl group attached to phenyl rings of the chains allow them to easily react with various kinds of organic moieties through nucleophilic substitution reactions [2]. Copper-mediated polymerization techniques can be easily identified in the literature by the use of an alkyl halide in conjunction with a ligated copper complex. Atom transfer radical polymerization (ATRP) is one of the most rapidly developing areas of polymer science. It allows control over molecular weight, preparation of polymers with narrow molecular weight distributions, incorporation of precisely placed functionalities, fabrication of various architectures, and synthesis of well-defined hybrid composites [3]. In this work, we tried to fabricate poly[St-co-CMS] via ATRP method in different styrene/4-(Chloromethyl)styrene (St/CMS) ratios. To incorporate silica nanoparticles into the polymer matrix, these nanoparticles are covalently linked to 4-(Chloromethyl)phenyltrimethoxysilane as the reaction initiator. Copper (I) chloride (CuCl) and bipyridine (Bipy) are also used as the polyaddition reaction catalyst and ligand, respectively (fig. 1). The resulting nanocomposites are fully charecterized by Fourier transform-infrared spectroscopy (FT-IR), thermogravimetric analysis (TGA), field emission-scanning electron microscopy (FE-SEM), and X-ray diffraction (XRD) techniques.

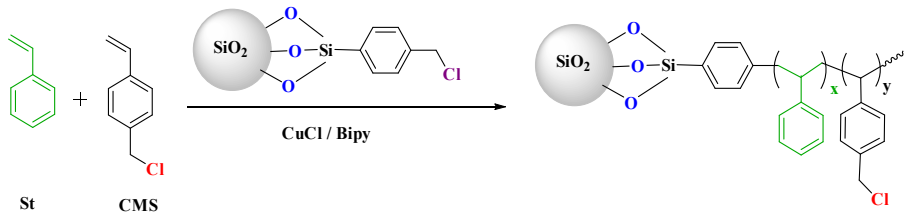

Fig. 1 Synthesis of [St-*co*-CMS] loaded by SiO_2 via ATRP method

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Paper code: 1106

Investigation of Dynamic Thermo-Mechanical Analysis on Epoxy/Silica Nanocomposites with Flexible Backbone

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Diglycidyl ether of bisphenol A (DGEBPA) is one of the most commonly used epoxy resins, which is cured with various types of hardeners such as isophorone diamine (IPDA) [1]. Although the resulted networks have high strength and modulus, their low toughness somewhat restricts their applications in some industrial fields [2,3]. In this study, our aim was to investigate the effect of network structure on the thermo-mechanical properties via employing binary epoxy resins and amine hardeners. One of the resins and hardeners used were chosen based on polyoxybutylene units, i.e., diglycidyl ether of polyoxybutylene (DGEPOB) and amine-terminated polyoxybuthylene (APOB). Moreover, to reinforce properties of the resulting epoxies, amine-functionalized silica nanoparticles with 5.0 wt.% were used during the curing process of the resin. The epoxy/silica nanocomposites obtained and their neat counterparts were fully investigated using dynamic mechanical thermal analysis (DMTA), and the results compared with each other.

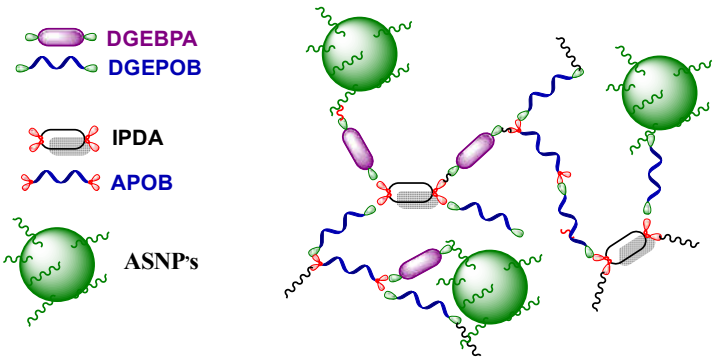

Fig. 1 ASNP's-loaded epoxy networks prepared from DGEBPA/DGEPOB binary resins and IPDA/APOB binary hardeners

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Paper code: 1107

Synthesis and Characterization of Magnetic Poly[St-*co*-CMS] Nanocomposites by ATRP Method

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Polymer-based magnetic nanocomposites have gained an increasing attention because of their potential applications [1,2]. A variety of functional polymers such as polystyrene have been used for the preparation of nanocomposites. This polymer is generally obtained via copolymerization of styrene (St) and chloromethyl styrene (CMS) monomers by using one of the controlled radical polymerization methods such as atom transfer radical polymerization (ATRP) [3]. In this study some poly[St-*co*-CMS]/Fe_3O_4 nanocomposites in different St/CMS ratios are synthesized through ATRP method starting from styrene/CMS monomers and magnetite-containing benzyl chloride initiator. In this rout, MNP's initially link to the polymerization initiator. The copolymers synthesized are thoroughly charecterised by Fourier transform-infrared spectroscopy (FT-IR), thermogravimetric analysis (TGA), field emission-scanning electron microscopy (FE-SEM), X-ray diffraction (XRD), and vibrating sample magnetometry (VSM) techniques.

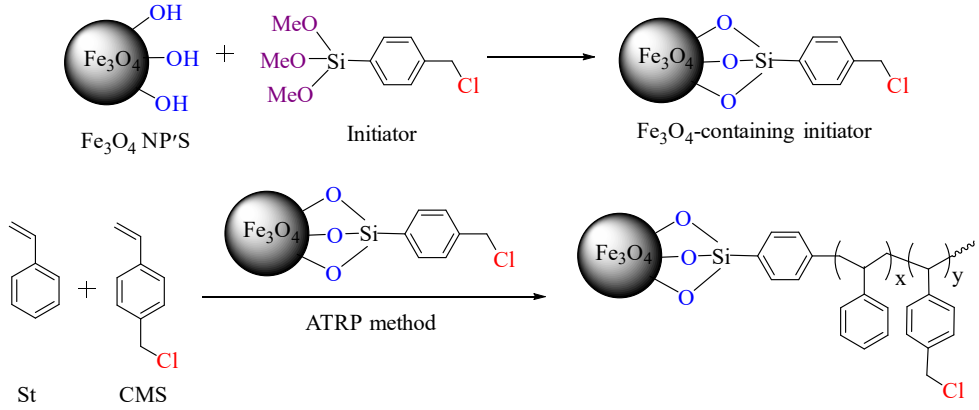

Fig. 1 Synthesis of magnetic [St-*co*-CMS] via ATRP method

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12-14 March, 2019

Paper code: 1109

Performance of Graphene Nanomaterial for Removal of Organophosphate Pesticide from Aqueous Solutions

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In recent years, water pollution and pesticide residues in food chain have become a seriousenvironmental problem [1]. Diazinon is a widespread organophosphorus pesticide which is used to control a variety of insects in agricultural applications and household environments [2]. This pesticide is known as a major contaminant in aquatic systems due to its potential toxicity to human and animals. Therefore, it is essential to remove from contaminants water [3]. Graphene oxide was prepared from the oxidation of graphite powder by a strong acid by Hummers-Offemane method [4]. Then these particles were decorated with zinc oxide in two steps [5]. Afterwards scanning electron microscopy, X-ray diffraction and Fourier-transform infrared spectroscopy were used to investigate morphological changes and chemical structure of the prepared adsorbent. At a regular time-interval, samples were taken, centrifuged and analyzed spectrophotometrically at absorption peak (245 nm) of diazinon. The effect of various parameters such as pH, contact time, diazinon concentration, temperature and adsorbent dosage on the process was investigated. The efficiency of removal of diazinon by applying optimal Taguchi conditions was 92% which include the contact time = 30 min, pH = 6.5, amount of sorbent = 15 mg and T = 20 °C. Accordingly, we concluded that GO/ZnO removed diazinon from aqueous solution to a great extent. The ability to remove this nanoparticle was also performed on chlorpyrifos (organophosphorus halogenated toxins) under the same experimental conditions of diazinon and the removal efficiency was 86%. So it was found that synthesized nano particles would be an appropriate adsorbent for eliminate the pesticide from contaminated water source.

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Paper code: 1111

1,10-Phenanthrolin-1-ium trinitromethanide (1,10-PHTNM) as a Nano Molten Salt Catalyst with Y-Aromatic Counter ion: Applications for the Synthesis of Organic Compounds

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1,10-Phenanthrolin-1-ium trinitromethanide (1,10-PHTNM) as a novel nano molten slat with Y-aromatic counter ion was synthesized and fully characterized by using various techniques such as FT-IR, ^{1}H NMR, ^{13}C NMR, mass, TGA, DTG, XRD, SEM and TEM. A series of organic compounds including 1,4-dihydropyrano[2,3-*c*]pyrazoles, tetrahydrobenzo[*b*]pyran, pyrano[4,3-*b*]pyrans, bispyrazole, 1*H*-pyrazolo[3,4-*b*]quinolones, hexahydroacridine-1,8-diones and methylenebis(3-hydroxy-5,5-dimethylcyclohex-2-enones) were synthesized in the presence of described 1,10-PHTNM as a novel and efficient proton sponge nano molten slat catalyst. These heterocyclces are considerable attention of organic chemists due to their broad range of pharmaceutical and biological properties containing arisugacins, anti-multidrug-resistant, anti-inflammatory [1], photodynamic therapy, inhibitors of human Chk1 kinase, spasmolytic, anti-filarial agents [2].

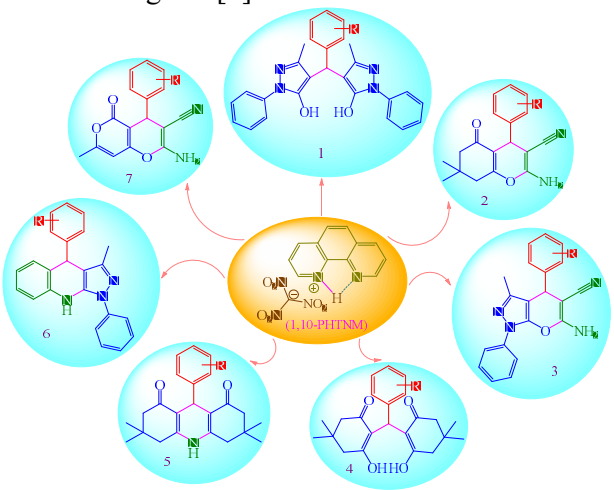

Fig. 1 Synthesis of a series of organic compounds using (1,10-PHTNM)

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The 26th Iranian Seminar of Organic Chemistry
University of Zabol
12-14 March, 2019

Paper code: 1112

Application of Pristine and Ni-Decorated Zigzag (8,0) Boron Nitride Nanotube for Adsorption of Methylamine and Ethylamine: A DFT Study

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In this study, density functional theory (DFT) method has been carried out to explicate the adsorption properties of methylamine (MA) and ethylamine (EA) on the surface of pristine and Ni-decorated $B_{32}N_{32}$ nanotube (BNNT). All calculations were carried out with the Gaussian 09 program at B3PW91/6-31G(d) level of theory. Electron density of states (DOS) was obtained to investigate HOMO and LUMO orbitals using GaussSum Software. Natural bond orbitals (NBO) calculations were done on the simulation models to predict the charge transfers [1]. The adsorption energies (E_{ad}) of the MA and EA on the surface of Ni-decorated BNNTs are defined as:

$$E_{ad} = E\text{ (MA- Ni-decorated BNNT)} - E\text{ (MA)} - E\text{ (Ni-decorated BNNT)} \quad (1)$$

$$E_{ad} = E\text{ (EA- Ni-decorated BNNT)} - E\text{ (EA)} - E\text{ (Ni-decorated BNNT)} \quad (2)$$

Our theoretical calculations show that the Ni atom can be adsorbed onto the surface of BNNT and it causes to significantly improve in the MA and EA adsorption energies on the surface of the pristine and Ni-decorated BNNT (Fig. 1). It is also discovered that the energy gap of pristine $B_{32}N_{32}$ nanotube decreases after complexation with Ni atom, and increases again upon adsorption of MA and EA molecules on its surface [2]. In addition, our results suggest that Ni-decorated $B_{32}N_{32}$ nanotubes show promise in MA and EA molecules adsorption.

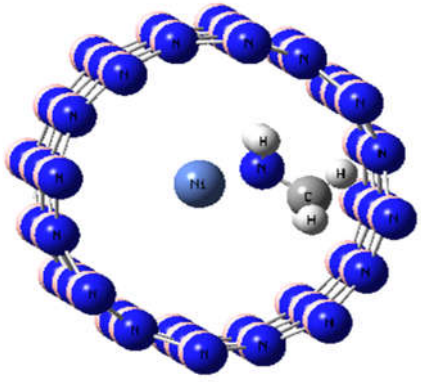

Fig. 1 Adsorption of MA onto the surface of Ni-decorated zigzag (8,0) BNNT

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Paper code: 1113

7α–Acetoxyroyleanone Terpenoid Extracted from Salvia Virgatae Collected in Northern Iran

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Salvia extracts have been used widely for various medicinal applications. The Most biological activity is dedicated to abietane diterpenoids, as a major content of extract. This terpenoid has antibacterial, antifungal, anti-Alzheimer, insecticide, cardiovascular disease Treatment Properties [1]. Seventeen species of Salvia are endemic in flora of Iran. Salvia Virgata is a member of Iranian endemic species on whose content there is no phytochemical studies [2]. Isolation and purification of compounds was done using column chromatography technique. Finally, 25 major fraction were selected after comparing thin layer chromatography. Crystalline samples were recrystallized with different solvents. A pure substance was identified using ^{1}H-NMR, ^{13}C-NMR and Mass spectra. An abietane diterpenoid (7a -acetoxyroyleanone) was newly identified for the first time in this specie (Fig. 1).
Diversity of flavonoid and terpenoid compounds in genus Salvia, along with little phytochemical researches, promises the potential of discovery of new medicinal phytochemicals in this specie.

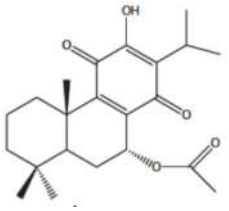

Fig. 1. 7α –Acetoxyroyleanone

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Paper code: 1115

Synthesis of a Novel Dendrimer Based on Poly Ethylene Glycol for Gene Transfection into the HEK-293T Cells

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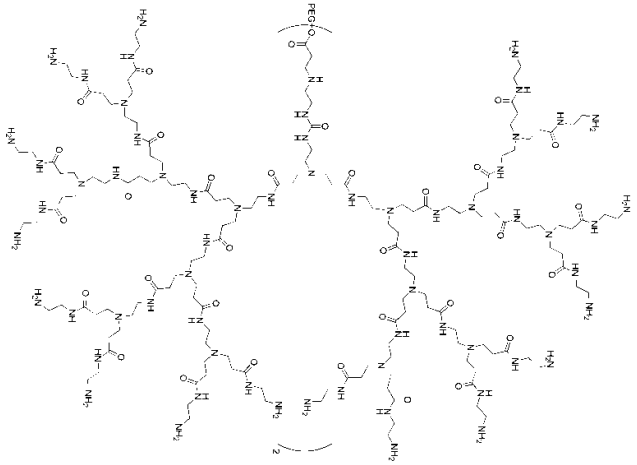
The delivery of the gene is a process in which external DNA is introduced into the host cell. Different methods have been developed for gene transfer in a variety of cells and tissues, from bacteria to humans. In order to carry out a good gene transfer, the outer DNA needs to survive in host cells so that it can integrate with its gene [1]. Gene transplantation in therapeutic programs uses non-immune carriers that are appropriate to the cell's characteristics, which can transmit enough transgene expression and result in an arbitrary effect [2]. In this paper, we synthesized a novel dendrimeric carrier based on a novel functionalized polyethylene glycol (PEG) to access the immunity and minimum of toxicity. The addition of step-by-step of ethylenediamine and methyl methacrylate to the functionalized PEG. Then, the dendrimeric carrier was used to transfer the plasmid to HEK-293 T cells.



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The 26th Iranian Seminar of Organic Chemistry
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12-14 March, 2019

Paper code: 1116

Optimization, Kinetics, and Equilibrium Studies on the Removal of Beta-Lactam Antibiotics from Industrial Waste Water Using Functionalized Magnetic Multi-Walled Carbon Nanotube as a Novel Adsorbent

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In the recent years, residual antibiotics are considered to be nascent environmental pollutants due to their continuous input and persistence into the aquatic ecosystem even at low concentrations. Therefore, these are necessary to develop efficient methods for the waste water treatment [1-3]. The presence studied describes the efficiency of magnetic multi-walled carbon nanotubes (MMWCNT) for the adsorption of the selected beta-lactam antibiotics (penicillin G procaine, Amoxicillin trihydrate) from wastewater samples. The functionalized MMWCNT were characterized by Fourier transform infrared spectroscopy (FT-IR), scanning electron microscopy (SEM). The obtained antibiotic percentage of sorption was evaluated by quantitative assessment using high-performance liquid chromatography(HPLC) coupled with the Ultraviolet Detector. In order to optimize the operating conditions, the effects of pH, Time contact, Agitation speed, adsorbent dosage, and antibiotics initial concentration were investigated by taquchi experimental design method [1]. The data were fitted tothe Pseudo first-order kinetic, Pseudo second-order kinetic, Langmuir, Freundlich and Dubinin-Radushkevich (D-R) equation to estabilish the sorption kinetics and isotherms of antibiotics removal by MMWCNT [4]. The best percentages of removal were obtained for penicillin 90%, and amoxicillin 86.5%.

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Paper code: 1117

Carbonaceous Materials Functionalization with Multicomponent Reactions: Novel Drug Delivery Platforms

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Materials functionalization with multicomponent reactions (MCRs) has definitely grabbed a lot of attention nowadays due to the integration of outstanding features of MCRs with materials domains for the construction of neoteric bio-functional materials [1]. What causes the MCRs in the spotlight as unparalleled strategies for carbonaceous materials functionalization is their "power of one-pot" which is the dream of many researchers. In this regard and based on our previous researches in this field [2, 3], the extraordinary empirical discovery of single-pot isocyanideand Meldrum's acid-based MCR [4] for the covalent functionalization of graphene oxide (GO) and carbon nanotubes (CNTs) has been reported. Meanwhile, the organic motifs that prepared with this approach are pentaamide structures that fully coated the surface of the carbonaceous materials and make it a great candidate for medicinal applications. The new synthesized pseudopeptide nanohybrids were fully characterized. Importantly, the nanobiohybrids showed unprecedented high and long-term dispersity and stability in water. The performance of the nanobiohybrids for the controlled release of Tenofovir, as a model drug, was investigated and the results depicted slow drug release behavior of nanobiohybrids. In addition, biocompatibility and cytotoxicity of nanobiohybrids were examined and no obvious adverse effects on the viability of MCF-7 breast cancer cells were observed. The results manifested its valuable applicability for the emerging drug delivery platforms.

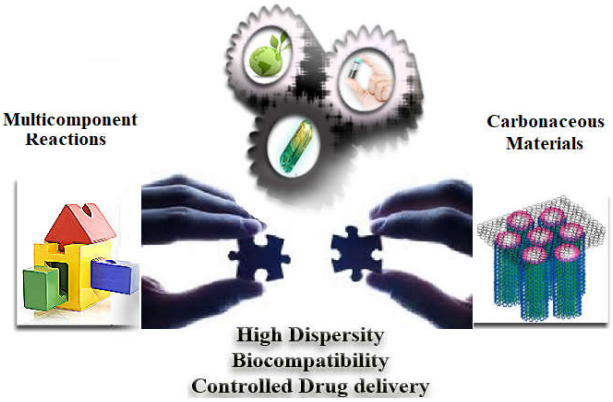

Fig. 1 Multicomponent reactions as novel versatile tools for functionalization of carbonaceous materials

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Paper code: 1118

Multilinker Phosphorous Acid Anchored En/MIL-100(Cr) as a Novel Nanoporous Catalyst for the Synthesis of New *N*-heterocyclic Pyrimidoquinolines

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Nowadays, solid compounds with crystalline structure formed by inorganic clusters or metal ions (generally transition metals) linked by two or multifunctional organic units, which called metal-organic frameworks (MOFs). In recent years, metal-organic frameworks (MOFs) are valuable materials because of their applications on the preparation of adsorption, catalysis, sensors, electronics, selective separation, fuel cells, petrochemistry, large scale of industrial products and drug delivery [1-2]. *N*-Heterocyclic compounds such as uracil derivatives are one of the important categories of compounds in the organic synthesis. Quinoline and pyrimidine derivatives containing uracil in their structure are interesting classes of organic compounds because of their pharmacological activity including antitumour, cardiotonic, hepatoprotactive, antihypertensive, antibronchitic and antifungal activity. Pyrimido[4,5-*b*]quinolone derivatives are a category of fused quinolines separated from the marine bacteria having antibacterial and antifungal activities [3-4]. In the present research, we explored MOFs chemically modified by organophosphonic acid MIL-100(Cr)/NHEtN($CH_2PO_3H_2$)$_2$ based on En/MIL-100(Cr) by a heterogeneous synthetic method, and used it as a task-specific, recyclable and reusable catalyst for the operational and one-pot synthesis of new *N*-heterocyclic compounds such as tetrahydropyrimido[4,5-b]quinoline-2,4,6(1*H*,3*H*,7*H*)-trione, tetrahydropyrimido[4,5-*b*]quinoline-4,6(3*H*,7*H*)-dione and octahydropyrimido[4,5-*b*]quinolin-6(1*H*)-one derivatives (Fig. 1).

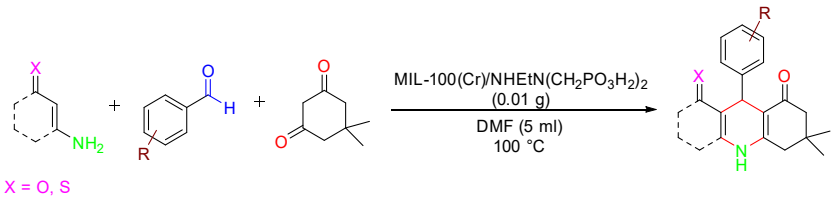

Fig. 1 Synthesis of pyrimido[4,5-*b*]quinolone derivatives using MIL-100(Cr)/NHEtN($CH_2PO_3H_2$)$_2$

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The 26th Iranian Seminar of Organic Chemistry
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12-14 March, 2019

Paper code: 1119

Design, Synthesis and Application of a Novel Nanomagnetic Functionalized Acetic Acid as a Catalyst for theSynthesis of Amidoalkyl phenols

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Activity and reusability of a catalyst should be considered in designing of it. Homogenous catalysts have higher activity than heterogeneous catalysts, but their separation and recycling is more difficult than heterogeneous ones. On the other hand, activity of heterogeneous catalysts is low, however their separation and reusability is easy [1]. 1-Amidoalkyl-2-naphtols have biological importance because they can be converted to 1,3-oxazine [2]. 1,3-Oxazine derivatives have pharmaceutical and biological properties such as anti-tumor, anticonvulsant, antimalarial, analgesic, antibiotic, antianginal, antirheumatic and antihypertensive [3-5]. Herein, we wish to introduce $[Fe_3O_4@SiO_2@(CH_2)_3\text{-im-}CH_2CO_2H]Br$ as a novel nano magnetic catalyst and use it as an efficient and reusable catalyst in the synthesis of amidoalkyl phenols under solvent-free condition (Fig. 1).

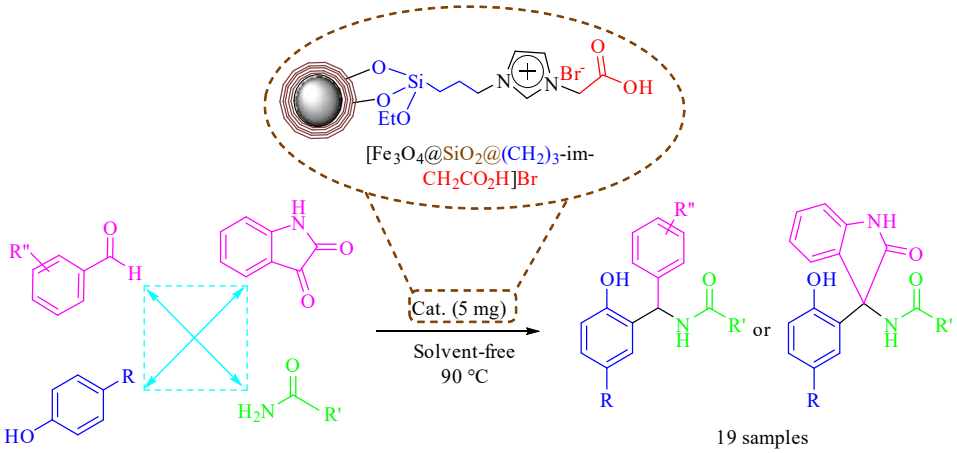

Fig. 1 Preparation of amidoalkyl phenol derivatives using $[Fe_3O_4@SiO_2@(CH_2)_3\text{-im-}CH_2CO_2H]Br$ as a novel nano magnetic catalyst

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Paper code: 1120

Synthesis of New (3′-Indolyl)pyrazolo[3,4-*b*]Pyridine *via* Vinylogous Anomeric Based Oxidation under Mild and Green Conditions

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In recent years, phosphorus acid tag is a valuable synthon due to its application at the preparation of catalysts, inhibitors, metal adsorbent and extractants [1]. Molecules with indole nucleus have attracted great interest due to the very important biological and pharmacologicalactivities, such as antibacterial, antifungal, antiviral, anticonvulsant, cardiovascular, optimal inhibitory, antihypertensive, anticholinergic and antiproliferative activities [2-3]. Pyridine moiety is one of the most important scaffolds which has found in the many pharmaceuticals and natural products due to their biological and medicinal properties such as inhibiting HIV protease, antidepressant, anti-inflammatory, inhibiting acetylcholinesterase, treating hypotension or hypertension [4]. Herein, we wish to develop vinylogous anomeric based oxidation mechanism at the preparation of (3′-indolyl)pyrazolo[3,4-*b*]pyridines from aryl aldehydes, 3-(1*H*-indol-3-yl)-3-oxopropanenitrile and 3-methyl-1-phenyl-1*H*-pyrazol-5-amine in the presence of a catalytic amount of melamine hexakis(methylene)hexakis(phosphonic acid) [MHMHPA] under mild and green conditions (Fig. 1).

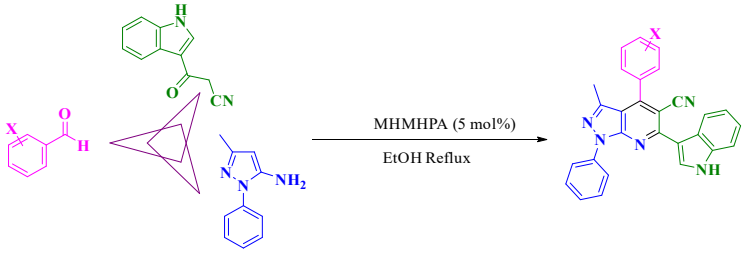

Fig. 1 Catalytic synthesis of (3′-indolyl)pyrazolo[3,4-*b*]pyridines in the presence of MHMHPA

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Paper code: 1121

Synthesis and Application of a Novel Ionically Tagged Polymer as a Nano-Heterogeneous Catalystfor Synthesis of *N*-Heterocycle Spiropyrans under Mild and Green Conditions

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Nowadays, ionically tagged polymers including cations such as imidazolium, pyrrolidonium, pyridinium and anions such as tetrafluoroborate, hexafluorophosphate, triflates incorrectly have been called polymeric ionic liquids PILs [1] .Organic and biological based solid acids are one of the most applicable compounds which have been used for acid-promoted processes and chemical methodologies. Solid acids have received great attention as general materials for a variety of chemical processes because of their reasonable properties such as nonmetallic, nontoxic, with no generated hazardous waste, reusability and high turnover [2]. Recently, application of solid acids with sulfonic acids tags as catalysts comprehensively reviewed [3]. The research and application of various multi-SO_3H functionalized solid acids are interesting due to their nano structures, Brønsted acidic and environmentally friendly, good candidates for replacing of conventional solid acids, which could be used as a catalyst and reagent [5]. Spiro compounds as drug candidates are target molecules for pharmaceutical investigations. The unpleasant effects of oxidative stress on human health have become a serious issue. Herein, a novel ionically tagged polymer was synthesized and used as an efficient and reusable catalyst for the synthesis of spiropyran derivatives (Fig. 1).

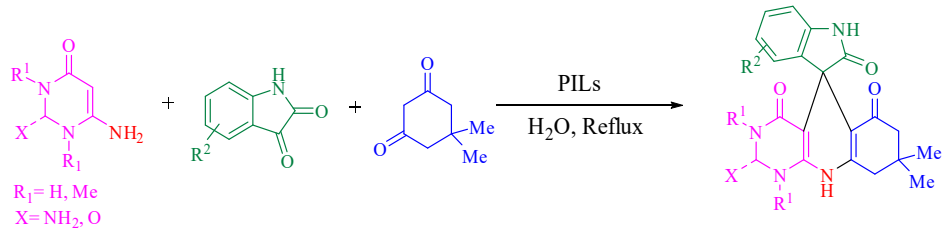

Fig. 1 Synthesis of *N*-heterocycle spiropyrans derivatives usingPILs

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Paper code: 1122

Synthesis of Pyridinioum Based Nano Molten Salts as Dual Role Catalysts: Application for the Synthesis of *O*-Heterocycle Compounds

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Nowadays, diversity of ionic liquids (ILs) or organic molten salts (MSs) can be achieved via anion exchange and is a subjective way for designing ILs and MSs with anions that cannot be directly prepared. Over the years, much attention has been paid to the study of exchanges in the properties of ILs and MSs by the replacement of their counter ions, which is changing physical and chemical properties such as viscosity, melting point, vapor pressure of fluids and fluorescence properties [1-2]. Ionic Liquids and molten salts as efficient solvents, catalysts and reagents have been applied for nitration reaction, regioselective sulfonation, preparation of high-energy compounds and organic synthesis under milder conditions [3-4]. Herein, we applied an anion exchange method for the synthesis of nano molten salts [$PySO_3H$]X as magnetic (with magnetic counter ion) and non-magnetic catalysts. These nano molten salts [$PySO_3H$]X utilized as efficient and reusable catalysts for the synthesis of a wide range of *O*-heterocyclic compound (Fig. 1).

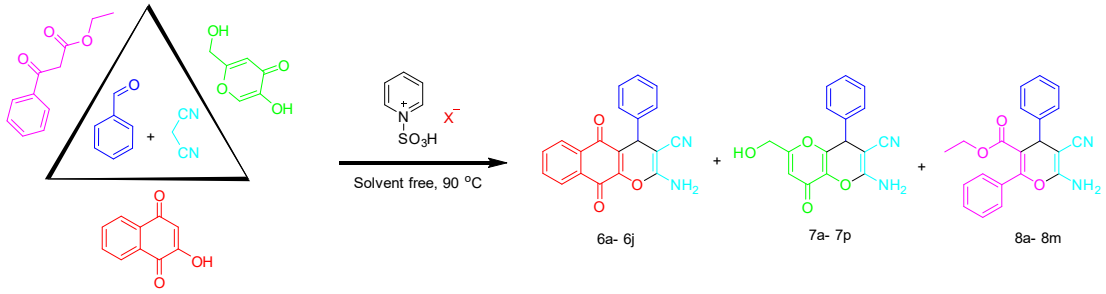

Fig. 1Synthesis of *O*-heterocyclic compounds using [$PySO_3H$]X

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Paper code: 1123

Synthesis and Antibacterial and Antifungal Evaluation of Novel Dithiocarbazinate Derivatives

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Dithiocarbazinate derivatives are key intermediates in the synthesis of a wide variety of biologically active heterocyclic compounds. In addition, they were applied as ligands in for complex formation with transition metals. For example, dithiocarbazinate provides intermediates for the production of novel 1,2,4-triazole derivatives as potential anticancer, antioxidants, antibacterial and antifungal agents [1-3]. The resistance of bacteria and fungi to antibiotics is still increasing and can be a serious threat to human health in the future. New antimicrobial agents must be designed and identified to confront these pathogens. In this research project, different alkyl or aryl hydrazides were reacted with carbon disulfide in the presence of potassium hydroxide in absolute ethanol to afford dithiocarbazinate compounds (Fig. 1). The molecular structurs of all synthesized compounds were characterized with IR, ^{1}H NMR, ^{13}C NMR spectra. Inhibitory activities of synthetic compounds were assessed on some pathogenic bacteria and fungi. The results were reported as MIC (Minimum Inhibitory Concentration), MBC (Minimum Bactericidal Concentration) and MFC (Minimum Fungicidal Concentration) values. The result of this study showed that dithiocarbazinate compounds are potential antibacterial andantifungal agents due to their significant inhibitory effects.

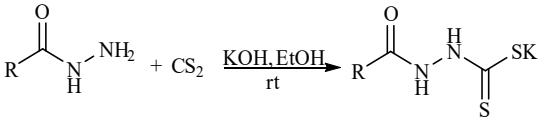

Fig. 1 Multicomponent synthesis of dithiocarbazinate

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12-14 March, 2019

Paper code: 1124

Application of MIL-101(Cr) in the Synthesis of *N*-Amino-2-pyridones and 1,4-Dihydropyrano[2,3-c]pyrazoles

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In recent years, metal–organic frameworks (MOFs) have been considered as a new category of nano-porous materials which are suitable for storage and separation of gases, catalysts, heavy metal adsorbents. MOFs, based on the type of ligand and functional groups on their surface, exhibit various properties. MOFs exhibit a unique catalytic role in the preparation of hydrogen and methane gas and the synthesis of a wide range of chemical and pharmaceutical compounds [1-2]. *N*-Amino-2-pyridones and 1,4-dihydropyrano [2,3-c]pyrazoles have been applied to the treatment of rheumatoid arthritis, psoriasis, cancer, Parkinson's disease, Huntington's disease, Alzheimer's disease, Down's syndrome, AIDS, schizophrenia, and myoclonus as well as demonstrating biological properties such as antiviral, , pheromonal, and central nervous system activity [3-4]. In this work, we have designed and synthesized a MOF, MIL-101(Cr), as an efficient catalyst for promoting the described four components reactions under refluxing water conditions (Fig. 1).

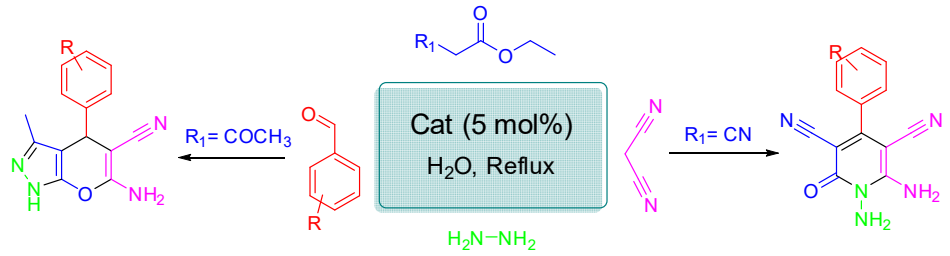

Fig. 1 Synthesis of *N*-amino-2-pyridones and 1,4-dihydropyrano [2,3-c]pyrazoles using MIL-101(Cr)

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12-14 March, 2019

Paper code: 1125

A New Ecofriendly Methodology for the Synthesis of Spiro-Oxindole Derivatives *via* Alcoholic Extract of Angustifolia Leaves as the Solvent and Catalyst

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The spiro-oxindole indwells a special place in heterocyclic chemistry because of the attendance of this 'privileged structure' in a wide spectrum of natural products , medicinal and organic chemistry [1]. Spiro-oxindole scaffold represents the pharmacological properties such as anti-tumor, anti-fungal, anti-microbial, anti-oxidant, anti-malarial, due to its unique chemopreventive and biological activities of the spiro-oxindole skeleton, the expansion of synthetic methods providing facile reaches to this heterocycle are still favorable [2-4]. Herein, we report Angustifolia leaf extract as a new catalyst to a known synthesis of spiro-oxindole derivatives via condensation of malononitrile, isatin derivatives, and 1,3-dicarbonyl compounds under mild reaction conditions (Fig. 1). This efficient and green methodology has a number of advantages such as short reaction time, high yields (87–95%), use an alcoholic extract of Angustifolia leaves as the solvent and catalyst, simple workup procedures and avoidance of hazardous or toxic catalysts and organic solvents. Chemical structure of all desired structures was identified by melting points and spectral data and elemental analyses.

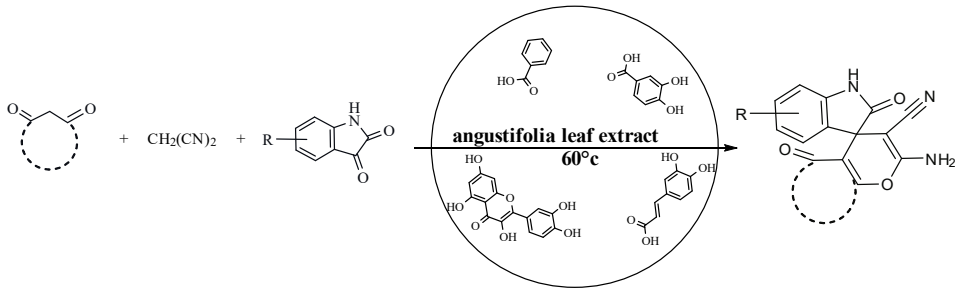

Fig. 1 Synthesis of spiro-oxindole-pirane derivatives in Angustifolia leaf extract

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Paper code: 1126

$Co(NO_3)_2$: An Efficiental Catalyst for Synthsis of Dihydropyrimido[4,5-*b*]quinolinetrione Derivatives Using a Multi-Component Reaction

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Pyrimidine derivatives have a biological and medicinal activity such as anticancer and anti-human immunodeficiency virus (HIV). Pyrimidine fused heterocycles have attracted great interest and biological activities such as inflammatory, antioxidant, anticancer, antitumour, antimicrobial, and antiviral actions from pyrimidine fused heterocycles have been reported. Many of alkaloids, drugs, antibiotics, agrochemicals, and natural products contain pyrimidine fused heterocycles [1]. Multicomponent reactions (MCRs) are an attractive strategy, in the field of medicinal chemistry and used to obtain desired biologically active compounds [2]. In this study $Co(NO_3)_2$ has been introduced as efficient catalyst for synthesis of the novel 8,9-dihydro-8,8-dimethyl-5,10-diphenylpyrimido[4,5-*b*]quinoline-2,4,6(1*H*,3*H*,5*H*,7*H*,10*H*)-trionederivatives via a four-component reaction of aldehydes, amines, dimedone, and barbituric acid with high efficiency and sutable time.

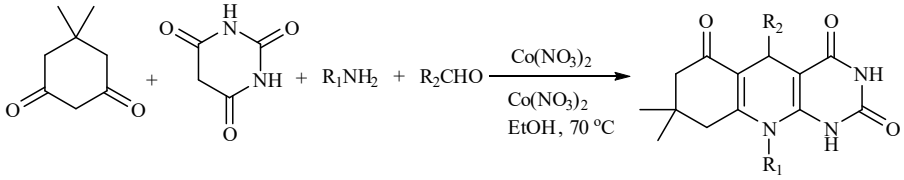

Fig. 1 Multicomponent synthesis of 8,9-dihydro-8,8-dimethyl-5,10-diphenylpyrimido[4,5-*b*]quinoline-2,4,6(1*H*,3*H*,5*H*,7*H*,10*H*)-trione with $Co(NO_3)_2$ as catalyst

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12-14 March, 2019

Paper code: 1127

Green Multicomponent Synthesis of Pyrido[2,3-d]pyrimidine Derivatives Catalyzed by a Novel LDH Modified Clinoptilolite Nanocatalyst

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Fused pyrimidine derivatives have participated in the structure of various medicinally significant compounds especially as the privileged motifs for anticancer agent's design purposes [1]. Among fused pyrimidine derivatives, pyrido [2,3-d]pyrimidines have been the subject of study in recent years for their diverse bioactivity effects [2, 3]. In the present study, some novel pyrido [2,3-d]pyrimidine derivatives were synthesized through a green and efficient multicomponent procedure in the presence of a novel prepared LDH modified Clinoptilolite nanocatalyst. 4(6)-Aminouracil derivative, malononitrile, benzaldeyhyde derivatives were used as starting materials in the presence of the designed nanocatalysts in DMF as medium. This protocol has been previously reported under several reaction conditions [4]. The reactions were carried out smoothly and the products were obtained with good to excellent yields within relative short reaction times. The nanocatalyst was easily separated by centrifugation from the reaction mixture. The products were simply obtained by aqueous dilution of the organic layer and washed with hot ethanol whenever necessary.

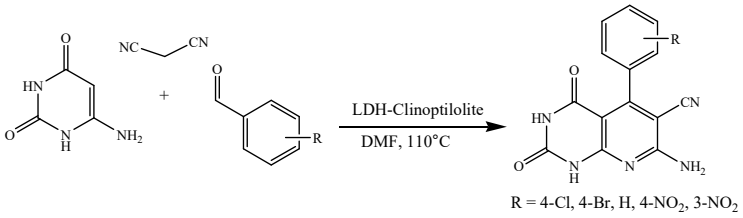

Fig. 1 Efficient multicomponent synthesis of pyrido[2,3-d]pyrimidine derivatives catalyzed by a novel LDH modified Clinoptilolite nanocatalyst

References

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Paper code: 1128

Core-Shell Fe_3O_4@SiO_2-SO_3H Nanoparticles as Efficient Catalyst in the Synthesis of Dihydropyrano [3,2-c]chromenes

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Pyrano[3,2-c]chromenes have received considerable attention in medical chemistry due to their unique biological and pharmacological properties. They exhibite biological activities such as anticancer, anti-inflammatory, antimicrobial, and antihyperglycemic activities. [1-3]
Paying attention to green chemistry concept efforts are conducted to use less toxic chemicals and less organic solvents in synthetic chemistry. Therefore, one pot multi-component reactions are receiving more attention as an alternative for multi-step reactions. The synthesis of pyrano[3,2-c]chromenes via multicomponent requires long reaction time while giving moderate production yields. However, employing a proper catalyst may boost the yield in shorter reaction time.
In the current research paramagnetic core-shell nanoparticles of Fe_3O_4@SiO_2 and sulfuric acid-functionalized one (Fe_3O_4@SiO_2-SO_3H) were synthesized and characterized by FT-IR, XRD, and SEM. [2,3] They have been employed as catalysts in one pot synthesis of dihydropyrano[3,2-c]chromenes via reaction of 4-hydroxycoumarin, malononitrile and a wide range of functionally substituted benzaldehydes. Catalyst Fe_3O_4@SiO_2-SO_3H which showed higher activity was separated from the reaction mixture and reused for three times without loss in its catalytic activity.

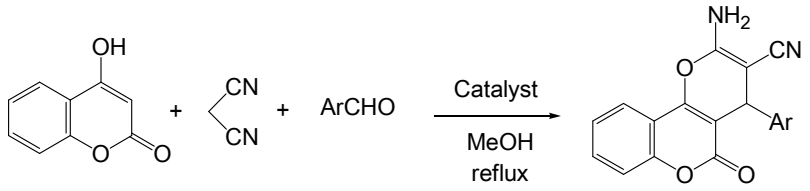

Fig. 1 One-pot multi-component synthesis of 3,4-dihydropyrano[3,2c]chromenes

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12-14 March, 2019

Paper code: 1129

Synthesis of Hydrophobin-Coated Niosome for Stealth Delivery of Anti-cancer Drugs

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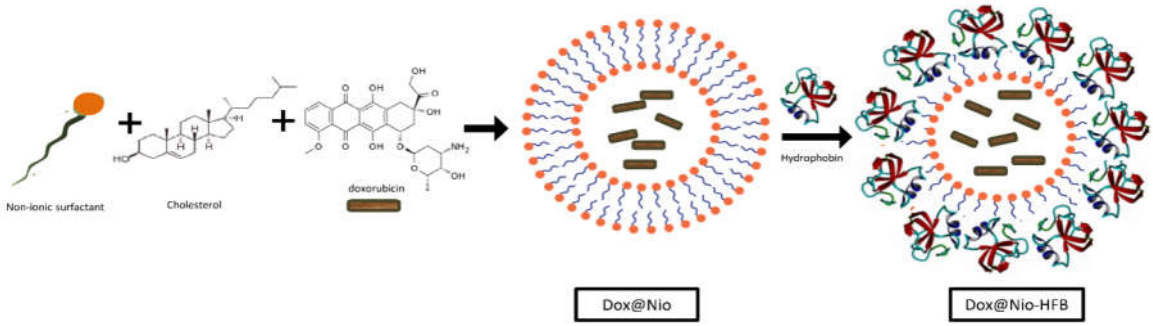
HFB-1 on the surface of fungal spores plays a role in the lack of antigen recognition by the host immune system [1]. The present study aimed to evaluate the hydrophobin-1 (HFB-1)–coated niosome formulations based on Span 40 and Tween 40 non-ionic surfactants to analyze the potential application of this novel formulation for the stealth delivery of doxorubicin (Dox) into the MCF-7 cell line [2]. The surface layer of HFB-1 on the niosomes leads to the hypothesis that these proteins could confer shielding against immune-system recognition in vivo and prevent the immune response. Thus, HFB-1 became a promising alternative to PEG. Here, Dox-loaded niosome was prepared using the thin-film hydration (TFH) method [2]. Physicochemical characteristics of constructed formulations analyzed in different pH (2, 5.2 and 7.4) (because of different pH values in the path of arriving the carrier to its target) from the aspects of the size, zeta potential, polydispersity index, morphology, entrapment efficiency (EE), and in-vitro cytotoxicity. Results showed that loaded niosomes exhibited a small mean size (338±3.14 – 593±3.12 nm), narrow size distribution, negative zeta potential, high EE (45±1.67 – 75±1.22), and high antitumor activity. By coating HFB-1 on niosomes, the size, stability, and EE% of the niosomes increased. Also, the HFB-1-coated niosomes had a more sustained release profile in comparison to niosomes without an HFB-1 shell. Our findings suggest that this drug delivery system that uses HFB-1-coated niosomes can be an efficient drug delivery system for the treatment of cancer.



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Paper code: 1130

Synthesis of 3,4-Dihydropyrimidin-2(1*H*)-ones using Boric Acid Aqueous Solution System

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Preparation of 3,4-dihydropyrimidin-2(1*H*)-one (DHPMs) are significant due to their therapeutic and pharmacological properties [1]. The Biginelli reaction was introduced for the first time by Pietro Biginelli [2]. In this reaction, 3,4-dihydropyrimidin-2(1*H*)- ones (DHPMs) were prepared by three-component condensation reaction of aldehyde, urea and *ß*-ketoester as interesting compounds with a potential for pharmaceutical applications. Various catalysts were reported for this reaction such as [bmim][$MeSO_4$] [3], $FeCl_3$ [4], $RuCl_3$ [5], and TMSCl [6]. Due to important properties of these compounds, finding the new methods for the synthesis of 3,4-dihydropyrimidin-2(1*H*)-ones are still needed. Herein, we have reported the preparation of 3,4-dihydropyrimidin-2(1*H*)-ones in the presence of boric acid, at 90 °C under aqueous conditions (Fig. 1). The prepared compounds were identified by ^{1}HNMR, ^{13}C NMR and IR analysis.

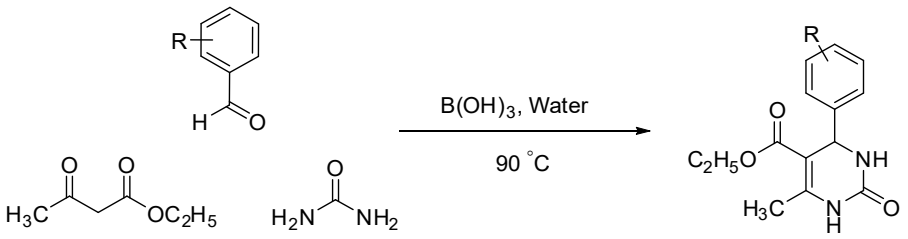

Fig. 1 The one-pot three-component synthsis of 3,4-dihydropyrimidin-2(1*H*)-ones using boric acid

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12-14 March, 2019

Paper code: 1131

Synthesis of Polycyclic 1,4-Dihydropyridine Derivatives in the Presence of a Ionically Tagged Nanomagnetic Catalyst

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Polycyclic 1,4-dihydropyridine derivatives are very important class of heterocyclic molecules as they represent remarkable pharmacological behavior. This versatile structure can be applied for treatment of Alzheimer's disease. Also, they applied as anti-tumor, anti-diarrhea and antimicrobial agent [1]. On the other hands, one-pot multicomponent strategy has an influential position in the domain of green chemistry. This manner presents diverse merits such as effective and rapid production of desired molecules accompanied with economic and ecological insight [2-3]. In this research project, we decided to present an easy and applicable synthetic procedure for the preparation of polycyclic 1,4-dihydropyridine derivatives in the presence of a ionically tagged nano magnetic catalyst (Figure 1).

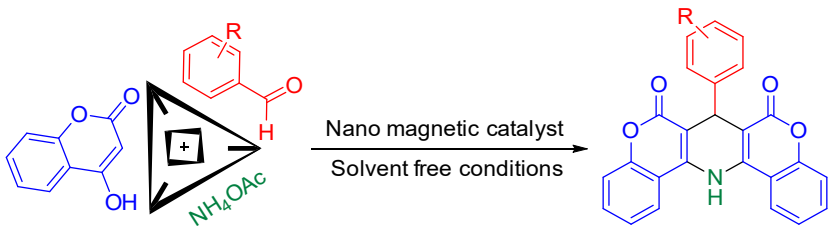

Fig. 1 Synthesis of polycyclic 1,4-dihydropyridine derivatives using a ionically tagged nano magnetic catalyst

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12-14 March, 2019

Paper code: 1139

Synthesis of a Novel and Reusable Acidic Nanomagnetic Catalyst: Application for the Synthesis of New 2-Amino-3-cyanopyridines *via* Vinylogous Anomeric Based Oxidation

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Functionalized nanomagnetic catalysts represent paramount characteristics such as high surface to volume ratios, high surface energies, enhanced dispersion, high catalytic performance, easy recoverability, and reusing without loss of their catalytic activity which these parameters make them versatile apparatus in the different fields of science [1-2]. Among the functionalized pyridine systems, 2-amino-3-cyano pyridine derivatives are prevalent. 2-Amino-3-cyano pyridines are versatile intermediates towards the synthesis of varied heterocyclic molecules such as vitamins [3]. In this study, we have reported the synthesis and catalytic application of a novel magnetically separable catalyst at the preparation of amino-3-cyano pyridines *via* vinylogous anomeric based oxidation (Figure 1).

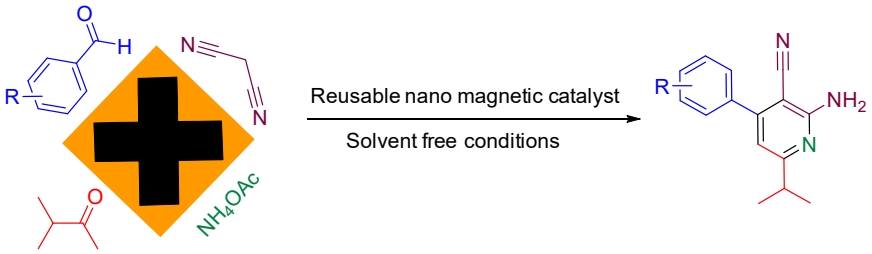

Fig. 1 Synthesis of new 2-amino-3-cyano pyridines using a novel magnetically separable catalyst

References

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Paper code: 1140

Novel Phosphonium Based Ionic Liquid Catalyzed One-Pot Multicomponent Synthesis of 2-Oxo-4,6-diphenyl-1,2-dihydropyridine-3-carbonitrile Derivatives

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Compare with conventional multi-step preparation processes, multi-component reactions represent elegant advantages such as convergence nature, facile automation, simplicity of operational protocols, reduce the number of work-up steps, minimizing waste production, and rendering the transformations based on green chemistry metrics [1-2]. On the other hands, ionic liquids represent unique features including excellent thermal and chemical stability, high electrochemical properties, good solubility, excellent potent of recyclability [3]. In this exploration, we combined the elegant characteristic of multicomponent reaction process and ionic liquids to present a facile synthetic routs for the preparation of 2-oxo-4,6-diphenyl-1,2-dihydropyridine-3-carbonitrile derivatives under mild reaction conditions (Figure 1).

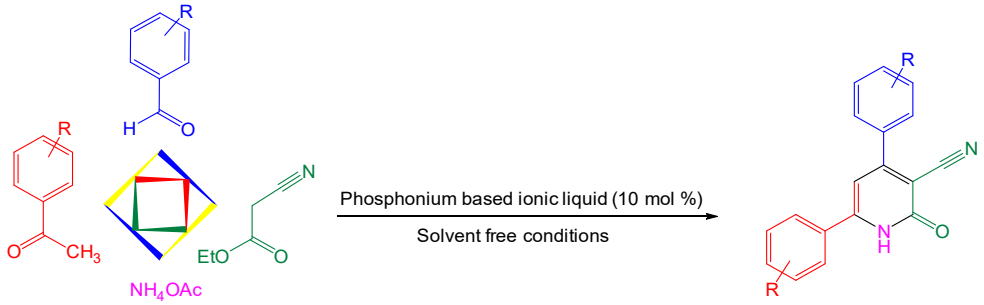

Fig. 1 Synthesis of 2-oxo-4,6-diphenyl-1,2-dihydropyridine-3-carbonitrile derivatives using phosphonium based ionic liquid as catalyst

References

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12-14 March, 2019

Paper code: 1142

Multi-Component Reactions for the Synthesis of Arylsulfonyl hydrazide Derivatives

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Most of the biologically active compounds include sulfonamides, and they are an important class of drugs showing various activities such as antimicrobial, antitumor, anticonvulsant, anticancer, anti-inflammatory, antidiuretic, antihydrod, insulin-releasing and hypoglycemic. They also act as inhibitors, e.g., histone deacetylase (HDAC), carbonic anhydrase and HIV protease. The chemotherapeutic derivatives of this class are extensively employed as antibacterial and antiviral agents. Since, they are structural analogues of *p*-aminobenzoic acid necessary for the production of folic acid. If they are substituted for *p*-aminobenzoic acid, the production of folic acid stops and ultimately bacterial growth stops. Sulfonyl hydrazones exhibit interesting chemical properties and are useful intermediates in organic synthesis.

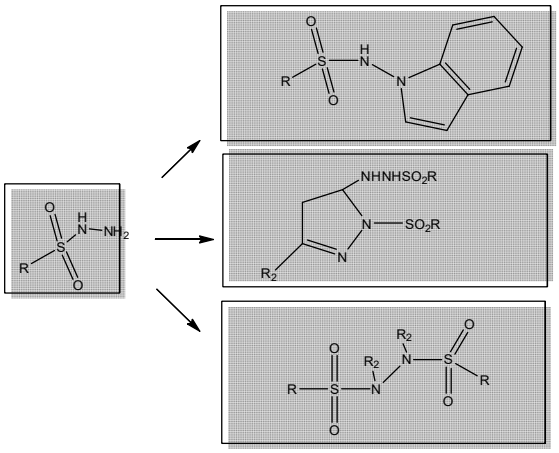

Fig. 1 Multicomponent synthesis with aryl sulfonyl hydrazides

References

[1] A. Siddiqa, A. Rehman, M.A. Abbasi, S. Rasool, *Tropical Journal of Pharmaceutical Research*, **2014**, 13 (10):1689-1696.
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The 26th Iranian Seminar of Organic Chemistry
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12-14 March, 2019

Paper code: 1144

Application of Dendrimer-Coated Magnetic Nanoparticles as a Heterogeneous and Reusable Catalyst for the One-Pot Synthesis of Acridinedione Derivatives

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Acridinediones are heterocyclic compounds containing nitrogen that are the core structure of a number of biologically interesting compounds. They contain a 1,4-dihydropyridine ring similar to nicotinamide adenine dinucleotide. Furthermore, acridinedione derivatives are known to be biological agents with anti-fungal, anti-tumor, anti-cancer, and anti-glaucoma properties [1]. There are many reported methods for the synthesis of acridinedione derivatives including multi-component condensation. In this paper, an efficient and green method for the synthesis of acridinedione derivatives via a one-pot, multi-component condensation of dimedone, various aromatic aldehydes and various aromatic amines using dendrimer super acidic magnetic nano particles as a heterogeneous nano catalyst under ambient and solvent-free conditions is described (Fig. 1) [2, 3]. Simple procedure, high yields, short reaction times and reusability of the catalyst are advantages of this protocol. The Synthesized compounds are characterized using spectroscopic (IR, ^{1}H-NMR) techniques.

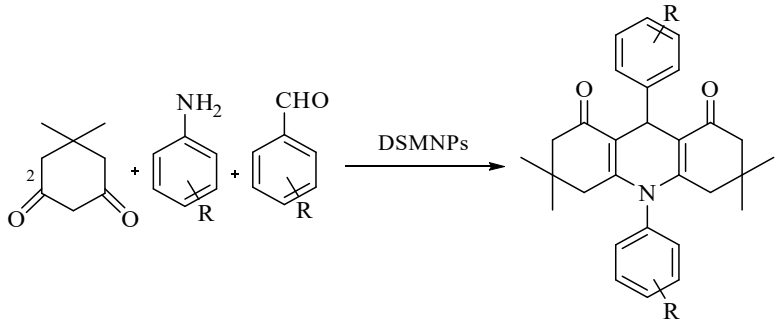

Fig. 1 Multicomponent synthesis of Acridinedione derivatives using DSMNPs

References

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Paper code: 1145

Organocatalyzed Synthesis of Dihydropyrimidinone/Thiones *via* Biginelli Condensation Reaction

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Compounds containing 3,4-dihydropyrimidonone/thione frameworks are best known for their biological and pharmacological activities. Due to the therapeutic properties of some 3,4-dihydropyrimidonones (DHPMs) and their applications in the pharmaceutical industry, discovery efficient and cost-effective methods for the synthesis of these compounds is a concern of many organic chemists. In general, the main method for the synthesis of DHPMs is a one-pot multicomponent reaction (MCR) of 1,3-dicarbonyl compounds, various aldehydes, and urea/thiourea derivatives called Biginelli reaction. Generally, this MCR has been catalyzed using various reagents such as Lewis acids, organoacids, organic and inorganic bases, inorganic acids, nanomaterials, supported catalysts, and metal-organic frameworks [1-3]. In the present work, we have synthesized 2-benzyl-1-sulfopyridin-1-ium *via* sulfonation processand used it to the synthesis of DHPMs through a MCR technique. The three-component reaction of ethyl acetoacetate, various aromatic aldehydes, and urea/thiourea under solvent condition in the presence of 2-benzyl-1-sulfopyridin-1-ium led to the formation of 3,4-dihydropyrimidonone/thione heterocycles in good to excellent yields (Fig. 1). This procedure has notable features, including relatively shorter reaction times, simplicity, and environmentally friendliness.

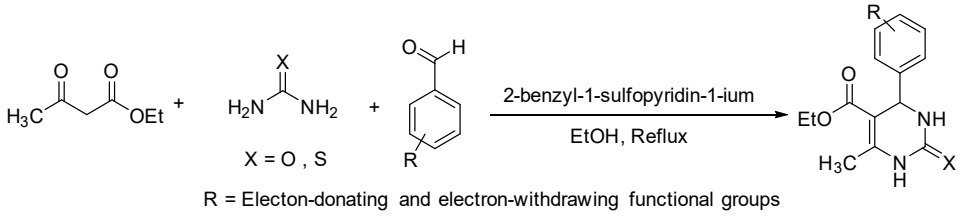

Fig. 1 The MCR synthesis of 3,4-dihydropyrimidonone/thiones

References

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Paper code: 1147

Green and Expeditious Synthesis of Isoxazol-5(4*H*)-ones *via* Three-Component Reaction

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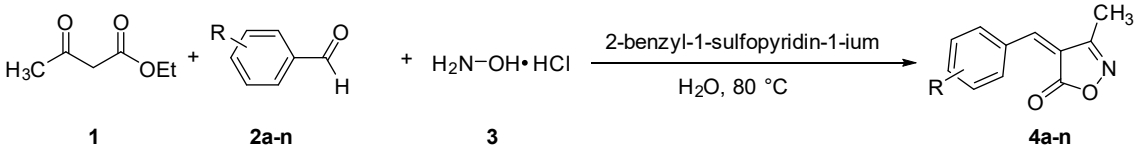
Organosulfonic acids demonstrate an important generation of organocatalysts in organic synthesis, which have been successfully applied in different types of acid-catalyzed organic transformations [1]. Isoxazole and its derivatives are good synthetic targets on account of their important applications, including pharmaceutical functions in medicine as antimicrobial, antiviral, anticancer, anti-inflammatory, immunomodulatory, anticonvulsant or anti-diabetic agents, pest control in agriculture, and also convertible to other heterocyclic compounds through catalytic processes [2]. Multi-component reactions (MCRs) are one of the most synthetically areas in modern organic synthesis for the synthesis of high levels of molecular diversity from three or more substrates with a minimal number of operations. Some obvious advantages of MCRs include atom-, and step-economy, cost-effectiveness, no need for isolation of intermediates, and manufacture of heterocyclic compounds with high diversity in one synthetic step. These characteristics together with the associated reduction of waste make a greener alternative to multistep synthesis [3]. In the present work, catalytic amounts of 2-benzyl-1-sulfopyridin-1-ium have been used for the synthesis of isoxazol-5(4*H*)-ones through a MCR procedure. This eco-friendly, one-pot, three-component process was performed using ethyl acetoacetate, various aromatic aldehydes, and hydroxylamine hydrochloride as reactants, and above-mentioned catalyst under aqueous conditions (Fig. 1). The heterocyclic products were obtained in good to excellent yields and relatively shorter reaction times.



R: H, 3-NO_2, 4-CH_3, 4-CH_3O, 4-NO_2, 3-Cl, 3-OH, 2-OH, 4-OH, 4-$N(CH_3)_2$, 3,4-di-CH_3O, 2-OH-3-CH_3O, 4-OH-3-CH_3O, 3,4,5-tri-CH_3O,

Fig. 1 MCR synthesis of isoxazol-5(4*H*)-ones

References

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12-14 March, 2019

Paper code: 1148

Magnetic Nanoparticles with Acidic Tags Promoted the Synthesis of Pyridine Derivatives *via* Vinylogous Anomeric Based Oxidation under Mild Conditions

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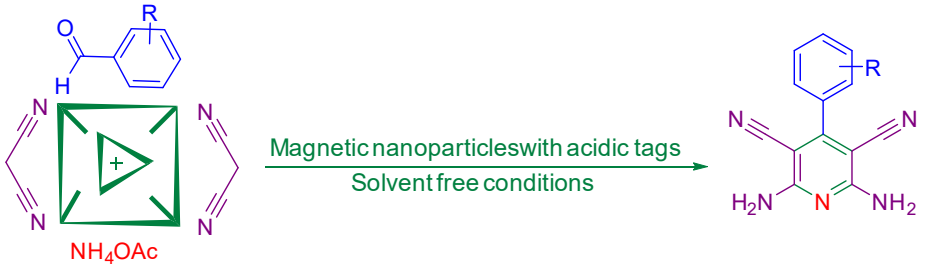
Nowadays, due to the biological importance of pyridine derivatives, these versatile molecules have found several applications in both medicinal and industrial fields. Highly substituted pyridines are applied as nonlinear optical materials, electrical materials, chelating agents and fluorescent liquid crystals. Also, these heterocyclic structures represent varied pharmaceutical activities. Pyridine derivatives can be found in several biologically active compounds, like antitumoral 2-amino-4-aryl-6-dialkylamino-3,5-dicyanopyridines and antiproliferative 2,6-dibenzylamino-3,5-dicyanopyridines [1-3]. In this study, a green protocol has been reported for the synthesis of highly substituted pyridine derivatives using magnetic nano particles with acidic tags as recoverable catalyst under solvent free conditions via a vinylogous anomeric based oxidation mechanism. The reported method represents varied merits such as clean reaction profile, short reaction time, high to excellent yields and simple workup procedure.



R= H, 4-Me, 4-OMe, 3,4-$(OMe)_2$, 4-Cl, 2-Cl, 4-Br, 4-CF_3

Fig. 1 Catalytic synthesis of pyridine derivatives *via* anomeric based oxidation process

References

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12-14 March, 2019

Paper code: 1149

Synthesis of Quinoline-3-carbonitrile Derivatives in the Presence of a Novel and Reusable Nanomagnetic Catalyst

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One of the interesting choices for the heterogenization of the homogeneous catalysts is the stabilization of catalytic active structure onto the surface of magnetic nanoparticles such as Fe_3O_4 nano particles. This process is an efficient strategy to overcome difficulties connected to cumbersome process of isolation and separation of the homogeneous catalytic system [1-2]. On the other hands applying one-pot multicomponent reactions strategy for the rapid synthesis of target molecules accompanied with economic and ecological insight in highly valuable [3]. In this investigation we combined excellent merits connected with nano magnetic heterogeneous catalysts and one-pot multicomponent reactions strategy and present an applicable route for the synthesis of quinoline-3-carbonitrile derivatives under mild reaction conditions (Figure 1).

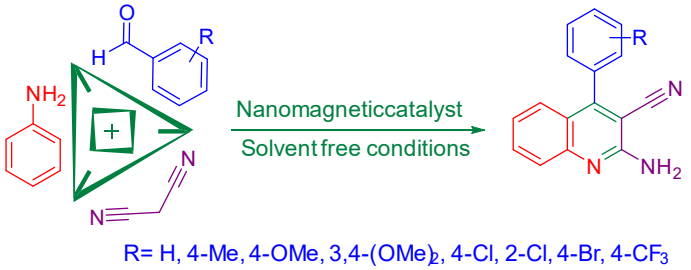

Fig. 1 Catalytic synthesis of pyridine derivatives *via* anomeric based oxidation process

References

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Paper code: 1150

Biological Based DES Shows Brilliant Catalytic Activity at the Synthesis of Linked Pyridine Derivatives

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Deep eutectic solvents (DESs) rapidly emerging in the domain of green chemistry area as green alternatives for hazardous and volatile common organic solvents. These compounds represent varied merits including availability, non-toxicity, biodegradability, recyclability, flammability, and inexpensive [1-2]. On the other hand, linked pyridine derivatives are ubiquitous within the nature and have a significant location in the pharmaceutical and medicinal industries and can applied for different goals such as anti-tumor, analgesic, anti-inflammatory, antipyretic, anti-microbial and cardiotonic activities [3]. In this investigation, we present an elegant strategy for the preparation of linked pyridine derivatives using biological based DES (Fig. 1).

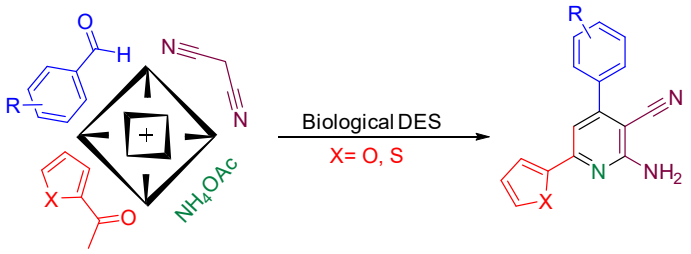

Fig. 1 Synthesis of new 2-amino-3-cyano pyridines using biological based DES

References

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Paper code: 1151

Co(II)@KCC-1 as a Novel Metal Salen Complex for the Synthesis of Spirooxindole Derivatives

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Homogeneous metal salen complexes were developed for the synthesis of a variety of organic compounds. Despite good catalytic activity, some drawbacks such as contamination of products and tedious work up as well as lack of economic efficiency restricted the use of these catalysts. Covalent attachment of metal salen complexes on a solid support such as polymer, zeolite and silica have recently been reported as innovation in the catalytic properties of such compounds [1]. Fibrous Nano-Silica (KCC-1) which has excellent physical properties, including high surface area, fiber morphology, good thermal properties and high mechanical stability are a good candidate for supporting metal salen complexes [2]. On the other hand, the oxindole compounds containing a spiro-cyclic stereo center are an important class of oxygen-containing heterocycles and medicinal scaffolds which are widely distributed in natural compounds such as alkaloids as well as synthetic drugs. Spirooxindoles have a wide range of biological activities including antiviral, anticancer, anti-inflammatory and antimicrobial activities [3]. Therefore, the synthesis of spirooxindole derivatives is still the subject of extensive research. In this study, we synthesized the Co(II) salen complex and supported on KCC-1 corresponding Co(II)@KCC-1 and the synthesis of spirooxindole derivatives was investigated in the presence of this catalyst in green media (Fig. 1).

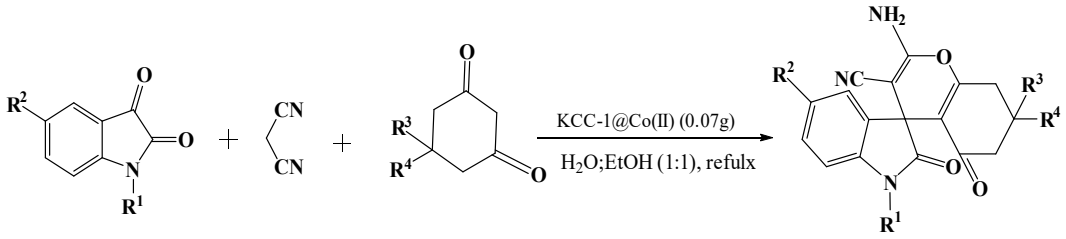

Fig. 1 The synthesis of spirooxindole derivatives was investigated in the presence of Co(II)@KCC-1 in green media

References

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Paper code: 1152

Zr-based MOF as a Novel Nanoporous Catalyst for the Synthesis of Dihydropyrido [2,3-*d*]pyrimidines

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As an emerging class of highly ordered crystalline porous materials, metal-organic frameworks (MOFs) with various potential applications have become a new research hotspot in chemistry and materials during the last few decades, which is mainly attributed to their exceptionally high surface area, tunable pores, as well as intriguing functionalities [1]. Some advantages of these porous materials are high surface area, and thermal stability of their chemical structure [2]. The improvement in the stability of MOFs can expand their applicable fields, and make them applicable on the other topics such as catalysis, adsorption and separation, and biomedicine. Zirconium is widely distributed in nature and is found in all biological systems. The rich content and low toxicity of Zr further favor the development and application of Zr-MOFs. Hantzsch 1,4-dihydropyridines (1,4-DHP) are an important class of compounds with vital medicinal value which are used for the treatment of cardiovascular disease such as hypertension and angina pectoris [3]. Indole nucleus is a prominent structural subunit present in many naturally occurring compounds that possess significant pharmacological and biological properties. A number of indole derivatives having heterocycles at the 3-position have been obtained from nature with potential biological activity [4]. Herein, the nano Zr-based MOFs utilized as an efficient and reusable catalyst for the synthesis of a wide range of dihydropyrido[2,3-*d*]pyrimidine compounds (Figure 1).

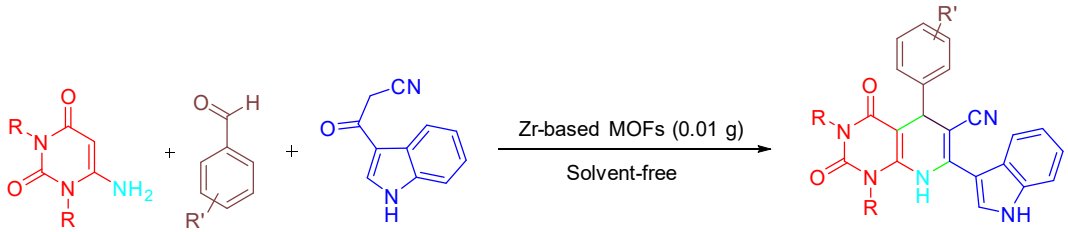

Fig. 1 Synthesis of dihydropyrido[2,3-d]pyrimidine derivatives using Zr-based MOFs

References

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Paper code: 1153

A New Schiff Base Complex of Aminoguanidin Established on γ-Fe_2O_3 for the Synthesis of Hexahydroquinolins

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Hexahydroquinolines (HHQs) are the unsymmetrical derivatives of 1,4-DHPs with an improved structural scaffold and many pharmacological properties such as antihypertensive, antimalarial, antiasthmatic and tyrosine kinase inhibitory activities [1,2]. Generally, HHQs are synthesized by the Hantszch condensation method, which involves a one-pot four-component condensation reaction of aryl aldehydes, β-ketoesters, 1,3-cyclohexanedione derivatives, and ammonium acetate. Several catalysts were reported for the synthesis of HHQs. Even though, synthesis of HHQs could be proceeded by these methods, there still exist some problems related to the use of metal catalysts, expensive reagents, non-recoverable catalysts, difficult work-up, high reaction temperature, long reaction times, and effluent pollution. Therefore, the design of a reusable heterogeneous catalyst for the synthesis of HHQs is a key aspect of achieving the aim of sustainable chemical synthesis. In this paper, in continues of our recent works on the introduction of new heterogeneous catalysts [3,4], we have synthesized a new Schiff base complex of aminoguanidin established on γ-Fe_2O_3.After its characterization by different methods, we have used it as a new heterogeneous catalyst for the synthesis of HHQs by one-pot four-component condensation reaction of aryl aldehydes, β-ketoesters, 1,3-cyclohexanedione derivatives, and ammonium acetate. By this method various HHQs were synthesized in good to high yields. The catalyst was easily isolated by an external magnet and reused five times without any loss in its catalytic activity.

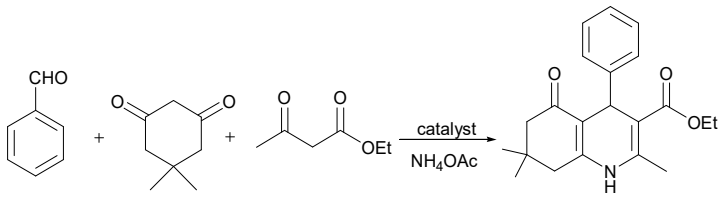

Fig. 1 Synthesis of HHQs via one-pot four-component condensation

References

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12-14 March, 2019

Paper code: 1154

Synthesis of 2-Amino-5-hydroxy Pyrimidines as the Novel Analogues of Tyrosinase Substrate

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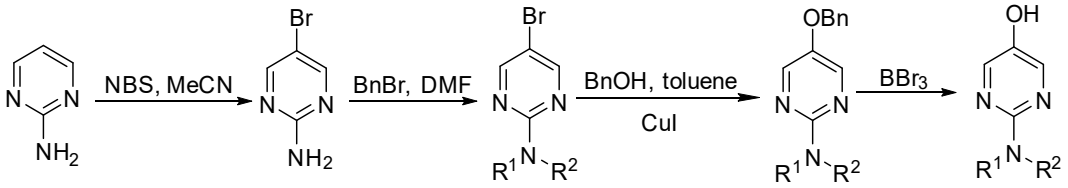
Tyrosinase is an oxidoreductase enzyme which catalyzes *o*-hydroxylation of monophenols into their corresponding *o*-diphenols. It also oxidizes *o*-diphenols to the corresponding *o*-quinones using molecular oxygen. Due to the high chemical activity, o-quinones participate in further chemical reactions and form macromolecules known as melanin which are the core substances of natural pigment of skin, eyes, and hair [1]. The synthesis of *o*-diphenols is a potentially valuable catalytic ability and thus tyrosinase has attracted a lot of attention with respect to industrial applications. Various dermatological disorders, such as melanoma, age spots, and sites of actinic damage arise from the accumulation of an excessive level of epidermal pigmentation originated from hyper activity of tyrosinase. In addition, unfavorable enzymatic browning of plant-derived phenolic compounds by tyrosinase causes a decrease in nutritional quality and economic loss of food products [2]. Consequently, a great deal of research has been directed toward finding compounds that can inhibit tyrosinase activities. Based on the scientific literature in this field, some 5-hydroxy pyrimidine derivatives were designed to work as analogues of tyrosinase substrates.



$R^1 = R^2 = PhCH_2$
$R^1 = H, R^2 = PhCH_2$
$R^1 = R^2 = H$

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The 26th Iranian Seminar of Organic Chemistry
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Paper code: 1155

$CoFe_2O_4@SiO_2$-NH_2-Co^{II}Magnetic Nanoparticles as a Highly Efficient Nanocatalyst for the Synthesis of Spirooxindole Derivatives

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The synthesis of oxindole derivatives as an important type of heterocyclic compounds is still a challenge in the field of organic chemistry and industrial science. Oxindole derivatives possess good biological and pharmaceutical activities [1]. Spirooxindoles have a wide range of biological activities including antiviral, anticancer, anti-inflammatory and antimicrobial activities. Therefore, the synthesis of spirooxindole derivatives is still the subject of extensive research [2]. Numerous homogeneous and heterogeneous catalysts were used for the synthesis of spirooxindole derivatives. In this study, $CoFe_2O_4$ was synthesized from $Fe(NO_3)_3$ and $Co(NO_3)_2$ in aqueous media. Core-shell nanoparticles ($CoFe_2O_4@SiO_2$) were prepared by precipitating silica on the surface $CoFe_2O_4$ [2]. In the following step, functionalization of $CoFe_2O_4@SiO_2$ NPs was performed by the treatment with (3chloropropyl) triethoxysilane and further reaction with triethylenetetramine to afford aminated $CoFe_2O_4@SiO_2$ followed by immobilization of Co^{II} corresponding heterogeneous magnetic nanocatalyst ($CoFe_2O_4@SiO_2$-NH_2-Co^{II}NPs).

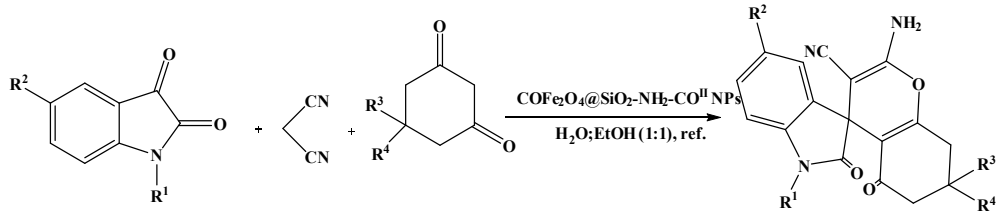

Fig. 1 Spirooxindole derivatives catalyzed by $CoFe_2O_4@SiO_2$-NH_2-Co^{II} magnetic NPs

The synthesis of spirooxindole derivatives was investigated in the presence of $CoFe_2O_4@SiO_2$-NH_2-Co^{II} NPs in H_2O/EtOH (1:1) at reflux conditions and the results shown that the corresponding products were synthesized in excellent yields.

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Paper code: 1156

$CoFe_2O_4@SiO_2$-NH_2-Co^{II} magnetic NPs as a novel, inexpensive and highly efficient magnetic nanocatalyst for aldol-condensation reaction

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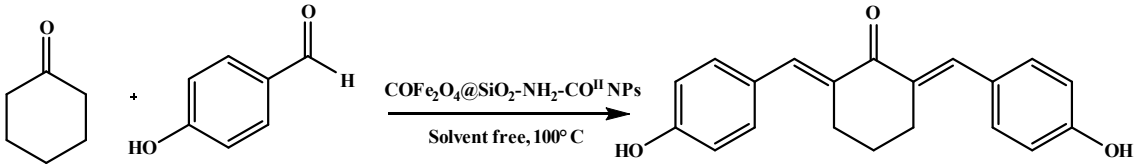
Aldol-condensation as a powerful C-C forming reaction which is used for the synthesis of α, β–unsaturated ketones is an important reaction in the biosynthesis of carbohydrates, and great number of valuable intermediates in organic synthesis [1]. Many solid platform were used for heterogenization of catalysts in the aldol-condensation reactions. Cobalt-ferrite ($CoFe_2O_4$) nanoparticle as a magnetic sold support is a good candidate for the immobilization of homogeneous catalysts. In this study, $CoFe_2O_4$ was synthesized from $Fe(NO_3)_3$ and $Co(NO_3)_2$ in aqueous media. Core-shell nanoparticles ($CoFe_2O_4@SiO_2$) were prepared by precipitating silica on the surface $CoFe_2O_4$ [2]. In the following step, functionalization of $CoFe_2O_4@SiO_2$ NPs was performed by the treatment with (3-chloropropyl) triethoxysilane and further reaction with triethylenetetramine to afford aminated $CoFe_2O_4@SiO_2$ followed by immobilization of Co^{II} Corresponding heterogeneous magnetic nanocatalyst ($CoFe_2O_4@SiO_2$-NH_2-Co^{II} NPs).



Scheme 1: Aldol-condensation reaction catalyzed by $CoFe_2O_4@SiO_2$-NH_2-Co^{II} magnetic NPs

The aldol-condensation reaction was investigated in the presence of $CoFe_2O_4@SiO_2$-NH_2-Co^{II} NPs in solvent free conditions at 100 ^{0}C and the results shown that the α,ά-bis(substituted-benzylidene) alkanones were synthesized in good to excellent yields.

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12-14 March, 2019

Paper code: 1157

Efficient Synthesis of Some New Oxazolone Based Azo Dyes

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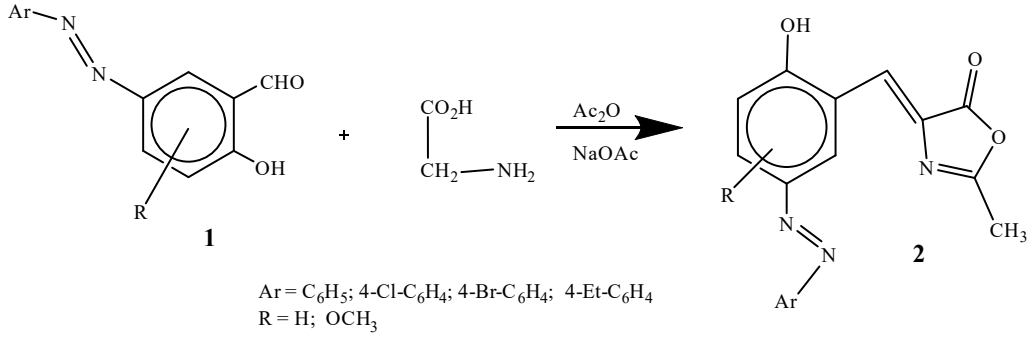
As one of the largest and oldest classes of synthetic industrial dyes, azo compounds have been used in a wide variety of applications including but not limited to textile industry, inkjet printing, LEDs, data storage, dye-sensitized solar cells, sensors [1], and also pharmaceuticals, foods and cosmetics [2]. In continuation of our quest for the synthesis of new azo dyes [3] and our previously reported synthesis on oxazolones [4], herein we wish to report one-pot, solvent free synthesis of oxazolone based azo dyes **2** (Fig. 1). In the present method, 5-aryl azo salicylaldehydes **1** and glycine in the presence of acetic anhydride and sodium acetate can produced oxazolones **2** in fairly high yields. The structure of the products is elucidated from IR, UV, ^{1}H, ^{13}C NMR spectra as well as mass spectral data. Limitation and challenges of this procedure will be presented and discussed.



Ar = C_6H_5; 4-Cl-C_6H_4; 4-Br-C_6H_4; 4-Et-C_6H_4
R = H; OCH_3

Fig. 1 Synthesis of oxazolone based azo dyes

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Paper code: 1158

Synthesis, Antimicrobial and Antioxidant Evaluation of 3-(2-Phenylhydrazono) indolin-2-one Derivatives by $Co(NO_3)_2$ as Powerful and Efficient Catalyst

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Schiff bases synthesized from the reaction of primary amines with aldehydes and ketones in specific conditions. These compounds widely used in organic chemistry and exhibit biological properties such as antiviral, antipyretic, anti-inflammatory, antifungal, antibacterial, antimalarial properties also used as pigments and dyes, catalysts, intermediates in organic synthesis, and polymer stabilisers [1-2]. Isatin is a natural product that found in a number of plants, various derivatives of isatin have pharmacological properties such as antibacterial, antifungal, anti-HIV and antiviral activity [3]. In this research some derivatives of 3-(2-phenylhydrazono)indolin-2-one using isatine derivatives, Phenylhydrazine derivatives and Co(NO3)2 as a catalyst with high efficiency and short time were Synthesized. The synthesized compounds showed biological activity such as antimicrobial properties (against standard pathogens strain and aquatic pathogens strain), antifungal activity and antioxidant property on DPPH.

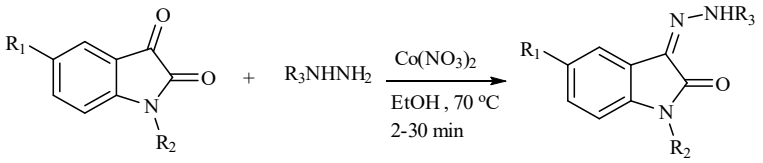

Fig.1 Synthesis of 3-(2-phenylhydrazono)indolin-2-one derivatives by $Co(NO_3)_2$ as catalyst

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The 26th Iranian Seminar of Organic Chemistry
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Paper code: 1159

Green Synthesis of 1,2,4-Triazole Derivatives and Evaluation of their Antimicrobial Effects

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Triazoles are an important class of five-membered aromatic heterocycles containing three nitrogen atoms. They are contained in two resonance forms [1]. The triazole ring system is found in a variety of naturally occurring compounds and biologically active molecules [2]. They are used in medicine as antifungal agents [3]. The resistance of bacteria and fungi to antibiotics is still increasing and can be a serious threat to human health in the future. New antimicrobial agents must be designed and identified to confront these pathogens. In this study, 1,2,4-triazole derivatives were obtained *via* reaction of benzamidine and hydrazides in the presence of K_2CO_3 in water (Fig. 1). The molecular structure of all synthesized compounds were characterized with IR, ^{1}H NMR, ^{13}C NMR spectra. Finally, the inhibitory effect of the synthesized derivatives has been investigated on several Gram-positive and Gram-negative bacteria and pathogenic fungi. The result of this study showed that triazole compounds are potential antibacterial and antifungal agents due to their significant inhibitory effects.

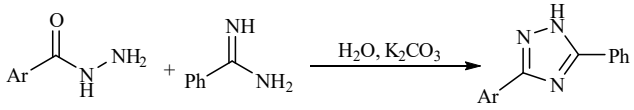

Fig. 1 Green synthesis of 1,2,4-triazoles

References

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Paper code: 1161

Alcohol Oxidation by TBHP Using Molybdenum Oxide Immobilized on Mesoporous Silica

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The molybdenum (VI) oxide nanoparticles were prepared inside the channels of mesoporous silica support via incipient-wetness impregnation method by taking appropriate concentration of Ammonium hepta molybdate tetrahydrate [1,2]. These compounds were characterized by XRD, TEM, BET, FT-IR and ICP. The XRD pattern showed high crystalline MoO_3 phase. TEM image presented hexagonal array of uniform channels of SBA-15 with diameter of 7 nm that were retained after impregnation and calcination. The N_2 adsorption-desorption isotherms illustrated decrease of surface area and pore size after immobilization. Infrared spectra indicated change in peaks intensity and create of new vibration at support when Mo introduce. The Molybdenum loading was obtained %17.15 on SBA-15 supports using ICP analysis. The catalytic activity of MoO_3/SBA-15 was investigated for the oxidation reaction of alcohols. This catalyst can catalyze the alcohol oxidation reactions with TBHP as oxidant at 80 °C in solvent free conditions (Fig. 1). The heterogeneous behavior of the catalyst was remained during the reactions, and various ranges of alcohols were converted to carbonyl compounds.

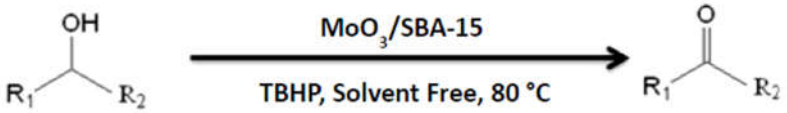

Fig. 1 Alcohol oxidation by TBHP using the Catalyst

Reference

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Paper code: 1162

An Efficient Regioselective Synthesis of Functionalized Spiropyrrolizidines through Azomethine Ylides Intermediate

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Pyrrolizidines (4-azabicyclo[3.3.0]octane) are substantial core structures of many natural products resembling alkaloids, and also occur in synthetic compounds with considerable bio-activities [1]. In particular, spiropyrrolizidines possess a privileged heterocyclic skeleton that is recognized in a large family of synthetic compounds exhibiting versatile biological and medical activities, such as antimycobacterial, antitumor, antifungal, and antiviral properties [2]. Another privileged structural core in the target compounds is rhodanine moiety, which has long been sought after by pharmacologists as an important structural motif in medicinal chemistry[3]. Herein we describe an efficient approach for the construction of functionalized spiropyrrolizidine-linked rhodanines **4** through the 1,3-dipolar cycloaddition reaction of an azomethine ylide, generated in situ from *L*-proline (**1**) and dialkyl acetylenedicarboxylates, with rhodanine derivatives **3** for the synthesis of **4** in EtOH (Fig. 1). The structures of products were characterized by their IR, mass spectral data, ^{1}H NMR, ^{13}C NMR, and X-ray crystallography. Various advantages of these transformations will be presented and discussed.

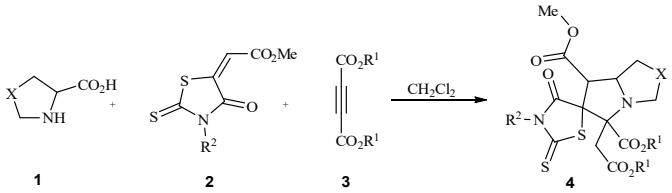

Fig. 1 Regioselective synthesis of spiropyrrolizidine derivatives

References

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Relative Stability of Clonidine Isomers

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Clonidine (CND), an alpha-2-adrenergic agonist, is used as an adjuvant with local anesthetics. However, due to its capacity in lowering blood pressure, CND has been successfully employed in the treatment of hypertension for over 25 years [1]. On based the position of Cl substituents, CND has several isomers with different chemical and biological activities (CND2-CND2-3, see Fig. 1). The relative stability of CND isomers in the gas phase and aqueous solution has been investigated using DFT calculations. The geometry optimizations have been performed at the B3LYP/6-31G(d,p) level of theory using the Gaussian09 program package [1,2]. The trend in the stabilities of isomers estimated in the gas phase and aqueous solution is CND2-3 > CND2-2>CND2>CND2-1. The ortho/para isomer (CND2-1/CND2-3) is the least/most stable isomer because of the electronic and steric effects.

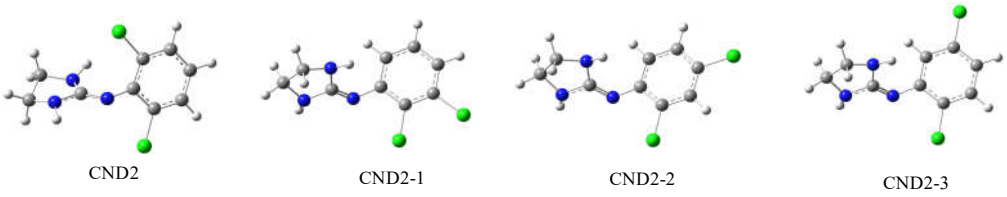

Fig. 1. The structures of CNDisomers.

Table 1. The relative energies of CNDisomers (in kcal mol^{-1})

i	ΔE_{gas}	ΔE_{water}
CND2	1.27	0.91
CND2-1	2.92	2.96
CND2-2	0.47	0.79
CND2-3	0.00	0.00

References

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Paper code: 1165

Preparation of New Hydrogels Based on Polyurethane/Polyoxyethylene/Silica Components *via* Click Chemistry

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Hydrogels are crosslinked hydrophilic polymer structures that can imbibe large amounts of water or biological fluids [1]. Hydrogels have been considered as promising materials in tissue engineering and biomedical area [2]. Because of its high hydrophilicity nature, polyethylene glycol (PEG) is one of the most extensively used monomers for preparing different types of hydrogels [3]. In this work, silica nanoparticles (SNP's) were homogeneously trapped into a polyurethane (PU)-based hydrogel during its preparation (Fig. 1). The effect of the nanoparticles on the thermal behavior as well as the amounts of water uptake were thoroughly studied. Briefly, an azide-containing and polyoxyethylene (POE)-based polyurethane (PU) was synthesized starting from PEG, ε-caprolactone (ε-CL), and methylene diphenyl diisocyanate (MDI). Next, an yne-terminated PEG was used as the crosslinker in the presence of SNP's in 2.5, 5.0, and 10.0 wt.%. In this stage, a thermally-induced copper (I)-catalyzed 1,3-dipolar azide-alkyne cycloaddition (CuAAC) was performed. FT-IR, XRD, ^{1}H-NMR, FE-SEM, and TGA/DTG techniques were used to characterize the desired samples.

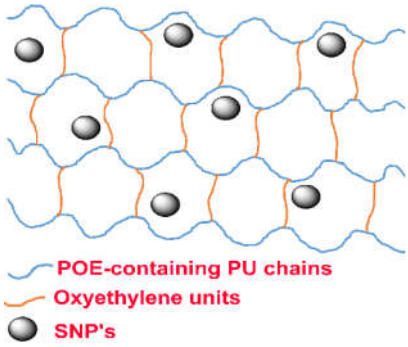

Fig. 1 Synthesis of new PU/POE/SiO_2 hydrogels

References

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Paper code: 1166

Chlorosulfonic Acid Supported Piperidine-4-carboxylic acid Functionalized Fe_3O_4 Nanoparticles: A Green Catalyst for the Synthesis of 2-Arylbenzimidazoles under Solvent Free Conditions

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Benzimidazoles are an important class of heterocycles that are frequently used in drug and agrochemical discovery programs. Recent medicinal chemistry applications of benzimidazole analogs include antibacterial and antifungal agents, anthelmintic agents, HIV-1-induced cytopathic inhibitor, and receptor agonists or antagonists [1]. Therefore, the construction of these heterocycles has always been of great interest to organic and medicinal chemists and has consequently received much attention. The classical and most common methods to assemble benzimidazoles involve the condensation of benzene-1,2-diamines with aldehydes, carboxylic acids, or their derivatives under strong acid/high temperature conditions or using a stoichiometric oxidant [2–4]. Although these transformations are widely used owing to their inherent simplicity, this method is restricted to the available starting materials and involves harsh reaction conditions. In this study, we report a highly versatile and efficient synthesis of 2-arylbenzimidazoles**3** from *o*-phenylenediamine, aldehyde and catalytic amounts of the catalyst (Fe_3O_4-PCA) under solvent-free conditions in high yields (Fig. 1).

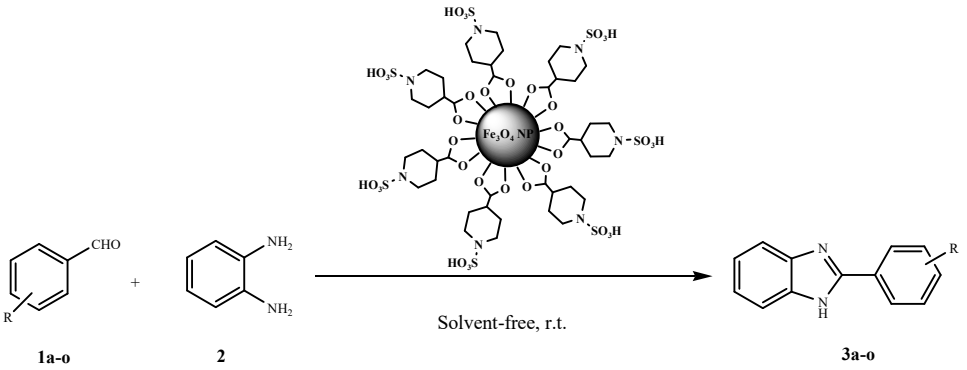

Fig. 1 General reaction scheme for the synthesis of 2-arylbenzimidazoles

The main advantages of the presented protocol are mild, clean and environmentally benign reaction conditions, as well as the high yields, simple work-up, ease of separation, and recyclability of the magnetic catalyst.

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Paper code: 1167

Antibacterial Activity and DNA Binding Studies of Co^{3+}, Cu^{2+}, Zn^{2+} and Pd^{2+} Complexes: Investigating Antibacterial Combination Therapy on These Complexes

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Therapy with antimicrobial combinations has been used since antimicrobials have been accessible [1], although clinical data from prospective randomized trials, fulfilling the criteria of evidence- based medicine, are rare [2]. In this study, four Co(III)-, Cu(II)-, Zn(II)- and Pd(II)-based potent antibacterial complexes of formula $K_3[Co(ox)_3].3H_2O$ (**I**), [Cu(phen)(bpy)Cl]Cl (**II**), $([Zn(bpy)_2(phen)]Cl_2.6H_2O$ (**III**) and $[Pd(bpy)(phen)](NO_3)_2$ (**IV**) (where ox is oxalate, phen is 1,10-phenanthroline and bpy is 2,2′-bipyridine) were synthesized. They were characterized analytically and spectroscopically by elemental analyses, molar conductance measurements, UV–Vis, FT-IR and 1HNMR spectra. These metal complexes were ordered in three combination series of **I+II**, **I+II+III** and **I+II+III+IV**. Antibacterial activity was tested for each of these four metal complexes and their combinations against gram positive *(Staphylococcus aureus* and *Enterococcus faecalis*) and gram negative *(Escherichia coli* and *Pseudomonas aeruginosa*) bacteria. All compounds were more potent antibacterial agents against the gram negative than those of the gram positive bacteria. The four metal complexes showed antibacterial activity in the order **I > II > III > IV** and the activity of their combinations followed the order of **I+II+III+IV > I+II+III > I+II**.

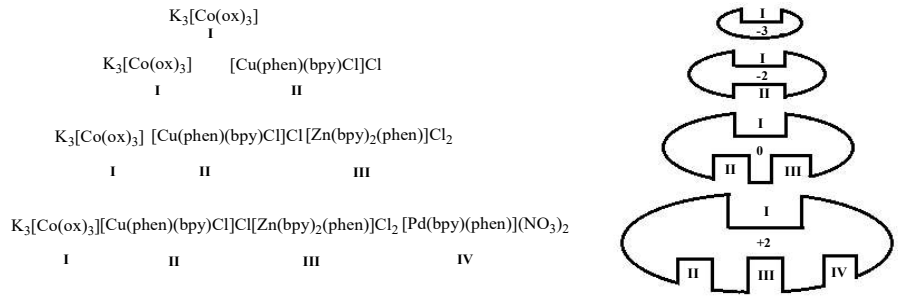

Fig. 1 Combination scheme a) $K_3[Co(ox)_3]$ complex(**I**) and its three combinations (**I+II, I+II+III, I+II+III+IV**) and b) Total charges of complex ions present on each combination (-3, -2, 0, +2)

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University of Zabol
12-14 March, 2019

Paper code: 1168

The Aromaticity of Aromatic Rings in Pyrroloquinoline Quinone Isomers

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Pyrroloquinoline quinone (PQQ) is a small, redox active molecule that serves as a cofactor for several bacterial dehydrogenases.PQQ has four isomers with three aromatic rings (1-3 in Fig 1.) [1]. The aromaticity of rings can affect the biological properties of compounds. In this work, the aromaticity of rings were estimated by the aromatic fluctuation index (FLU). The geometries of compounds were optimized at the B3LYP/6-31G(d,p) level of theory using the Gaussian 09 program [2]. The FLU index is in a sense based on the ρ values calculated using the AIM analysis. The results show that the trend in the aromaticity of rings 1–3 in PQQisomersis 3 > 1 > 2. The rings 3 and 1 are six and five membered rings, respectively and generally, where the former is more aromatic than latter. The ring 2 is less aromatic than other two rings, because two electron-withdrawing group, C=O, disturb the charge distribution of ring 2.

Fig. 1 The structure of PQQ with aromatic rings 1-3.

Table 1 The values of FLU index for rings 1-3 in PQQ isomers

i	1	2	3
Iso1	0.0171	0.0654	0.0089
Iso2	0.0170	0.0643	0.0082
Iso3	0.0181	0.0647	0.0079
Iso4	0.0165	0.0640	0.0077

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Paper code: 1169

A Green Synthesis of Substituted Bis(indolyl)methanes Using Chlorosulfonic Acid Supported Piperidine-4-carboxylic acid (PPCA) Functionalized Fe_3O_4 Nanoparticles (Fe_3O_4-PPCA) as Recyclable Catalyst

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Bis(indolyl)methane and their derivatives are members of an important class of heterocyclic compounds that display diverse biological properties, and can act as a selective colorimetric sensor for F^- and also as a highly selective fluorescent molecular sensor for Cu^{2+} [1]. In the past years, various methods were mentioned for the synthesis of bis(indolyl)methanes, generally, these compounds could be obtained by the cascade reaction between indole and aromatic (or aliphatic) aldehydes in the present of protic or Lewis acids, such as I_2, Ionic liquids, $CeCl_3 \cdot 7H_2O$, AuCl, SBA-15/SO_3H and zeolites [2-4]. However, all of the synthetic protocols reported so far suffer from disadvantages such as, use of metal and expensive reagent, prolonged reaction time, use of organic solvent, harsh reaction condition, use of excess indole and low yield. In continuation with the search for simple non-hazardous methods for the transformations in organic synthesis, herein we report a highly versatile and efficient synthesis of bis(indolyl)methanes (**3**) from indole (**1**), aldehyde (**2**a-j) and catalytic amounts of nano Fe_3O_4-PPCA under mild reaction in high yields (Fig. 1).

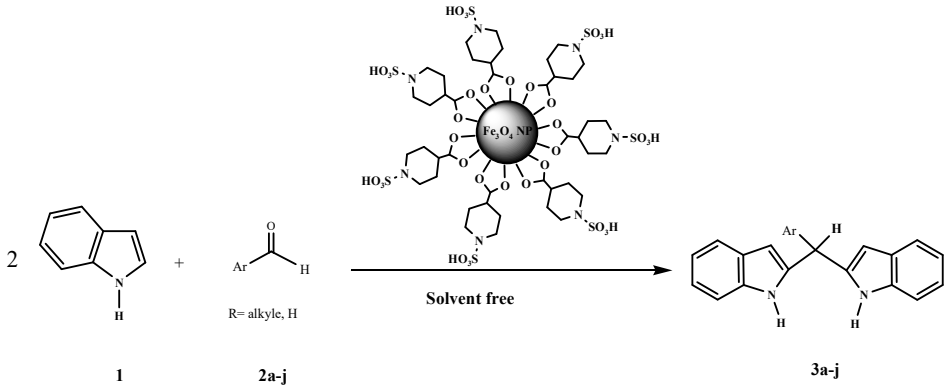

Fig. 1 General reaction scheme for the synthesis of bis(indolyl)methanes

This method provides several advantages, such as safety, mild condition, short reaction times, neutral conditions, non-toxic, environment friendly solvent, high yields and easy workup procedure compared to the traditional method of synthesis.

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Paper code: 1170

Green Multi-Component Reaction of α-Haloketoneswith Acetylenic Esters in the Presence of Papaverine (Poppy alkaloid)

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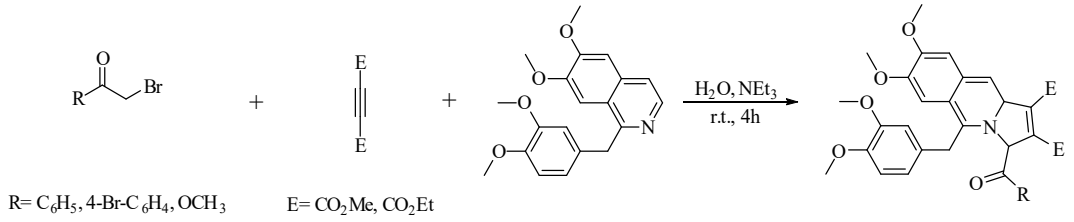
Multi-component reactions (MCRs) are useful organic reactions in which three or more starting materials react to give a product [1]. A poppy plant consists a lot of alkaloids and this plant has been used for medical purposes since ancient times.Some opium alkaloid derivatives have been medicinal properties, including oxycodone, oxymorphon, buprenorphine, nalbuphon [2-4]. In continuation of our quest for the synthesis of heterocyclic compounds [5], here in we describe a three-component condensation of α-haloketones**1**react with acetylenic esters**2**in the presence of papaverine **3**in water at room temperature by vigorous stirring to afford products **4**in good to high yields.



1 **2** **3** **4**

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Paper code: 1173

Classification and Discrimination of Pyridine-Based Compounds with Various Substitutions Using Fluorescent Carbon-dots Sensor Array

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Pyridine derivatives are important chemical compounds with widespread applications in various fields [1]. Several pyridine derivatives play important roles in biological systems [1]. This ring system is present in a number of natural products such as vitamins, niacin, niamide, vitamin-B6, alkaloids, nicotine, and pipeline [1]. So, detection and identification of different pyridine-based compounds with similar structures is of great interest. Carbon dots (C-dots) are kind of fluorescent materials that have drawn increasing attention in recent years owing to exceptional advantages such as high optical absorptivity, chemical stability, biocompatibility, and low toxicity [2]. Moreover, fluorescence quenching is a promising technique for chemical sensing applications and widely used for identification and quantitation of various analytes [3]. In this work, we have developed a facile fluorescent sensor array based on fluorescent carbon dots for detecting and differentiating some pyridine derivatives. Three kinds of nitrogen-doped carbon dots have been synthesized. These carbon dots have various surface states and thus exhibited diverse quenching responses to different target analytes. The fluorescence response was measured after incremental addition of analyte solutions i.e. 4-methyl pyridine, 4-pyridine carboxylic acid, 4-pyridinol, 2,3-pyridindiol, pyridine-3-carboxylic acid, 3-pyridine carboxamide, and 2-pyridine carboxylic acid. Implementation of the principal component analysis (PCA) and linear discriminant analysis (LDA) to the collected data matrices allowed the successful classification of all seven pyridine compounds with good accuracy. In addition, the binary and ternary mixtures of the seven pyridine compounds can also be well recognized with this sensor array. This method is simple, and the sensor arrays could be obtained easily with low-cost.

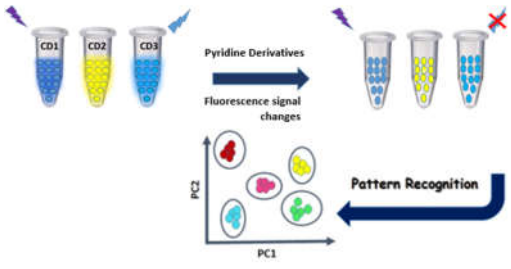

Fig. 1

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Paper code: 1176

Application of Hydrophilic Palladium Complex in Cyanation Reactions

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Aryl nitriles are important structural units of various natural products, polymers, pharmaceuticals and dyes [1]. Nitriles are also key intermediates in the synthesis of heterocycles, as they are easily converted into a variety of functional groups such as carboxylic acids, oximes, amines, amides and ketones [2]. Transition-metal-catalyzed cross-coupling reactions between aryl halides and metal cyanides such as CuCN, NaCN, and $Zn(CN)_2$ are an efficient alternation for the synthesis of aryl nitriles in relatively mild reaction conditions and with high yields [3]. However, many of the cyanide sources are highly toxic, hence the industrial applications of such reactions are often limited. Recently, Beller *et. al*. reported the use of $K_4[Fe(CN)_6].3H_2O$ as a safe cyanide source for cyanation of aryl halides. This is non-toxic and commercially available compared to the other cyanide ion sources. By the way, a general problem of metal catalyzed cyanationreactions is related to the high affinity of cyanide ion towards the metal catalysts. By considering the above mentioned facts, in the current study. A new hydrophilic Pd-based catalyst was successfully synthesized and used for the cyanation reactions of aryl halids using $K_4[Fe(CN)_6].3H_2O$ as a safe cyanide source. Significantly heterogeneous magnetically-recyclable catalyst can be separated easily using a magnetic bar and reused nine times without any drastic loss of its catalytic activity. Using water as a green solvent, facile catalyst recovery and reuse, simple work-up and not requiring any additive or promoter make this method desirable from the environmental and economic point of view, to use in such coupling reactions.

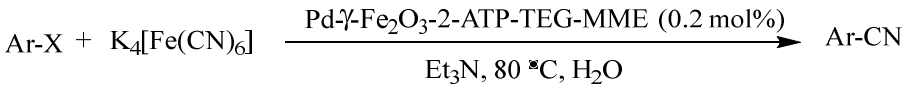

Fig. 1 Cyanation reaction using the catalyst

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Paper code: 1177

Removal of Methyl Orange Dye by Absorbent Carbon Nanotubes with Response Surface Experimental Design and Genetic Algorithm

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Water pollution, as a result of inadequate discharge of urban and industrial wastewater, the presence of toxic contaminants and inappropriate management of solid waste, seriously affects human health. Considering the huge volume of wastewater produced, efforts to achieve proper disposal of sewage in the environment are necessary [1,2]. The evacuation of colored wastewater from various industries such as textiles, paper, wood, cosmetics, agriculture, plastics and leather will cause severe environmental problems. Among the industries mentioned, the textile industry has the highest consumption and produces a large volume of wastewater with a high concentration of color in the range of 10-200 $mg.L^{-1}$ [3,4]. The purpose of this study was to optimize methyl Orange dye removal from aqueous solutions by carbon nanotube using Response Surface Method and Central Composite Design methods and Genetic Algorithms. The batch experiment was conducted to evaluate the effects of independent variables such as pH, dye concentration, dose of sorbent and contact time. For the experiment, Response Surface and Central Composite Design methods were applied to evaluate the effects of these variables. Analysis of variance (ANOVA) was used for statistical analysis. The optimum conditions for basic methyl orange dye removal were pH = 2, dye concentration = 20, absorbent dose = 0.009g and contact time = 20 min. The verified model is Quadratic and R-squared value of this Study was obtained to be 95.49%, The R-Squared Adjusted was obtained to be 90.63% and The Squared predicted R2 was obtained to be 65.71%. Investigation of the isotherm and kinetic models showed that the experimental data were correlated with Langmuir adsorption isotherm model (R^2 = 0.9334) and pseudo-second order kinetic (R^2 = 0.9998). The equation obtained from CCD with genetic algorithm was studied and optimal conditions were obtained with this software. Finally, the water of the city of Omidieh was studied.

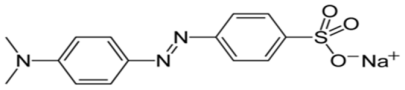

Fig. 1 Methyl organge structure

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Paper code: 1179

Acetic Acid as a Green Catalyst for the Synthesis of *N*-Aminotriazolethione Azomethine Derivatives

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Amino-mercapto-1,2,4-triazole are five-membered heterocycles compounds containing vicinal nucleophiles (NHR, SH) group which constitutes a ready-made building block for construction of various organic heterocycles. 1,2,4-Triazoles ring attracts considerable attention in organic chemistry owing to their biological activity [1] such as analgesic, antimicrobial, antiviral, antioxidant, anticancer, anticonvulsant, anti-inflammatory, and antihypertensive properties. Various methods have been reported for the synthesis of N-Aminotriazolethione Azomethine derivatives [2, 3]. In view of these above, we have reported the synthesis of Schiff bases incorporating 1, 2, 4-triazole scaffold derived via green and efficient procedure. 4-amino 5-methyl-1, 2, 4-triazole-3-thione with different aryl aldehydes resulted in the formation of the corresponding imines in the presence of acetic acid as the catalyst and solvent (Fig. 1). *N*-Aminotriazolethione Azomethine derivatives were obtained in excellent yields and short times. Chemical structure of all molecules was characterized by their spectral data and elemental analyses.

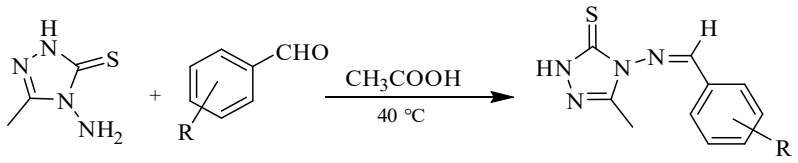

Fig. 1 Synthesis of azomethine of *N*-amine derivatives in acetic acid

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Paper code: 1181

Removal of phenol from Synthetic Waste Water by Fenton Method with Taguchi Test Design

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Phenol has a special importance among the various pollutants found in most industrial wastewater. Phenol is a hydrocarbon that the US Environmental Protection Agency has placed it in the category of first-class pollutants. This material and its derivatives are used in various industries such as resin and plastic manufacturing industries, paints, pesticides, pharmaceuticals, petroleum refineries, petrochemicals, coal mines, steel and aluminum and lead industries, detergents, artificial textiles and leather. And is therefore considered as an important pollutant in the sewage sludge mentioned above [1]. Phenol with the general formula C_6H_5OH is also known as hydroxyl benzene and carboxylic acid. Phenol is one of the most important organic compounds used in industry, which is used in many industries as a raw material [2]. In this study, removal of phenol from effluent by Fenton oxidation method was investigated using iron catalyst and H_2O_2 addition. Different conditions and quantities used in the experiment were designed using Taguchi technique, and finally, the optimal values of temperature, iron catalyst and the amount of H_2O_2 was used. The optimal results of these values were obtained at 25 °C, pH = 3, H_2O_2 equal to 5 g, and iron amount 5 g. Finally, under optimal conditions, by analyzing the actual sample, the removal of more than 80% of the phenol content We were in the wastewater. This method is one of the best methods for removing phenol from industrial effluent, due to its cost-effectiveness and rapid analysis and availability of used materials.

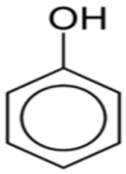

Fig. 1 Phenolic Chemical Structure

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Paper code: 1183

Theoretical Investigation of Methylpentynol-AzideIntermolecular H-Bonding and Regiochemical Outcome of Its 1,3-DC Reactions

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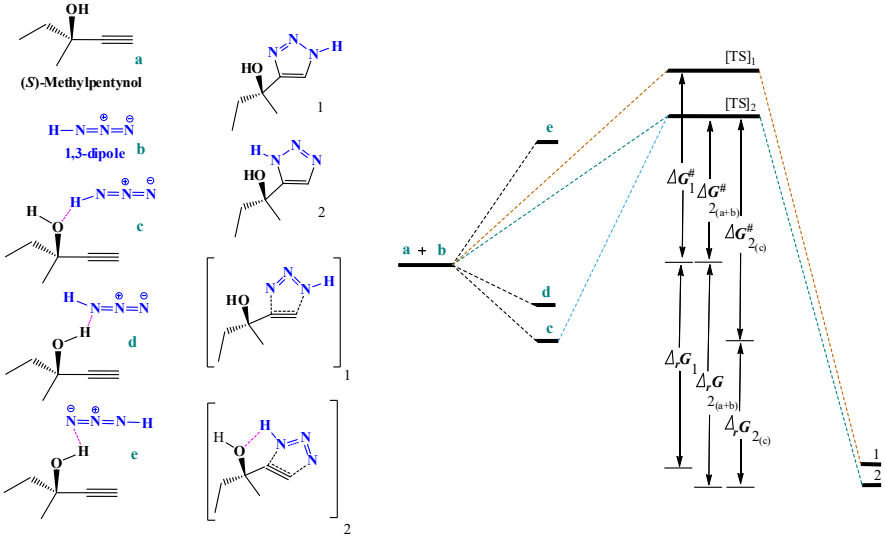
This study was focused on the theoretical and computational studies of the Hydrogen bonding effect on the regioselectivity of the 1,3-dipolar cycloaddition (1,3-DC) reactions. 1,3-DC Reactions have been applied in a number of diverse fields [1]. Stereochemistry in these reactions is spotlight, recently [2]. The five-membered heteroaromatic rings that achieved by 1,3-DC were widely used as an important role in various biochemical processes [3]. Here in, Methylpentynol (**a**) which is a treatment of insomnia was used as a dipolarophile. Cycloaddition of **a** to azide (**b**) can lead to regioselective 1,2,3-triazoles due to H-bonding between the hydrogen of azide (**b**) and the oxygen of hydroxy group in methylpentynol **(a)** as a hydrogen acceptor or H-bonding between the hetro atom of Azide (**b**) and the hydroxy group of methylpentynol **(a)** as a suitable hydrogen donor. In this study, the energy levels of the reactants (**a**,**b**), H-bonding arrays (**c**-**e**), transition state (TS), products (**1**,**2**), the free energies (in kcal mol^{-1}) of reaction ($\Delta_r G$ and $\Delta G^{\#}$), rate constants by using *Eyring*'s equation (k), structural data were calculated and obtained by DFT-B3LYP/6-31G* method.



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Paper code: 1185

1,3-Dipolar Cycloaddition Reactions on Medicine Dimethisterone: A Computational Insight

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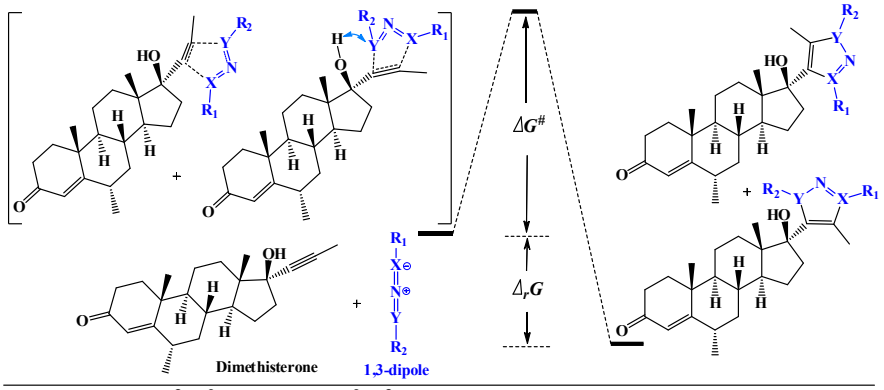
The different types of 1,3-dipolar cycloaddition (1,3-DC) reactions have been widely used in various fields. Based on the recent researches, stereochemistry of these reactions is spotlight [1]. In this study, the theoretical aspects of the electrostatic attraction effect on the regioselectivity of the 1,3-DC reactions to dimethisterone was assessed which it is a progestin medication [2] as a dipolarophile white nitrile imine (**a**), nitrile oxide (**b**) and azide (**d**) as 1,3-dipoles. Cycloaddition of dimethisterone to each of **a-d** can lead to regioselective five-membered heteroaromatic rings, the 4- and/or 5-substituted, due to secondary effect between the hetro atom of 1,3-dipoles and the hydroxy group in dimethisterone. These heteroaromatic rings were widely used as an important role in various biochemical processes [3]. In this study, the (1,3-DC) reaction of dimethisterone with **a-d** were utilized to produce the five-membered aromatic heterocyclic rings, i.e. pyrazole, isoxazole and triazole derivatives. Data were calculated and obtained by DFT-B3LYP/6-31G* method.



1,3-dipoles	$R_1—X\equiv\overset{\oplus}{N}—\overset{\ominus}{Y}—R_2 \leftrightarrow R_1—\overset{\ominus}{X}=\overset{\oplus}{N}=Y—R_2$		Products	
a	$Ph—C\equiv\overset{\oplus}{N}—\overset{\ominus}{N}—Ph \leftrightarrow Ph—\overset{\ominus}{C}=\overset{\oplus}{N}=N—Ph$	Nitrile imine	4- & 5-substituted pyrazole derivatives;	1 , 2
b	$Ph—C\equiv\overset{\oplus}{N}—\overset{\ominus}{O} \leftrightarrow Ph—\overset{\ominus}{C}=\overset{\oplus}{N}=O$	Nitrile oxide	4- & 5-substituted isoxazole derivatives;	3 , 4
c	$\overset{\oplus}{N}\equiv N—\overset{\ominus}{N}—Ph \leftrightarrow \overset{\ominus}{N}=\overset{\oplus}{N}=N—Ph$	Azide	4- & 5-substituted triazole derivatives;	5 , 6

References

[1] (a) S. Taban, A.A. Taherpour, *Letters in Organic Chemistry,* **2017**, 14:159-163. (b) K.A. Kumar, *International Journal of ChemTech Research.* **2013**, 5:3032-3050. (c) K.V. Gothelf, K.A. Jørgensen, *Chemical Reviews,* **1998**, 98:863-910.

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[3] D.K. Dalvie, A.S. Kalgutkar, S.C. Khojasteh-Bakht, R.S. Obach, J.P. O'Donnell, *Chemical Research in Toxicology*, **2002**, 15:269-299.

The 26th Iranian Seminar of Organic Chemistry
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12-14 March, 2019

Paper code: 1186

The Aromaticity of Rings in Some Pterin-Based Inhibitors of Dihydropteroate Synthase

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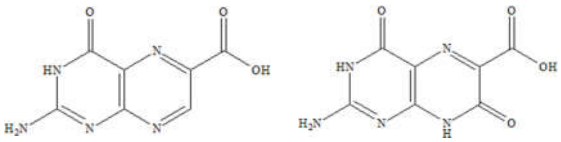
Dihydropteroate synthase (DHPS) is a key enzyme in bacterial folate synthesis and the target of sulfonamide class of antibacterials. Several pterin-based inhibitors (PBI) of DHPS with aromatic ringshave been identified. The estimation of aromaticity of rings (pyrimidine (1) and pyrazine (2)) of these inhibitors (see Fig. 1) is important in the prediction of inhibitory activity [1]. In this work, the aromaticity of some inhibitors have been estimated using the aromatic fluctuation index (FLU). The geometries of compounds were optimized at the B3LYP/6-31G(d,p) level of theory using the Gaussian 09 program [2]. The FLU index which is based on the ρ values was calculated using the AIM analysis on the wave functions obtained at the B3LYP/6-31G(d,p) level of theory. With respect to the FLU values, the ring 2 is more aromatic than 1. The largest aromaticitiy of rings 1 and 2 is corresponded to the cases in which one C=O functional group changes to NH_2 (in ring 1) or H (in ring 2).



A B C

Fig. 1 The structure of some PBIs

Table 1 The values of FLU index for rings 1 and 2 in PBIs

i	1	2
A	0.060	0.034
B	0.045	0.012
C	0.041	0.035

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University of Zabol
12-14 March, 2019

Paper code: 1187

A New Nanomagnetic Cobalt Catalyst for Copper-free Sonogashira Coupling Reaction in Water at Room Temperature

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Chitosan (CS), which is an *N*-deacetylated derivative of chitin, is an example of polysaccharide that is widely spread in living organisms.Surprisingly, chitosan have unique characteristics of the biomaterials; including the nontoxicity, biodegradability, environmentally friendly, renewability and abundance. More importantly, although, chitosan is a proper green and biodegradable catalyst by itself, the presence of hydroxyl and amine groups in the chitosan structure makes it possible to prepare the modified chitosan-based heterogeneous catalysts possessing new properties. However, chitosan is only soluble in acidic aqueous media while it is insoluble in basic aqueous medium, which is a necessary condition for cross coupling catalysis [1]. Carbon-carbon coupling reactions as a powerful synthetic tool and a major area in multiple organic transformations have recently been one of the most intensively studied subjects in organic synthesis which has been applied in various areas, including the synthesis of natural products, drugs and fine chemicals [2]. Nevertheless, these reactions suffer from problems associated with the separation and recovery of the homogeneous and costly Pd-based catalysts, which might result in undesirable metal contamination of the products. Therefore, to have an efficient recovery and recycling of the catalyst, the immobilization of homogeneous catalytic systems on different supporting materials has been the subject of intense researches. Recently, there has been an increased focus on palladium and copper free conditions in such reactions. These problems can be largely overcome by using other transition metals such as nickel, copper, iron and cobalt. This metals are low cost, nontoxic and available. Sonogashira reaction employing heterogeneous cobalt-based catalysts have been reported less frequently [3]. In this work, we have successfully prepared an economical, environmentally benign and heterogeneous cobalt-based catalyst. This newly synthesized catalyst was characterized by different methods such as XRD, SEM, FT-IR, TG and ICP analysis and used as an efficient heterogeneous catalyst in Sonogashira coupling reaction in water at room temperature (Fig. 1).

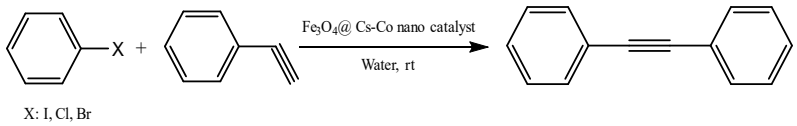

Fig. 1 The Sonogashira Coupling Reaction

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Paper code: 1188

Diasteroseletive Synthesis of Functionalized Cyclohexanones by Condensation of Acetoacetanilide and Various Aldehydes in the Presence of DMAP as Catalyst

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Functionalized cyclohexanones containing stereogenic centers as valuable building blocks are present at the core of an array of natural products candidates [1], that they are biologically active agents with antibacterial, and anticancer properties [2]. In this context, and in continuation of our previuos work [3], we reported a facial synthetic strategy for the diasteroselective synthesis of *N,N'*-diaryl-2-hydroxy-6-methyl-4-oxocyclohexane-1,3-dicarboxamide using DMAP as catalyst. Acetoacetanilide undergoes a diasteroselective condensation reaction with various aromatic aldehydes in EtOH at 50 °C to afford desirable products via one-pot pseudo-three-component reaction. The present protocol provides an inexpensive and efficient route to obtain functionalized cyclohexanones containing four quartetnary stereogenic centers with high yields from the simple and readily available starting materials undermild conditions in shorter reaction times. The products have been characterized by spectral data.

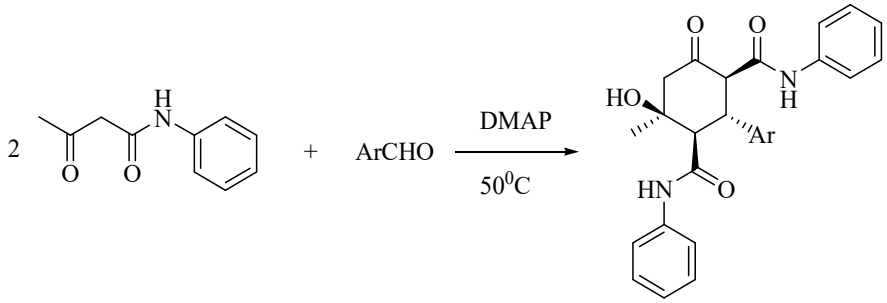

Fig. 1 One-pot pseudo-three component synthesis of *N,N'*-diaryl-2-hydroxy-6-methyl-4-oxocyclohexane-1,3-dicarboxamide

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Paper code: 1190

PTSA: A FacileCatalyst a One-Pot Synthesis of 2-Arylpyrrolo[2,3,4-kl]-1(2*H*)-one under Mild Conditions

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Synthesis of heterocycles has always been a topic of great interest owing to the agricultural, pharmacological, and industrial significance of the majority of heterocyclic structures [1]. Among an immense variety of N-heterocyclic compounds, acridine moieties are preeminent due to their multiple pharmacological and biological activities [2]. Many procedures have been extended for synthesis of these scaffolds via hantzch reaction. However, a vast survey of the literature disclosed that there are a few synthetic methods for construction of pyrroloacridines with three-component reaction of dimedone, various anilines, and isatin [3]. Hence, we developed the synthesis of medicinally important 2-arylpyrrolo[2,3,4-*kl*]acridin-1(2*H*)-ones by an efficient and convenient approach of three-component reactions of dimedone, various anilines, and isatin in the presence of PTSA as environmentally benign and effective catalyst. This work presented here has the merits of environmental friendliness, easy operation, simple work-up, excellent yields. Chemical structures of all molecules were characterized by spectral data and elemental analysis.

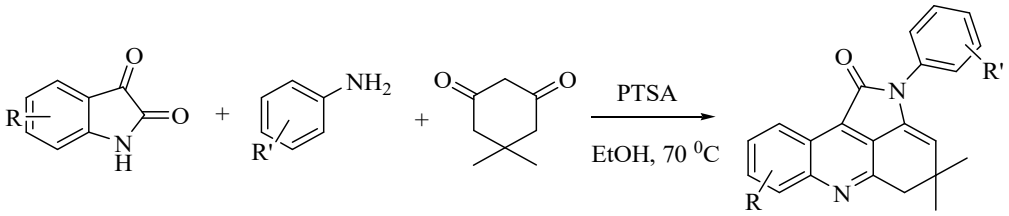

Fig. 1 Multicomponent synthesis of 2-arylpyrrolo[2,3,4-*kl*]-1(2*H*)-one catalyzed by PTSA

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Paper code: 1191

Ultrasound-Promoted One-Pot, Four-Component Synthesis of 1,6-Diamino-2-oxo-1,2,3,4-tetrahydropyridine-3,5-dicarbonitriles Using 4-Dimethylaminopyridine (DAMP) as Catalyst

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Multi-component reactions (MCRs) provide a convenient method for the preparation of new chemical entities required by agrochemical and pharmaceutical industries [1]. Also, MCRs have been applied to produce laborious biologically active compounds [2]. Nitrogen-containing heterocyclic molecules in five- and six-membered rings such as pyridine rings compose the considerable section of chemical identities which are predominant interest in medicinal chemistry due to industrial, pharmacological, biological activities such as anesthetic, antimalarial, antibacterial, antioxidant and antiparasitic properties [3]. In addition, an efficient method for synthesis of 1,6-diamino-2-oxo-1,2,3,4-tetrahydropyridine-3,5-dicarbonitrile derivatives by 4-(dimethylamino)pyridine as homogenous catalyst through a one-pot and four-component reaction is described. This work provides practical method and offer many advantages such as short reaction times, excellent yields, and easy work-up procedure.

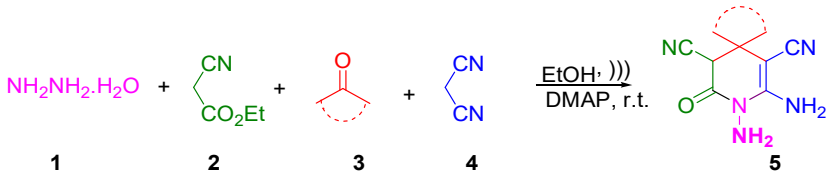

Fig. 1 Synthesis of 1,6-diamino-2-oxo-1,2,3,4-tetrahydropyridine-3,5-dicarbonitrile derivatives

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Paper code: 1192

Synthesis of New [1,2,4]triazolo[1,5-a]pyridine Derivatives by Reaction Pyridine-2-(1*H*)-ones and Aldehydes in the Presence of Acetic Acid as a Green Catalyst and Solvent

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Pyridines have been reported as biologically interesting molecules and precursors for the synthesis of triazolo[1,5-a]pyridines [1]. Triazolopyridines constitute an important class of heteroatomic compounds and frequently found in a variety of biologically active compounds such as antithrombotic, anti-inflammatory and antiproliferative agents [2]. Several methods have previously described for the synthesis of triazolo[1,5-a]pyridines [3]. In the present investigation the synthesis of some novel substituted triazolo[1,5-a]pyridines are attempted for their expected useful biological properties. New 1,2,4-triazolo[1,5-a]pyridine derivatives have been synthesis in high yields in the presence of acetic acid as both solvent and catalyst at 70 °C with the reaction of pyridine-2-(1*H*)-one derivatives and aldehydes. The Brϕnsted acid nature of acetic acid, promotes reaction by involving in both nucelophilic addition as well as in dehydration steps. Chemical structure of all molecules were characterized by spectroscopy and elemental analysis. The procedure offers several advantages, including green conditions, a simple work-up procedure, excellent yields and short reaction times.

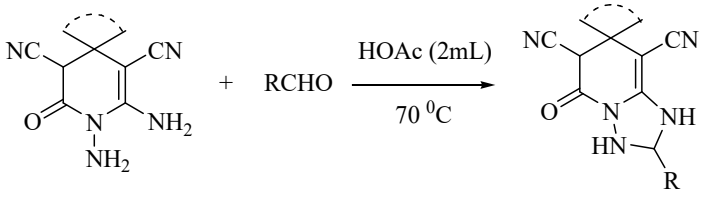

Fig. 1 Synthesis of triazolo[1,5-a]pyridines in the present of acetic acid as both solvent and catalyst

References

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Paper code: 1193

Application of Schiff Base Mn(III) Complexes Grafted to Crown Ether Rings as Catalysts for Oxidation of Benzyl Alcohol Derivatives by Oxone

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A combination of crowned Schiff base manganese(II) catalysts 1 or 2 and Oxone, as oxidant in $CHCl_3$ was used for the oxidation of various benzyl alcohol derivatives to corresponding aldehydes and ketones. the prepared catalysts in this research showed better efficiency in comparison of the identical crown free catalysts. Furthermore, Among the prepared catalysts, catalysts 1, containing pyridine ring, showed excellent catalytic efficiency. we think the presence of crown rings bonded to these complexes would not only increase the solubility of the oxidant ($KHSO_5$) in the organic phase, but also may facilitate bringing the $KHSO_5$ into the vicinity of the manganese [1], leading to faster oxidation of manganese (III) to oxo manganese (V) which is a better oxidant than $KHSO_5$ [2]. The addition of pyridine improved the chemical yields of all the reactions catalyzed by catalyst 2, but the reaction times of catalyst 1 remained nearly constant. It is concluded that the additional N atom on the bridge groups of catalyst 1 itself might play the role of axial base, therefore, the presence of pyridine as an external axial base only slightly improves corresponding reaction times in this case [3].

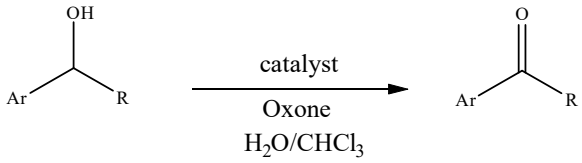

Fig. 1 Benzyl alcohols oxidation in the presence of the catalyst

References:

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Paper code: 1195

Simultaneous Removal of Organic Dyes from Environmental Samples by Using Sistan Sand as an Effective Sorbent

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Organic dyes are compounds with complex chemical structures, mostly of high hazard to human health. Moreover, they are one of the major pollutants, especially when entering environmental waters [1]. Many of dyes are not bio-degradable and must be removed from waters by physico-chemical processes. One of the most economical, easy and rapid methods to achieve this purpose is using an adsorbent [2]. In this work, Sistan sand was successfully used as a free and available sorbent for simultaneous removal of Malachite Green (MG), Rhodamine B (RhB) and Cresol Red (CR) dyes from environmental water samples. This sand can be found everywhere in Sistan area. We could show that each gram of this sand can effectively adsorb and remove high amount of 0.132 mg of CR, 0.109 mg of RhB and 0.120 mg of MG very rapidly. When these three dyes are in a mixture, Sistan sand can remove up to 83% of the dyes from the solution. In this regards, Sistan sand can be compared with some very high-priced nano-sorbents. Parameters affecting adsorption were optimized using both experimental design methods (Taguchi and Plackett-Burman) and experimentally. According to our kinetic studies, the pseudo-first-order equation was the best model for all three dyes. To the best of our knowledge, no other report can be found for the simultaneous removal of organic dyes by a natural sorbents.

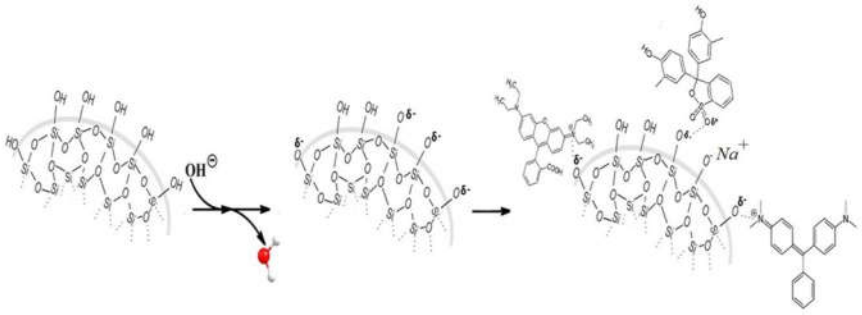

Fig. 1 Mechanism of simultaneous removal of Malachite Green, Rhodamine B and Cresol red by Sistan sand

References

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The 26th Iranian Seminar of Organic Chemistry
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Paper code: 1196

Adsorptive Schiff Base-Chitosan Nanocomposite for Removal of Pb(II) Ion from Aqueous Solutions

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A new chitosan-2-iminothiophenol methylbenzaldehyde Schiff base-based adsorbent (Fig. 1) was synthesized to be effective adsorbent for adsorption of Pb^{+2} from aqueous solutions. The adsorbent was characterized by FT-IR, SEM, EDX, DLS, VSM, and XRD. Batch adsorption experiments were done under various conditions, such as adsorbent dose, pH, and contact time. The equilibrium data were fitted to Langmuir and Freundlich isotherm models. The maximum monolayer capacity obtained from the Langmuir isotherm was 134.10 mg/g. The MCS-Sch was found to be regenerated effectively up to five efficient cycles of adsorption/desorption processes. The mechanism for Pb^{+2} adsorption onto MCS-Sch involved the interactions of N, O and S atoms and also aromatic rings with heavy metal followed by their adsorption on the MCS-Sch.

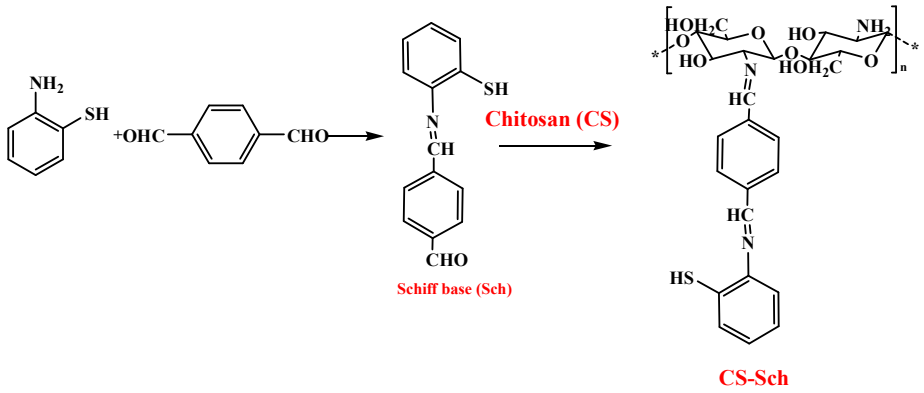

Fig. 1 Complete scheme for the synthesis of Schiff base ligand (Sch) and chitosan nanocomposite (CS-Sch).

References

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The 26th Iranian Seminar of Organic Chemistry
University of Zabol
12-14 March, 2019

Paper code: 1197

Synthesis and Application of Schiff Base Mn(III) Complexes Containing Crown Ether Rings as Catalysts for Oxidation of Sulfides by Oxone

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Two new crowned Schiff base manganese(II) catalysts 1 and 2 were synthesized and characterized by IR spectroscopy and CHNS microanalysis. A combination of Oxone, as oxidant and these catalysts in $CHCl_3$ was used for the oxidation of various sulfides to sulfones and sulfoxides. Compared with the crown free catalysts, the prepared catalysts in this research exhibited excellent efficiency. Additionally, among the prepared catalysts, catalysts 1, containing pyridine ring, showed better catalytic activity. we think the presence of crown rings bonded to these complexes would not only increase the solubility of the oxidant ($KHSO_5$) in the organic phase, but also may facilitate bringing the $KHSO_5$ into the vicinity of the manganese [1], leading to faster oxidation of manganese(III) to oxo manganese(V) which is a better oxidant than $KHSO_5$ [2]. The addition of pyridine improved the chemical yields of all the reactions catalyzed by catalyst 2, but the reaction times of catalyst 1 remained nearly constant. It is concluded that the additional N atom on the bridge groups of catalyst 1 itself might play the role of axial base, therefore, the presence of pyridine as an external axial base slightly improves the corresponding reaction times in this case [3].

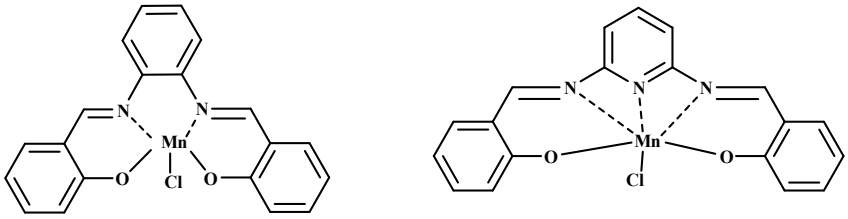

Fig. 1 The structures of catalysts 1 (right) and 2 (left).

References

[1] R. Wang, Z. Duan, Y. He, Z. Lei, *Journal of Molecular Catalysis A: Chemical*, **2006**, 260:280–287.
[2] K.C. Gupta, A.K. Sutar, *Journal of Macromolecular Science Part A Pure and Applied Chemistry*, **2007**, 44:1171–1185.
[3] K.C. Gupta, A.K. Sutar, *Polymers for Advanced Technologies,* **2008**, 19:186– 200.

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Nano Polymeric Biodegradable of Alginate-Arginine for Breast Anticancer Drug Delivery

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In this study, etoposide (ETO), a typical chemotherapeutic agent, was selected as themodel drug to evaluate of cysteine-modified sodium alginate (SA) nanoparticlesto load drug. The structure of nanoparticles was elucidated by fourier transform infrared spectroscopy (FTIR) (Fig. 1). The shape, and morphology were determined by scanning electron microscopy (SEM).In characterising the nanoparticles, physicochemical properties of particle size, poly-dispersity index (PDI), zeta potential (ZP), encapsulation efficacy (EE) and drug loading (DL) were investigated. The mean size, PDI and ZP of the obtained drug loaded nanoparticles were reported tobe 355.4nm, 0.309and -27.7 mV, respectivel [1,2]. The encapsulation effi-ciency, was between 80.50 and 90.77. Morever drug loading and drug release properties of the nanoparticles loaded with paclitaxel were also studied.The in-vitro drug release was stud-ied by using UV–Visible spectrophotometer at acidic environment (pH 5.0) and physiological pH (pH 7.4) and sustained release compared to the ETO alone. It was found that ETO drug is re-leased much faster in pH 5.0 than in the pH 7.4.

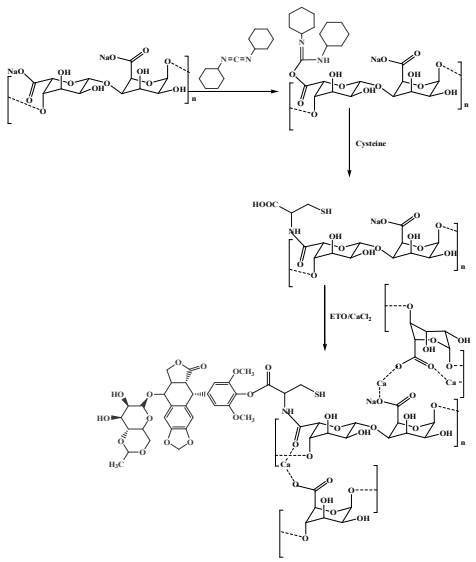

Fig. 1 Schematic synthesis of the polymer

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The 26th Iranian Seminar of Organic Chemistry
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12-14 March, 2019

Paper code: 1199

Magnetic Nanoparticles-Supported CuI-Caffeine: ARecyclable and Eco-friendly Catalyst for Green Synthesis of 1,2,3-Triazols from Organic Halides

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1,2,3-Triazoles as vital structural scaffolds are found in a large number of biologically active natural compounds and have extensive applications in medicinal chemistry, pharmaceutical industry [1], biochemical [2] and materials science [3]. Therefore, several investigations have focused remarkably on such well-known structure using different catalysts. In current research, we proposed a green and efficient method to prepare a value-added copper(I)–caffeine complex immobilized on silica-coated magnetite catalyst and then examined the catalytic activity in green synthesis of 1,2,3-triazoles through the three-component reaction of various terminal alkynes with in situ generated organic azides from organic halides in an aqueous medium in good yields (Figure 1). Moreover, final catalyst characterized well by FT-IR, XRD, SEM, ICP, TGA and VSM techniques. The immobilized catalyst with collecting ability via an external magnet, reused for at least five times with little loss in activity.

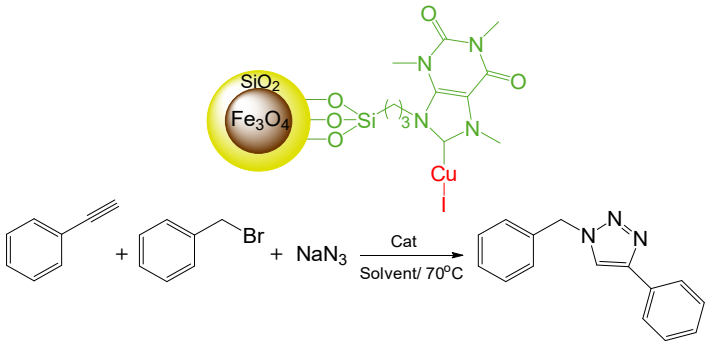

Fig. 1 Three-component click reaction of NaN_3, phenyl acetylene and benzyl bromide

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Paper code: 1201

Co(II) Immobilized on Functionalized Magnetic Hydrotalcite (Fe3O4/HT-NH2-CoII): A Green and Magnetically Recyclable Bifunctional Nanocatalyst for the Synthesis of Xanthenes

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Hydrotalicites (HTs) and magnetic hydrotalcites (MHTs) have been widely studied as promising supporting materials for catalysts in organic reactions. Hydrotalictes as a layer double hydroxide (LDH) with abundant surface hydroxyl groups consist of alternating cationic ($Mg_6Al_2(OH)_{16}^{+2}$ anionic (CO_3^{2-}) interlayers and Mg–Al mixed oxides which are chemically active sites (strong basic sites) for use in catalytic reactions and also act as the anchoring sites for metal nanoparticles. By considering the fact that the separation of hydrotalcite-based catalysts from the reaction mixture is difficult to some extent, replacement of conventional separation methods with magnetic separation approaches is a fascinating technique. Thus, incorporation of magnetic nanoparticles (MNPs) into the hydrotalcite structure provides easy separation of catalysts from the reaction mixture using a simple magnetic bar along with the prevention of MNP agglomeration, as well. A variety of amines and other functional groups have been utilized in nanoparticle preparation as stabilizers on surface of MHTs, which could be useful for immobilization of metal ions [1,2]. In recent times, xanthene derivatives have greatly drawn the attention of organic chemists as they are important motifs in a variety of biologically active compounds [3]. In summary we have successfully synthesized CO^{II} immobilized on functionalized magnetic hydrotalcite (Fe_3O_4/HT-NH_2-CO^{II}) from readily available starting materials. The applicability of nanocatalyst was explored in the synthesis of of xanthene derivatives through reaction aldehydes with 2-naphtol at 90 °C under solvent free conditions in excellent yields.

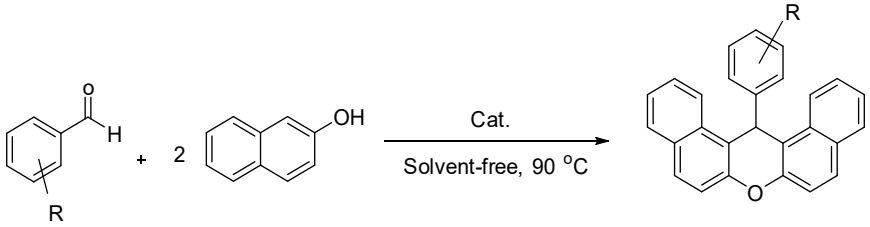

Fig. 1 Synthesis of of xanthene derivatives in the precence of the catalyst

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The 26th Iranian Seminar of Organic Chemistry
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12-14 March, 2019

Paper code: 1202

Preparation and Characterization of Ammonium-Based Ionic Liquids for Separation of Polycyclic Aromatic Hydrocarbons

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Polycyclic aromatic hydrocarbonssuch as drugs, dyes and PAHs are highly hydrophobic, non-polar, cytotoxic, mutagenic, carcinogenic and teratogenic [1]. Exposure to these aromatic compounds cause a variety of negative health impacts such as various cancers, breaking down hormone systems and depressing immune function. Determination and separation of aromatics is very important in industrial and medical applications. Ionic liquid (IL) has been used as green solvents instead of traditional organic solvents because of its special chemical and physical properties, such as high polarity and thermal stability, low volatility and wonderful miscibility [2]. Recently there are several novel sorbents using ionic liquids have been applied for trace enrichment of drug and aromatic residues in many samples. In this study we prepared tritely-n-octyl ammonium hexaflourophosphate (TAH) IL by mixing tritely amine and bromoalkane and refluxing for 48 h. Then, aqueous solution of KPF_6 added to resulted powder of previous step. ^{1}H NMR and FT-IR proved that IL was successfully synthesized. Many authors mentioned that ILs have a promising future as a sorbent in separation techniques [3].

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The 26th Iranian Seminar of Organic Chemistry
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Paper code: 1203

Effect of Vitamin C Template on Morphology and Structure of α–Alumina

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α-Alumina, a stable alumina polymorph, is usually formed by heat treatment of other polymorphs at temperatures higher than temperatures above 1000 °C, leading to severe surface area loss [1]. Nano α-Alumina particles can be utilized in polymer composites, paints, varnishes, coatings, in order to strengthen their mechanical properties. Furthermore, high strength ceramics can be produced from Nano α-Al_2O_3 powders at reduced temperatures [2].
In this research, α-Alumina powder was prepared *via* hydrolysis of aluminum isopropoxide, as inexpensive precursor, in the precence of vitamin C (as a chiral pool and a co-structural-directing-agent) in a facile and green procedure (Fig. 1). The influence of vitamin C and its degradation products on the texture and morphology of alumina was investigated by the means of XRD, SEM, TEM, EDX, BET, N_2 adsorption–desorption isotherm and optical rotation. The distinctive feature of this research is obtaining fine alpha-alumina with size less than 30 nm through a facile and green synthetic procedure using Vitamin C template-controlled pore size. Tthe surface area witnessed a significant fall with an increase of Vitamin C molar ratio.

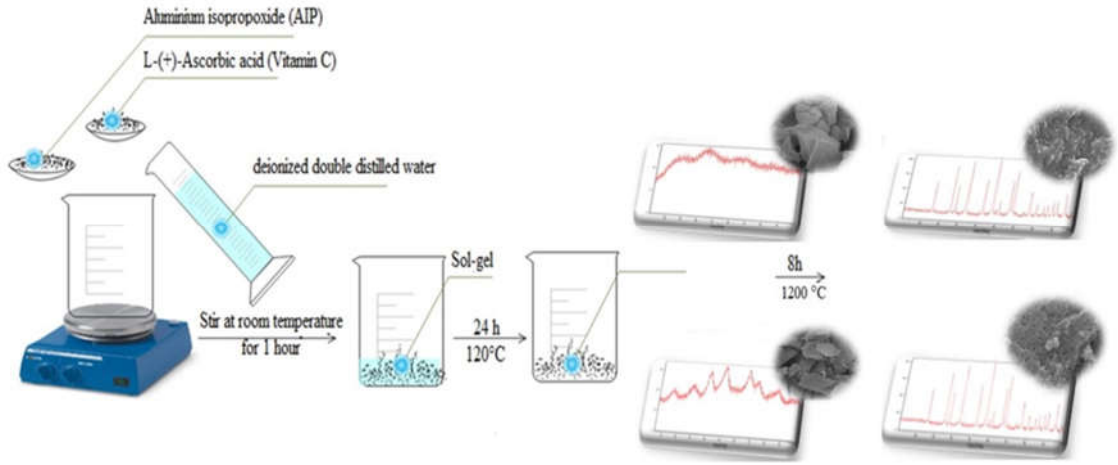

Fig. 1 Vitamin C template on the morphology and structure

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12-14 March, 2019

Paper code: 1205

The Study of Performance of Trachyspermum Ammi and Dimethicone in Bloating

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Bloating is one of the most common digestive problems in the community and many people suffer from it [1]. There are many medications to eliminate bloating that can be classified into three categories: synthetic, semi-synthetic and natural. The present paper reviews and compares the performance of the synthetic drug of dimethicone and the natural medicine Trachyspermum ammi, a medicinal plant, in an overview method of study. The studies show that the synthetic drug dimethicone has surfacatant, anti-surface tensile and anti-foam properties. Also the herbal medicine Trachyspermum ammi that has a warm and dry nature, has many properties, including anti-surface tensile strength, anti-foam, and exacerbates the intestine and stomach movements. The results of the present study indicate that both dimethicone and Trachyspermum ammi, due to the properties described above, can reduce bloating in the stomach and intestine, although they do not completely eliminate it. Regarding these results, although the therapeutic effects of dimethicone are higher than that of Trachyspermum ammi, the use of Trachyspermum ammi in comparison with dimethicone has less harm.

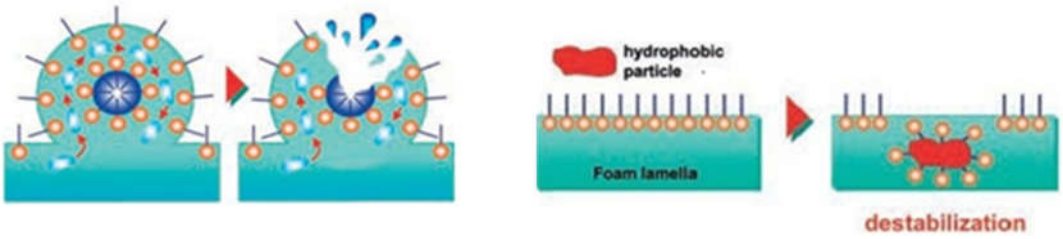

Fig. 1 Anti-foam action mechanism

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The 26th Iranian Seminar of Organic Chemistry
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Paper code: 1206

Salen Complex of Cu(II) Supported on Superparamagnetic Fe_3O_4@SiO_2Nanoparticles: An Efficient and Magnetically Recoverable Catalyst for the Synthesis of 1,4-Dihydropyridines

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The Fe_3O_4@SiO_2/Salen-Cu(II) nanocatalyst is reported as a thermally and air stable, economical, and magnetically recoverable heterogeneous catalyst for the selective and efficient 1,4-Dihydropyridines. Only by adding a small amount of the catalyst (0.4mol% Cu) to the reactants and heating under air, the new presented method provides a variety of functionalized1, 4-Dihydropyridines in good to excellent yields within short reaction times. The catalyst could be easily recovered with the aid of a permanent magnet and reused up to five consecutive runs without significant loss of activity. Also, the leaching of Cu was negligible after the fifth recycle. Particularly, ethyl acetoacetate and aromatic aldehydes as agents and the need of only small amount of the magnetically recoverable heterogeneous copper-based nanocatalyst make this method low-cost, environmentally benign, and easy to use.

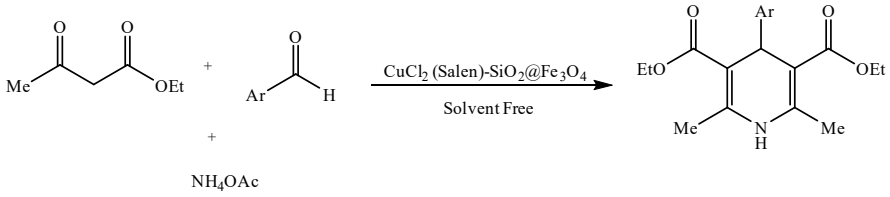

Fig. 1 Hantzsch synthesis of 1,4-dihydropyridines in the presence of Cu(Salen)-SiO_2@Fe_3O_4

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The 26th Iranian Seminar of Organic Chemistry
University of Zabol
12-14 March, 2019

Paper code: 1207

Magnetic Cellulose Nanofibers Supported Imidazolium-Based Ionic Liquid as a Biodegradable Catalyst for the Synthesis of Quinoline Derivatives

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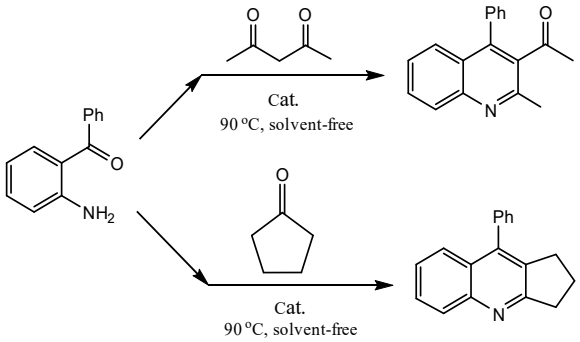
Ionic liquids are a class of liquids that are composed solely of ions. They are non-volatile, non-flammable, thermally stable, and have excellent solvation properties, thus find potential applications in catalysis, electrochemistry. Supported ionic liquid catalysis is a concept which combines the advantages of ionic liquids with those of heterogeneous support materials [1]. As an excellent support, cellulose is of great interest due to its good biocompatibility, biodegradation and non-toxicity. Furthermore, the cellulose nanofibers (CNF) has a large surface area, many available functional groups and high mechanical strength, which makes it an attractive candidate as a supporting material for the synthesis of heterogeneous catalysis. On other hand, as the recovery of the most heterogeneous catalysts from the final reaction systems requires filtration or centrifugation step as a time consuming and tedious process, for this reason, they have been coated with magnetic nanoparticles. Magnetically recoverable catalysts can be easily separated with an external magnetic field [2]. Because of quinoline importance as substructures in a wide range of natural and semisynthetic products, significant efforts are directed to the development and construction of new quinoline-based structures [3]. In this study we report the synthesis of imidazolium-based ionic liquid immobilizated on magnetic cellulose nanofibers (Fe_3O_4@NFC-IIL-HSO_4) and its identification by various techniques like FTIR, TGA, SEM, TEM, ICP-AES and VSM. The applicability of the constructed heterogeneous nanocatalyst was explored in the synthesis of quinoline derivatives through reaction of 2-Aminobenzophenones with ketones and diketones at 90 °C under solvent-free conditions in excellent yields.



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Paper code: 1209

Synthesis of Sulfonamide Derivatives Using Electrochemistry

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Sulfonamides are a class of antibacterial compounds, all of which contain the sulfonamido group, $-SO_2NH$. These compounds are used in both human and veterinary medicine. In human medicine they are widely used to treat various conditions including urinary tract infections, eye lotions, gut infections, and mucous membrane infections. Sulfonamides are classified in veterinary medicine as standard use, highly soluble, potentiated, and topical sulfonamides. While sulfonyl hydrazides are widely utilized in organic synthesis, it is only in recent years thatthey have emerged as powerful sulfonyl sources. The hydrazinyl group can be readily removed fromsulfonyl hydrazides under thermal, basic, oxidative, radical, and/or transition metal-catalyzedconditions, and subsequently, the remaining sulfonyl groups are able to form carbon-sulfur,sulfur-nitrogen, sulfur-halogen, sulfur-sulfur, and sulfur-selenium bonds with a wide variety oforganic compounds, providing alternative approaches to the preparation of sulfones, sulfonamides,sulfonyl halides, thiosulfonates, and selenosulfonates [1-3]. A variety of vinyl sulfones were prepared from alkenes and sulfonyl hydrazides via electrochemical oxidative sulfonylation. The reaction proceeds in an experimentally convenient undivided electrochemical cell equipped with graphite and iron electrodes employing KI as a redox catalyst and a supporting electrolyte. Applying extremely high current density up to 270 mA/cm^2 permits rapid synthesis in a compact reactor and with small surface area electrodes.

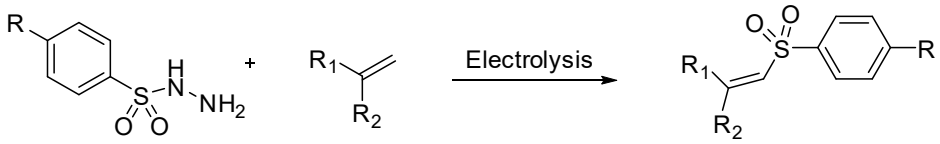

Fig. 1 Electrosynthesis of vinyl sulfones from sulfonyl hydrazides

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12-14 March, 2019

Paper code: 1214

Efficient and Facial Synthesis of Tetrahydrobenzo[*b*]pyrans using Sodium Cyclamate as a Green Catalyst

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Since its discovery in 1996 by Strecker, multicomponent reactions (MCRs) have been recognized as a powerful tool in synthetic chemistry to enable expedient access to various heterocycles and bioactive compounds. Since then, significant efforts have been devoted to expanding scope of the MCRs and achieving a number of molecules using various catalysts including, organocatalysts, natural catalysts, nanocatalysts, acidic organic and inorganic reagents, and ionic liquids [1]. Tetrahydrobenzo[*b*]pyrans as fused pyran scaffolds constitute an important class of heterocycles represent a "drug-like" structural motif with a wide range of applications in organic synthesis and medicinal chemistry. They display a wide range of biological and pharmaceutical activities. The MCRs of dimedone, aldehydes, and malononitrile toward the synthesis of tetrahydrobenzo[*b*]pyrans is catalyzed by a wide variety of catalysts, such as nanoparticles, Lewis acids, ionic liquids, and organocatalysts [1-3]. Herein, we report sodium cyclamate as a new organocatalyst for the synthesis of tetrahydrobenzo[*b*]pyrans in aqueous media under reflux conditions. Under the optimized conditions, various aldehydes, malononitrile, and dimedone substrates are able to provide good to high yields of the desired heterocyclic products. The structures of synthesized compounds were confirmed by IR, NMR spectroscopy, and melting point data.

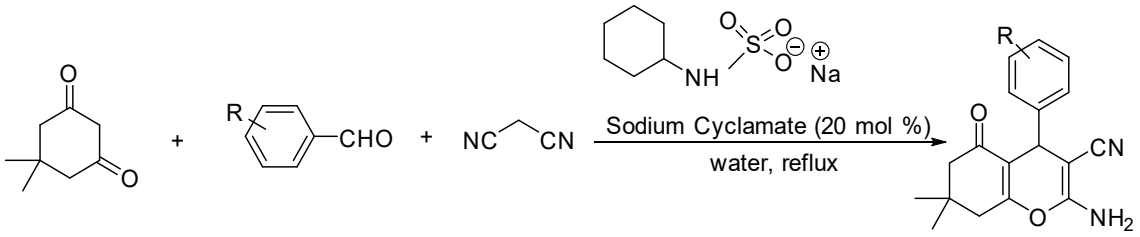

Fig. 1 Synthesis of tetrahydrobenzo[*b*]pyrans

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The 26th Iranian Seminar of Organic Chemistry
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Paper code: 1215

Antioxidant Function and *β*-LG Interactions of Zinc(II) Dithiocarbamate Complex

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A new dithiocarbamate complex was synthesized and characterized (Fig. 1) [1]. The *in vitro* antioxidant activity of Zn(II) complex was measured against 1,1-diphenyl-2-picrylhydrazyl radicals (IC_{50} = 36 mg L^{-1}). The interaction of the complex with bovine β-lactoglobulin (*β*-LG) presented that Zn(II) complex strongly quenched the fluorescence of carrier protein in static quenching mode. Thermodynamic analysis indicated that complex binding βLG was driven by favorable enthalpy and unfavorable entropy, and the major driving forces were hydrogen bonding and Van der Waals forces. The results of FT-IR and UV–visible measurements illustrated that the binding of complex to *β*-LG may induce conformational and microenvironmental changes of studied protein [2]. Molecular docking analysis confirmed that Zn(II) complex binds to residues located in the site II of *β*-LG.

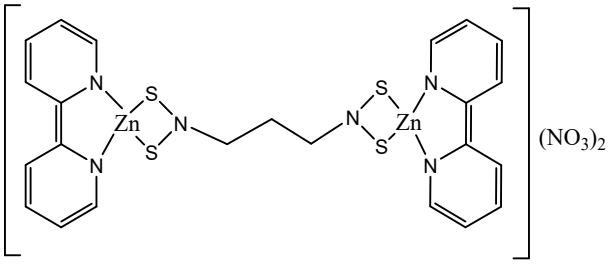

Fig. 1 The chemical structure of Zn(II) complex

References

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12-14 March, 2019

Paper code: 1216

Pd(II) Complex Based on the Propylenebis (Dithiocarbamate) Bridging Ligand: Synthesis, Characterization, Antioxidant Activity and Investigation on the Interaction with Human Serum Albumin

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A new bridging dithiocarbamate ligand and its Pd(II) metal ion complex (Fig. 1) was synthesized and characterized [1]. The *in vitro* antioxidant activity of the prepared complex was evaluated as radical scavengers against 1,1-diphenyl-2-picrylhydrazyl radicals (DPPH**.**). The results showed that this complex has a good antioxidant potential. The binding studies of this complexwith the model protein, human serum albumin (HSA), were investigated by employing biophysical techniques as well as computational modeling.The experimental results showed that the complex interacted with HSA by moderate binding affinity. Binding of complex to HSA caused strong fluorescence quenching of protein through static quenching mechanism. In the studied system, hydrogen bonds and Van der Waals forces were the major stabilizing forces in the drug-protein complex formation. Protein–ligand docking analysis confirmed that the Pd(II) complex bind to residues located in the subdomain IIA of HSA. All these experimental and computational results suggest that HSA may act as a carrier protein for the complex to deliver it to the target molecules.

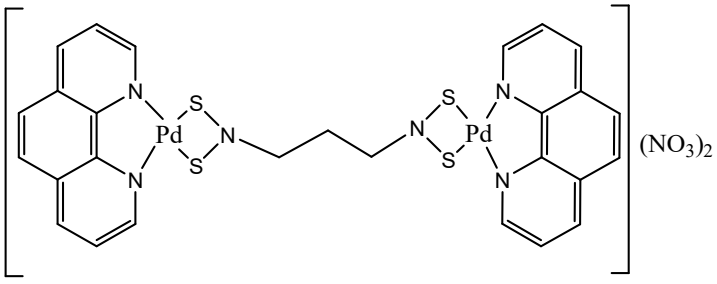

Fig. 1 The chemical structure of Pd(II) complex

References

[1] F. Shiri, S. Shahraki, S. Baneshi, M. Nejati-Y., M. Heidari, *RSC Advances,* **2016**, 108:106516-106526.

Paper code: 1218

Removal of Pb(II) Ion from Aqueous Solution by an Engineered Novel Chitosan Functionalized Schiff-Base Adsorbent

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A new adsorbent was synthesized to for the adsorption of Pb^{+2} from aqueous solutions. The magnetic chitosan-(d-glucosimine methyl) benzaldehyde, (MCS-Sch) was characterized by Fourier transform infrared spectroscopy (FT-IR), scanning electron microscope (SEM), energy dispersive X-ray spectroscopy (EDX), dynamic light scattering (DLS), vibrating sample magnetometer (VSM) and X-ray Diffraction (XRD) [1]. Batch adsorption experiments were done under various conditions, such as adsorbent dose, pH and contact time. The equilibrium data were fitted to Langmuir and Freundlich isotherm models [2]. The maximum monolayer capacity obtained from the Langmuir isotherm was 121.10 mg/g. The MCS-Sch was found to be regenerated effectively up to five efficient cycles of adsorption/desorption processes. The mechanism for Pb^{+2} adsorption onto MCS-Sch involved the interactions of nitrogen and oxygen atoms and also aromatic rings with heavy metal followed by their adsorption on the MCS-Sch.

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Paper code: 1219

Application of Modern Computers in *in-silico* Chemical Simulations

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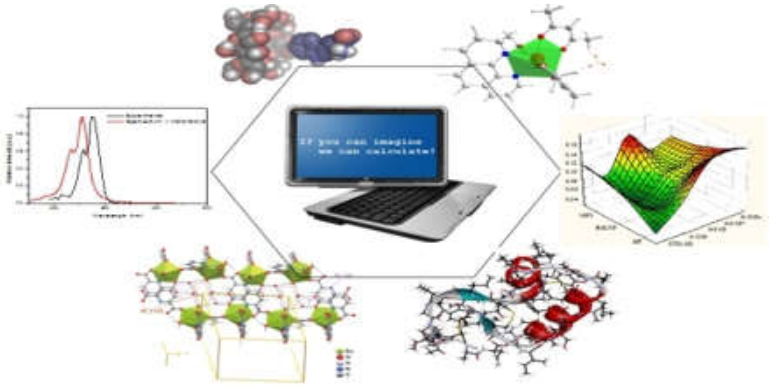
With the recent advances in computer hardware and programming codes for running quantum chemical and molecular dynamics simulations in a massively parallel manner, the *in-silico* tools have become a reality for modeling chemical systems of interest [1]. The software packages are becoming more advanced and intuitive. Their documentation has become very easy to follow and their graphical user interface, in some cases is so user-friendly that not much coding or quantum background is required for running simulations [2]. This provides an opportunity for the experimental chemical community to use these tools on a daily basis for exploring their systems. This project provides some examples of the application of quantum chemical calculations.



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The 26th Iranian Seminar of Organic Chemistry
University of Zabol
12-14 March, 2019

Paper code: 1220

Oxidation of Alcohols by TBHP Applying Fe(III) Complexes on the Magnetic Nanoparticles

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Fe_3O_4 nanoparticles were synthesized through co-precipitation method, and were coated with silica via a reverse microemulsion method [1]. Then iron(III) Schiff base complex was immobilized on the surface of Fe_3O_4@SiO_2. The Fe_3O_4@SiO_2/Fe(III) Schiff base catalyst was characterized with XRD, TEM, VSM and FT-IR techniques. XRD pattern of the catalyst showed a pure cubic phase. Spherical morphology with the size of about 60 nm was detected with TEM image of the catalyst. Also the paramagnetic property of the nanocatalyst was recognized using VSM technique, and FT-IR confirmed the grafting of iron complex on the Fe_3O_4@SiO_2 support. The catalyst was used for oxidation of alcohols in the presence of TBHP at 80 °C with conversion average 20-%95%, and 100% selectivity to corresponding carbonyls.

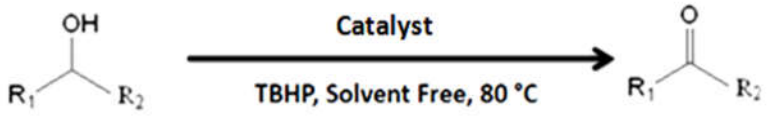

Fig. 1 Oxidation of alcohols in the presence of the catalyst

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The 26th Iranian Seminar of Organic Chemistry
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Paper code: 1221

Synthesis of Novel Spiro Uracil-1,4-dihydropiridine *via* One-Pot, Three Component Reaction

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Green synthesis of spiro uracil-1,4-hydropyridine has been reported via one-pot three component reaction in the presence of p-TSA as catalyst. Spiro oxindoles are classified as an important structural motif due to their distribution in diverse natural products, biologically and pharmaceutical activities such as the influenza virus [1], as inhibitors of the denque virus [2] and anti-cancer agents [3]. Therefore, we conducted a series of examination the chemistry of 5,6-dihydro-4*H*-pyrrolo[3,2,1-ij]quinolone-1,2-dione, in which the reactivity of the ketone carbonyl group of the 2-keto-amide unit was utilized. Thus, we were able to construct various spiro[3,3'-oxindoles] via three and four component combination [1-3]. Amongst, spirouracil-1,4-dihydropyridine moieties have shown important biological and medicinal activities. As a part of our ongoing interest in this context, we reported a simple and facile synthesis of a new type of spiro uracil-1,4-dihydropyridines (4) in the presence of *p*-TSA as catalyst (Figure 1) from starting 6-aminouracil (2), 3-oxo-3-phenyl propannitrile (3) and 5,6-dihydro-1*H*-pyrrolo[3,2,1-*ij*]quinolone 1,2(4*H*)-dione (1) in environmentally friendly solvent, EtOH/H_2O. The key features confirming the structures can be illustrated with the data of product (4).

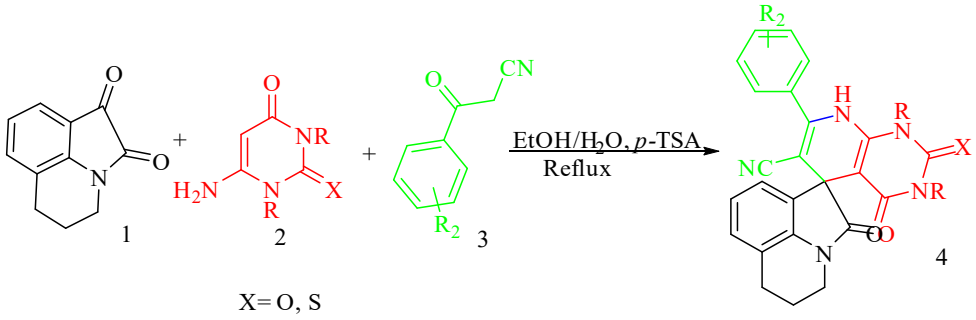

Fig. 1

Reference

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Paper code: 1222

Synthesis of Novel Tetrahydrospiro[1,4]diazepine

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Green synthesis of tetrahydrospiro[1,4]diazepine has been reported in EtOH/H_2O (1:1) in the presence of *p*-TSA as catalyst.Spirooxindoles are classified as important structural motifs due to their distribution in diverse natural products, biologically and pharmaceutical activities such as the influenza virus, as inhibitors of the virus and anti-cancer agents [1]. Therefore, we conducted a series of examination the chemistry of 5,6-dihydro-4H-pyrrolo[3,2,1-ij]quinolone-1,2-dione, in which the reactivity of the ketone carbonyl group of the 2-keto-amide unit was utilized. Thus, we were able to construct various spiro [3,3'-oxindoles] via three and four component combination [2-4]. Amongst, spirouracil-1,4-dihydropyridine moieties have shown important biological and medicinal activities. As a part of our ongoing interest in this context, we reported a simple and facile synthesis of a new type tetrahydrospiro[1,4]diazepine (3) in the presence of p-TSA as catalyst (Figure 1) by reaction of (*E*)-1-(2-oxo-2-phenylethylidene)-5,6-dihydro-1*H*-pyrrolo[3,2,1-ij]quinolin-2(4*H*)-one (1), 1,2-diaminophenyl derivatives (2) in environmentally friendly solvent, EtOH/H_2O.

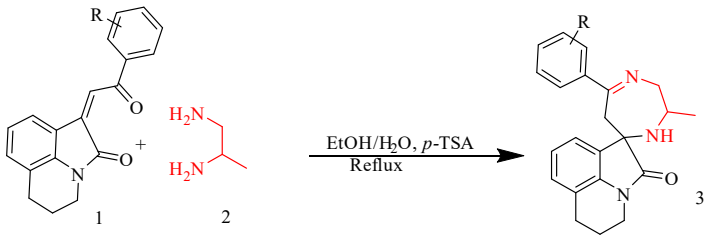

Fig. 1

References

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The 26th Iranian Seminar of Organic Chemistry
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12-14 March, 2019

Paper code: 1223

A Convenient Synthesis of Tetrasubstituted Pyrazoles from Nitrile Imines and 2-(Thioxothiazolidin-5-ylidene)acetates

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Pyrazoles are prominent structural motifs utilized extensively as pharmaceuticals and agrochemicals, as well as coloring agents [1]. For these reasons, the development of new methodologies for the synthesis of polysubstituted pyrazoles continues to be an active area of research in fine chemistry. Among the conventional approaches developed over the past decades for the construction of the pyrazole skeleton [2,3], the most commonly used the cyclocondensation of hydrazine derivatives with 1,3-disubstituted three-carbon units including 1,3-diketones and *α,β*-unsaturated ketones, and 1,3-dipolar cycloaddition reaction of nitrogen-based 1,3-dipoles with alkynes or alkenes. We now report a 1,3-dipolar cycloaddition/elimination process for the synthesis of pyrazole derivatives in the presence of Et_3N in acetonitrile (Fig. 1).

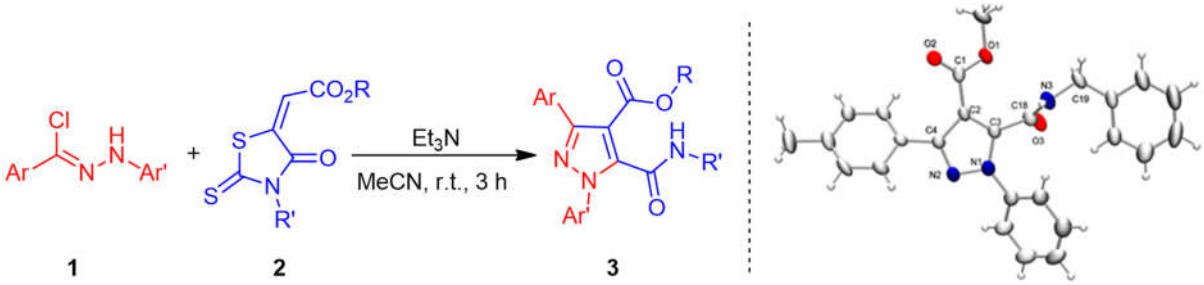

Fig. 1 Regioselective synthesis of tetrasubstituted pyrazoles.

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Paper code: 1224

Tautomerism in Phenytoin: A Theoretical Study in Gas Phase

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Phenytoin (Pht) has anticonvulsive, antiepileptic, and antiarrhythmic effects in the human organism (see Fig. 1). Tautomerismcan affect the chemical and biological activities of Pht. In the present work, the tautomerism in Pht has been investigated. The geometries of compounds were optimized at the B3LYP/6-31G (d,p) level of theory using the Gaussian 09 program [2]. As can be seen in Table 1, Pht with two H atoms on the N atoms of hydantoin ring is more stable than other tautomers with respect to the relative energy values (ΔE_g). The stability greatly decreases when two H atoms are located on the O atoms, (Pht4). The steric effects seem to be very effective in the stability of tautomers.

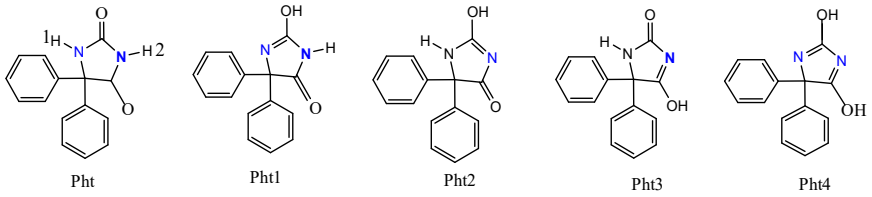

Fig. 1 The structures of phenytoin tautomers.

Table 1 The relative energies of phenytoin tautomers (in kcal mol^{-1}) in the gas phase

i	ΔE_g
Pht	0.00
Pht1	17.02
Pht2	18.61
Pht3	18.15
Pht4	31.54

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12-14 March, 2019

Paper code: 1227

Synthesize and Functionalize of the Novel Choline Chloride/2-Chloroacetylchloride/PEI Derivatives for Applications inEnzyme Stabilization

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Deep eutectic solvents (DESs) are new generation of solvents [1] which defined as a mixture of two or more components. DES may be solid or liquid which show a high melting point depression becoming liquids at room temperature. The DESs are so called natural deep eutectic solvents when constitute based on aminoacids, organic acids, sugars, or choline derivatives [2].

Herein, we present a novel DES based on functionalized polyethylene imine as hydrogen bond donor and choline chloride (Fig. 1). The application of the novel DES was investigated on the *uricase* stabilization and immobilization. The synthesized DES was shown high ability to the enzyme immobilization with interesting increase in the *uricase* activity up to 4 times.

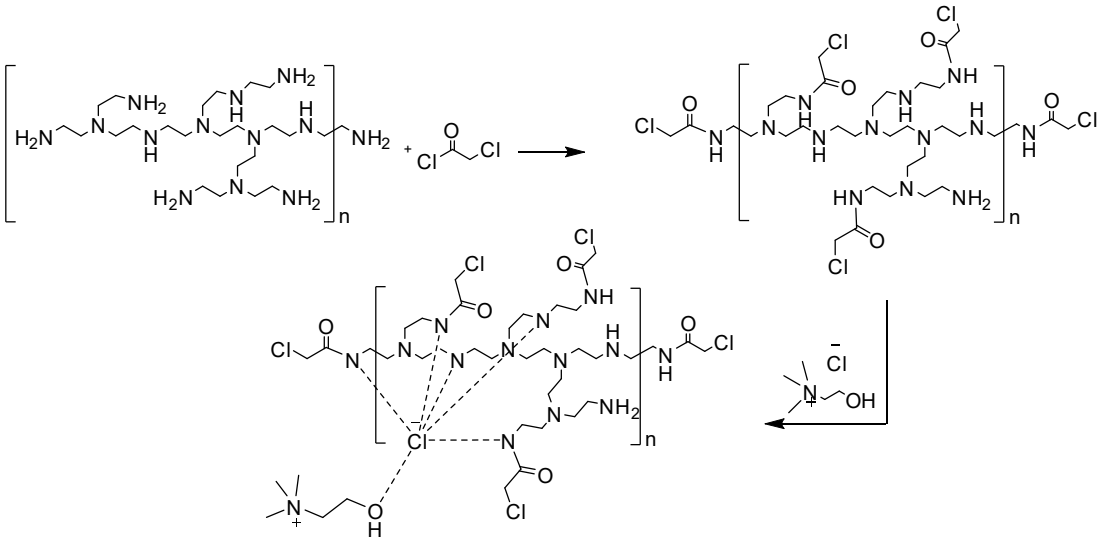

Fig. 1 Schematic synthesis of the novel deep eutectic solvent

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The 26th Iranian Seminar of Organic Chemistry
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12-14 March, 2019

Paper code: 1228

Synthesize and Functionalize of a Novel Organic-Inorganic Hybrid Material Based on Heteropoly Acid for Gene Delivery into the HEK-293T Cells

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[2] *Department of New Materials, Institute of Science and High Technology and Environmental Sciences, Graduate University of Advanced Technology, PO Box 76315-117, Kerman, Iran.*
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Gene therapy is a treatment option predicated on the underlying principle that disease can be addressed by introduction of exogenous genetic material into somatic cells of patients for the purpose of modulating gene expression of desired proteins [1] .Thus, the delivery of genetic material, DNA and RNA, can be utilized to combat various acquired or heritable diseases and under circumstances where natural immunity is abert has been reported here (Fig 1). In this regard, we report the synthesis of a novel hybrid materials based on heteropoly acid (HPA) for gene delivery application. At the first, choline chloride was reacted with 2-chloroacetyl chloride, and then heteropoly acid was added to the mixture. The synthesized organic-inorganic hybrid material was fully characterized and its biological application was investigated in gene delivery into the HEK-293T cell line.

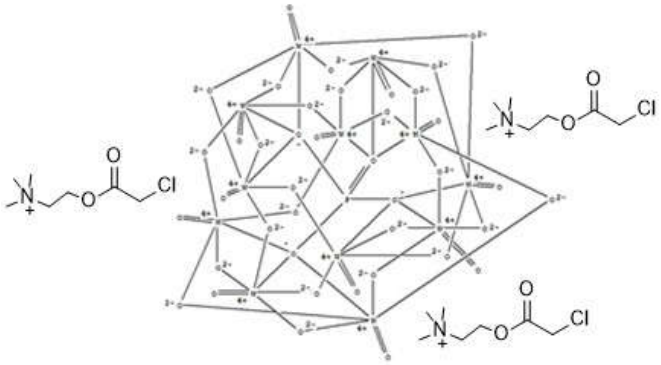

Fig.1 The chemical structure of the novel organic-inorganic hybrid material.

Reference

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The 26th Iranian Seminar of Organic Chemistry
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Paper code: 1229

Synthesis of Novel Bioactive Candidates 4-Aryl-1*H*-indeno [1,2-d]pyrimidine-2,5-diones using {[HMIM]C(NO$_2$)$_3$} as a Dual Role Ionic Liquid Catalyst: An Experimental and Theoretical Evaluation of Their Corresponding Antioxidant Activities

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An efficient one-pot multi-component reaction of 1,3-indanedione, arylaldehydes and urea leading to new series of 4-aryl-1*H*-indeno[1,2-d]pyrimidine-2,5-diones in the presence of a catalytic amount of 1-methylimidazolium trinitromethanide{[HMIM]C(NO$_2$)$_3$}, as a nano ionic liquid, at ambient temperature under solvent-free conditions is reported. Advantages of the present protocol are the operationally simple and simple work-up, good to excellent yields, short reaction times, dual catalytic activity and reusability of the described catalyst. Finally, considering the role of oxidative stress in the progress of many ailments, the synthesized indenopyrimidine derivatives were screened for their corresponding anti-oxidant activities. Theoretical investigation of anti-oxidant activities of the target molecules were also checked out.

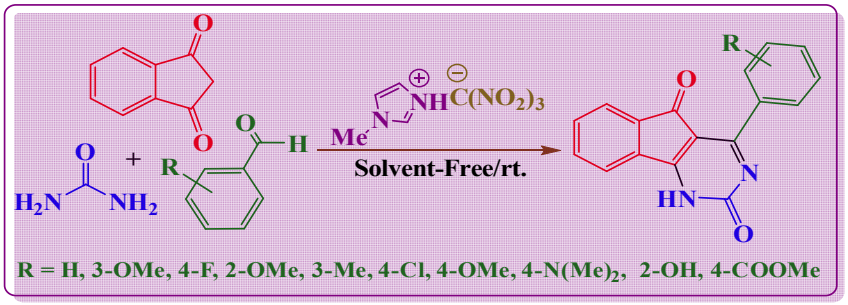

Fig. 1 Multicomponent synthesis of novel substituted 4-phenyl-1*H*-indeno[1,2-d]pyrimidine-2,5-diones

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12-14 March, 2019

Paper code: 1230

Synthesis and Antibacterial Activity of a New Bipyridyl Complex

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The Schiff base molecules are a significant category of organic compounds with biological activities such as antitumor, antifungal, antibacterial, antidiabetic and anthelmintic properties [1-3]. El-Sonbati and his colleagues [4] investigated the synthesis and characterization of Cu(II), Co(II), Ni(II) and Cd(II) complexes with 3-[(2-hydroxy-3-methoxybenzylidene) hydrazo]-1,3-dihydroindol-2-one ligand. The ligand and cadmium (II) complex exhibited good antibacterial properties against Staphylococcus aureus bacterium.

In this study, the synthesis, characterization and structure determination of a cadmium (II) complex with schiff base ligand of 2,5-bis(3-pyridyl)-3,4-diaza-2,4-hexadiene (3-bpdh) was reported. The antibacterial activity of the ligand and the complex against the Gram-positive bacterium of Staphylococcus aureus is evaluated using disk diffusion method. The results represented that the cadmium(II) acetate had the highest antibacterial activity in comparison to other compounds. Figure 1 shows the structure of complex with this Schiff base ligand.

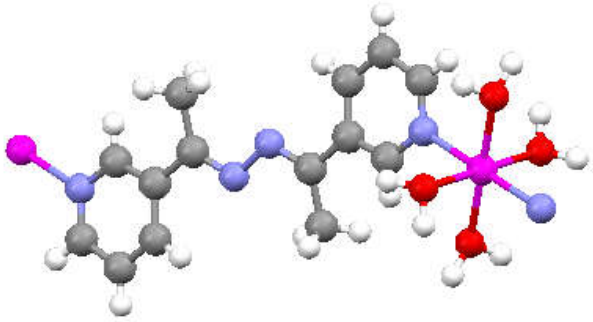

Fig. 1 Cadmium(II) complex structure

References

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The 26th Iranian Seminar of Organic Chemistry
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Paper code: 1231

Defect Engineering of a Chromium-Based Metal–Organic Framework for Catalysis

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MIL-101(Cr), one of the most robust and stable MOFs, is widely used in many scientific fields [1,2]. The presence and nature of structural defects of the MIL-101(Cr)-NO_2 has been recognized as a key factor shaping the material's physical and chemical behavior. In this work, the formation of the "missing linker" defects have been investigated for the Prins coupling of β-pinene and formaldehyde as shown in the Fig. 1. The results indicate that the defects have a significant impact on Lewis and Brønsted acidity of the MOF.

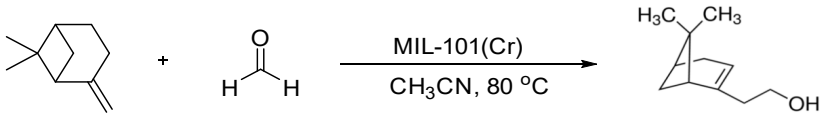

Fig. 1 The Prins coupling of β-pinene using MIL-101(Cr) as catalyst

References

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Paper code: 1232

Removal of Orange II R and Red 12 Dyes from Water with Montmorillonite and Chitosan Nanosheets

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[2] *Department of Chemistry, Safadasht Branch, Islamic Azad University, Tehran, Iran*
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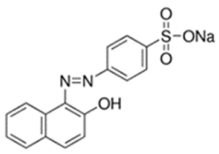
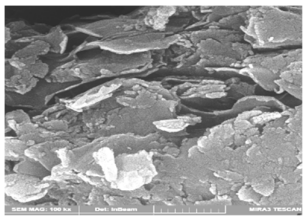
Colors are organic compounds with a complex, toxic, carcinogenic, mutagenic and non-degradable biological structure and one of the most important wastewater pollutants in textile Industries. The montmorillonite-chitosan composite could provide hydrophobicity and functional groups to enhance the performances of montmorillonite in wastewater treatment. The composites showed good abilities to remove the pollutant, such as heavy metals and dyes. In this work, montmorillonite was modified with Chitosan with the purpose of synthesizing multifunctional adsorbents to adsorb hydrophobic organic contaminants, heavy metal cations, and dyes from water [1]. Montmorillonite was modified with different amounts of chitosan to obtain chitosan/montmorillonite bio nanocomposites (CSMMT) which the sodium ions in montmorillonite layers are replaced by chitosan. The structural and surface characteristics of the raw materials and bio-nanocomposites were analyzed. XPS results showed that the obtained bionanocomposites had MMT-rich surfaces with chitosan essentially intercalated in the host clay galleries [2,3]. We have observed in our methods and with compared to MWCNT, That The obtained results suggested that C/T-Mt could be a multi-functional adsorbent for the effective up take of different types of contaminants from water.



Orange II R structure



CS-MMT Nanosheets

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12-14 March, 2019

Paper code: 1233

Post-modification a Mesoporous Metal-Organic Framework: Synthesis and Structural Studies

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In this work, a functionalization technique, solvent assisted ligand incorporation (SALI), was applied to efficiently incorporate carboxylate-based functionalities in a Zr-based metal-organic framework [1,2]. Unlike previous metal node functionalization strategies, which employ dative bonding to unsaturated metal sites, SALI presents functional groups as strongly bound moieties to the Zr_6 node. Using SALI, various compounds (2,2′-bipyridine-4-carboxylate, 2,2′-bipyridine-4-phosphonate, 4-TEMPO carboxylate and 4-aminobenzoate) on the Zr_6 nodes of the MOF efficiently were attached (Figure 1).

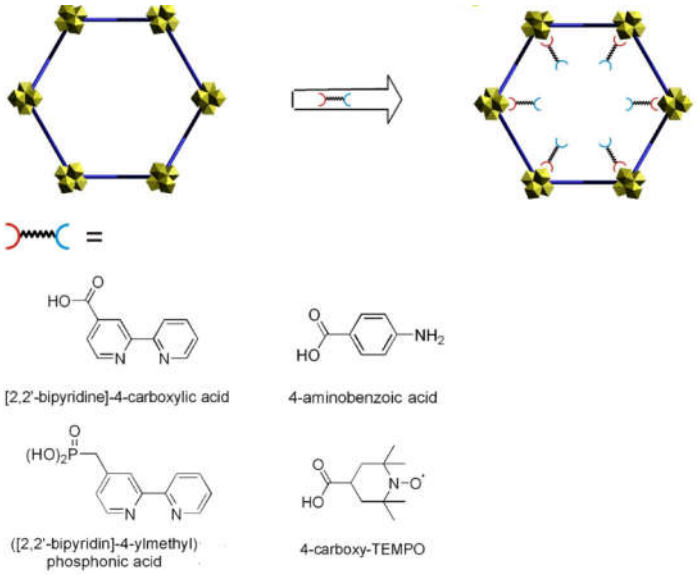

Fig. 1 Functionalization of the mesoporous MOF

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The 26th Iranian Seminar of Organic Chemistry
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Paper code: 1234

Advanced Computational Methods for Investigating in Liquid Phase

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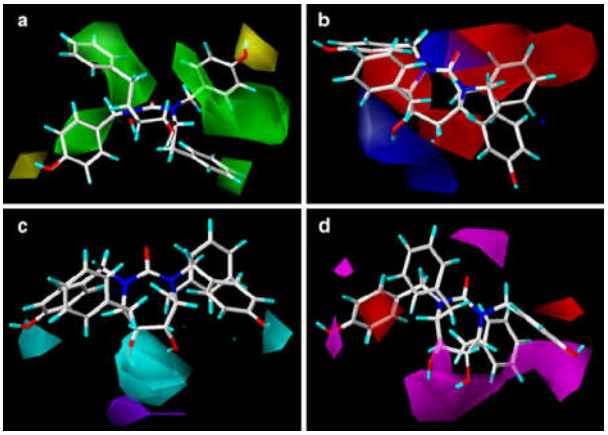
Knowledge about local properties is extremely helpful for the analysis of molecular structures and interactions. Moreover, it is a valuable source of information for the characterization of dynamic processes and facilitates the interpretation of experimental data. Calculations provide additional insight allowing the targeted study of specific structures. In this way, it is possible to quantify the contributions of, e.g., solute and solvent molecules [1] or adsorbents on solids. We present novel methods for the calculation of local properties with a focus on Raman [2] and Infrared spectroscopy [3] applied, among others, to solvents used in Li-ion batteries as well as an in-depth study of artificial water oxidation catalysts. In this study, all compounds in the liquid phase were investigated and all data were taken at the highest possible computational level.



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12-14 March, 2019

Paper code: 1236

Synthesis of Starch Nanocatalysts and Use in the Green Synthesis of Heterocyclic Naphthyropane Derivatives

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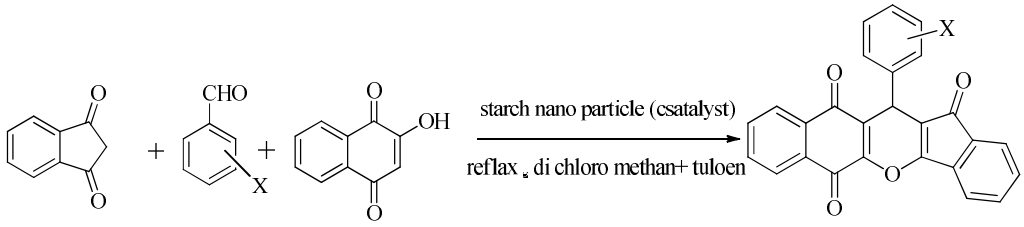
The development of environmentally benign, efficient, and economical methods for the synthesis of biologically interesting compounds remains a significant challenge in synthetic chemistry [1]. The use of Nano-catalysts to carry out and advance chemical processes today has become an integral part of the research on green chemistry. In this field, the use of modified catalysts with organic chemical particles or natural chemicals with specific chemical properties plays a role in the synthesis of organic compounds, especially derivatives of heterocyclic compounds [2]. Synthesis of nafthopyran is important because of its extensive biological and therapeutic properties such as anti-bacterial, anti-viral and anti-inflammatory [3]. Taking in to account the importance and the principles of green chemistry the use of solfonating starch nano particle as a new catalyst, non-toxic and effective for compression benzaldehyde derivatives, 2-hydroxynaphtalene-1,4-dione and indene-1,3-dionehas been used. One-pot quantitative procedure for the preparation of functionalized 12-arylbenzo[g]indeno[1,2-b]chromene-6,11,13(12*H*)-trione Derivatives in the presence of solfonating starch nano particle under reflux conditions:



The advantages of this approach are; the use of available, cheap and non-toxic catalyst, high efficiency, the short of time reaction with less pollution.

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The 26th Iranian Seminar of Organic Chemistry
University of Zabol
12-14 March, 2019

Paper code: 1237

Synthesis and Characterization of Copper-Salen Complex on Periodic Mesoporous Organosilica and its Application in Synthesis of Pyrano (2,3-d) Pyrimidine Derivatives

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Nanoporous materials are porous in the nanoscale and have very diverse, regular structure with a high ratio, selectivity of shape and size, which has resulted in their application in catalytsis, purification, and separation [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. In order to enhance the applications of nanoporous compounds in various fields such as catalysts, chemical sensors and chromatography, surface of silica mesoporous must be functionalized with appropriate functional groups [2, 3]. Herein, we report the synthesis of copper(salen) complex immobilized on periodic mesoporous organosilica and its application as catalyst for the synthesis of pyrano (2,3-d) pyrimidine derivatives by using aldehydes, malononitrile and barbituric acid under solvent-free conditions. The activity and recovery of the catalyst under reaction conditions were also examined (Fig. 1).

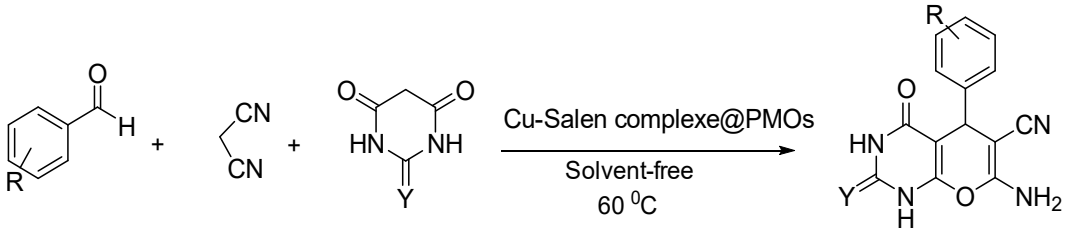

Fig. 1 Preparation of pyrano (2,3-d) pyrimidine derivatives catalyzed by the Cu(II)-Salen complex@PMOs

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The 26th Iranian Seminar of Organic Chemistry
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12-14 March, 2019

Paper code: 1238

Preparation of Sulfamic Acid-Functionalized Fe_3O_4@Carbon as an Efficient Nanocatalyst for One-Pot Synthesis of 9,9-Dimethyl-12-phenyl-8,9,10,12-tetrahydro-11*H*-benzo[a]xanthen-11-one Derivatives

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In the past decade, magnetic nanoparticles have attracted the attention of many researchers for their excellent properties. Magnetic nanoparticles, due to their large specific surface against oxidation and agglomeration are highly sensitive and chemically very reactive, the surface of magnetic nanoparticle can be modified with a layer of silica, polymer, carbon or metal hydroxides. Among these, carbon-coated magnetic nanoparticles have been considered for many advantages compared to polymer and silicone coatings. Carbon materials from this precursor, resorcinol-formaldehyde resin, glucose and dopamine, have a much higher chemical and thermal stability, and they are impermeable to most chemicals and fully protect internal magnetic cores [1,2]. One of the nano-structures that are nowadays of great interest is nanoparticles with core-shell structure. These nanoparticles have special applications in the biosensors, catalysts, and also in the paint industry. Providing a good surface for the stabilization of terminal functional groups [3] In this study, we fixed the sulfamic acid groups on the carbon-modified magnetic core-shell nanoparticles and applied as efficient and very active nanocatalyst for the synthesis of biologically active of 9,9-dimethyl-12-phenyl-8,9,10,12-tetrahydro-11*H*-benzo[a]xanthen-11-one derivatives (Fig. 1).

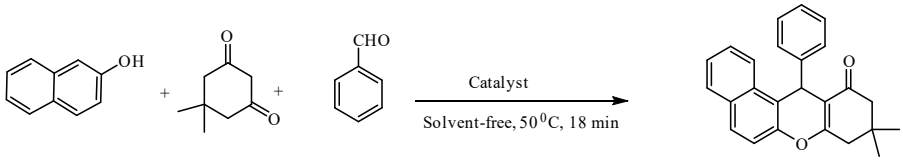

Fig. 1 Synthesis of 9,9-dimethyl-12-phenyl-8,9,10,12-tetrahydro-11*H*-benzo[a]xanthen-11-one derivatives

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12-14 March, 2019

Paper code: 1240

The Effect of Different Supports Calcineal at Different Temperatures on the Catalytic Activity for Fischer-Tropsch Synthesis

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In this research work, the alumina, titanium and zeolite supports, are meshed and then calcinated for 6 h at different temperatures, which has a great effect on the formed phases, surface area, cavity volume and cavity size [1]. A three-metal catalyst (Ce, Co and Fe) is provided with these supports using a wet impregnation method. The catalyst was tested for synthesis of gases to light olefins by Fischer-Tropsch synthesis reaction in a fixed bed micro-reactor and the analysis of the products was carried out using a chromatograph gas machine. For all cases, the functionality, selectivity and the ratio of o/p was investigated and the best reactor conditions for these catalysts were prepared by wet inoculation method as follows: The alumina support was entered the reactor at 400, 600, 700 and 800 ºC, and the best temperature was 700ºC which had high activity and light olfines. The titana support was entered the reactor at 400, 500, 600, 700, 800 and 900 ˚C, and the best temperature was 800° C which had high activity and light appropriate olfines. The zeolit support was entered the reactor at 400, 500, 600, and 800C, and the best temperature was 800 ºC which had high output. These temperatures were considered as optimal temperatures than the other temperatures. Finally, in order to determine the characteristics of the catalysts, pre-produded and calcinated samples were identified before and after the test of the reactor using techniques such as SEM (determine the catalyst texture) and BET (determine the surface area, size, and pore size).

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The 26th Iranian Seminar of Organic Chemistry
University of Zabol
12-14 March, 2019

Paper code: 1241

Zr-Based Metal-Organic Framework as an Efficient Nanocatalyst for Three-Component Synthesis of Quinazolin-4(1*H*)-one Derivatives

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The framework of UiO-66 ($Zr_6O_4(OH)_4(bdc)_6$; bdc^{2-}= 1,4-benzenedicarboxylate), a zirconium-based MOF with very high surface area, is constructed of $Zr_6O_4(OH)_4(O_2CR)_{12}$ clusters in which the μ_3-O and μ_3-OH ligands originate from water present during the synthesis and the carboxylate groups are part of the bdc^{2-} ligands linking the clusters together [1]. The remarkable thermal and chemical stability of this Zr^{4+} based MOF material prompted us to use this MOF for the first time as a catalyst for the synthesis of 2,3-dihydroquinazilin-4(1*H*)-ones [2, 3], employing three-component reactions of isatoic anhydride with primary amines (or ammonium acetate) and aldehydes under thermal solvent-free conditions (moderate to good yields) (Fig. 1). The catalyst is stable under the reaction conditions as confirmed by comparison of the powder XRD and FT-IR of the fresh and reused catalyst.

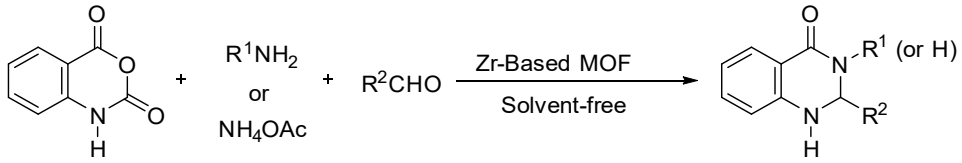

Fig. 1 Preparation of 2,3-dihydroquinazilin-4(1*H*)-ones using the Zr-based MOF

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The 26th Iranian Seminar of Organic Chemistry
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12-14 March, 2019

Paper code: 1242

Superparamagnetic Fe_3O_4 Nanoparticles Applicable in the Removal of Cd^{2+}

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Iron-based magnetic nanoparticles, such as magnetite (Fe_3O_4), have unique features, such as large surface area-volume ratio and diminished consumption of chemicals, reached without any secondary pollutant [1]. Fe_3O_4 nanoparticles with particle size less than 40 nmshows superparamagnetic behavior. Superparamagnetism is a magnetic behavior which appears in small ferromagnetic or ferrimagnetic nanoparticles when their particle size is smaller than a single domain and they have no magnetic memory [2,3]. In this study, we present synthesis of a new metal organic complex formulated as $[Fe(bpy)_3][Fe(dipic)_2]_2 \cdot 7H_2O$ (**1**) (Fig. 1), and preparation of superparamagnetic Fe_3O_4 nanoparticles by thermal decomposition of this complex at 600ºC. Fe_3O_4 nanoparticles were utilized for removal of Cd^{2+} from water. The results showed that Fe_3O_4 can act as an effective and recyclable adsorbent capable to remove Cd^{2+} from contaminated water.The adsorption of cadmium on the surface of the nanoparticles of Fe_3O_4 reaches equilibrium after 120 min at pH 6.

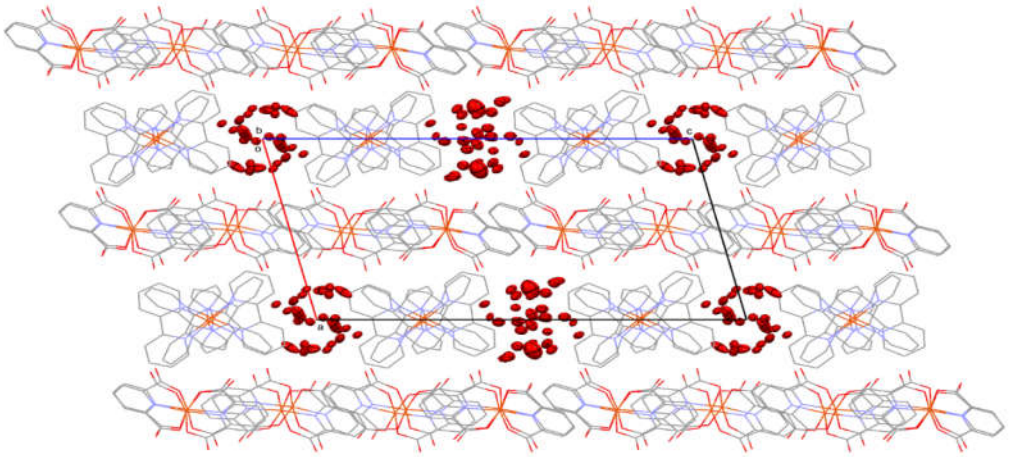

Fig.1 The view of solvent channels in the compound **1**

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The 26th Iranian Seminar of Organic Chemistry
University of Zabol
12-14 March, 2019

Paper code: 1243

New Complex Based on Zn(II) and Quinoline: A Supra Precursor for Fabrication of ZnO Nanoparticles

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Quinolines and their derivativesplay an important role in a variety of pharmacologically active synthetic and natural compounds such as antimalaria drug [1], effective against the parasites Leishmania, effective against the protozoan parasite Trypanosoma cruzyas agent of Chagas' disease as well as for a number of other diseases [2,3]. On the other hand, the synthesis of many antibiotics and anti-tumors is based on quinoline derivatives. In this study, a new complex of $[Zn(NCS)_4].2(C_9H_8N)$ **1** has beensuccessfully synthesized by sonochemical irradiationand structurally characterized by single crystal X-ray diffraction. In the crystal lattice of complex **1**, the $[Zn(NCS)_4]^{2-}$ complex anion are stacked in hexagonal-like columns forming 2D layers, each column includes an organic chain formed from one of $[C_9H_8N]^+$ organic cations where the other cation separates between layers. Magnetic studies at room temperature reveal that complex **1** is a weak ferromagnet.Complex **1** was used as a precursor for the preparation of ZnO nanoparticles with an average particles size of 50 nm by a thermal decomposition process.

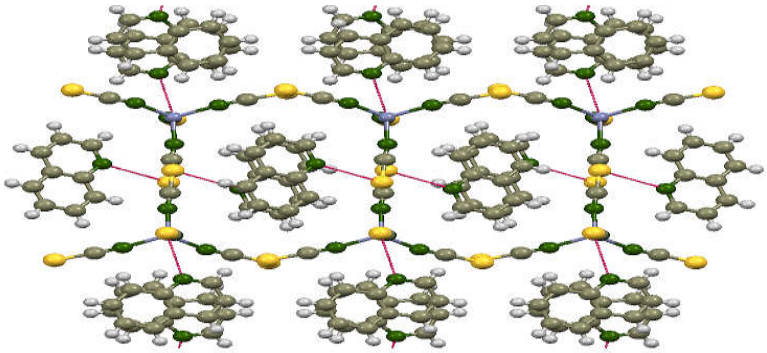

Fig. 1 Packing view of the structure of complex 1

References

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University of Zabol
12-14 March, 2019

Paper code: 1244

Doped Carbon Nanostructures; Synthesis by Chemical Vapor Deposition and Their Applications as Sensor, Catalyst and Adsorbent

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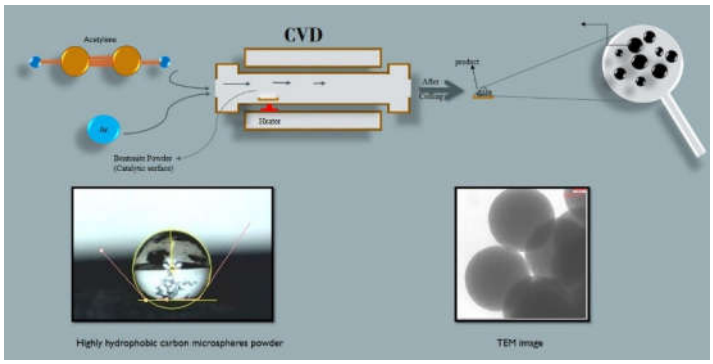
Doped carbon nanostructures (CNTs, graphenes, carbon fibers and fullerenes), have been attracted a worldwide interest as novel nanostructures [1]. Several methods such as spray pyrolysis, laser deposition, chemical vapor deposition (CVD) and hydrothermal have been employed to produce these materials. These materials could be used in electronic devices [2], supercapacitors, electrochemical catalysts, lithium ion batteries, Sensor and as the catalyst for chemical reactions [3]. However, many aspects in the synthesis applications of these compounds, especially in the case of doped materials, are unknown and needs to be investigated. Therefore, during the last 5 years, we have focused to develop efficient and economic methods for the synthesis of simple and doped carbon nanostructures. Moreover, some studies have been performed about the application of these compounds as catalyst in chemical and electrochemical reaction, adsorbent and sensors. It should be considered that because of the high surface/mass ratio of these compounds, they could be suitable nanocatalysts in various transformations. Meanwhile, they can be used as efficient sensors for different molecules such as toxic gases, pollutants and drugs. It is noticeable that when the nanostructures doped with heteroatoms (such as N, B, S and P), their properties will be changed effectively and doping is well-known as an efficient method to obtain the desired properties for each special application.



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Paper code: 1245

Preparation and Assesment of Althaea Officinalis -Loaded Electrospun Nano Fiber

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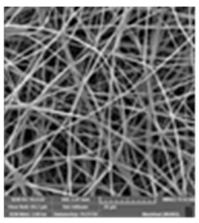
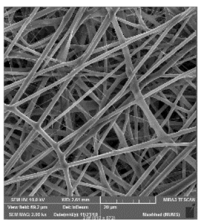
The use of nanofiber scaffold has attracted a lot of attention in recent years. For example, nanofiber scaffold is considered as suitable substrates for tissue engineering, enzymes and catalysts stabilization, wound dressing, controlled release of drugs and artificial vessels, and in cosmetic and sanitary industries. Edible and biodegradable microspheres of chitosan were prepared using glycolic acetic acid solvent [1,2]. Three different concentrations of chitosan and extract of *Althaea officinalis* solution (5%, 10%, 15%) was prepared. The optimization of electrospinning process and solution parameters, such as distance between needle tip, collector, electrical voltage, solution flow rate and needle size, was done by using response surface method to obtain uniform chitosan nanofibers(Fig.1). The electrostatic voltage at these three concentrations was 10 KV, the distance between the tip of the needle and the collector at three concentrations was fixed at 20 cm with the flow velocity constant of 0.5 ml/h. Based on the results, the concentration changes of the Althaea officinalis extract showed a significant effect ($p \leq 0 / 05$) on the diameter of the fiber. As the density of concentration of the extract Althaea officinalis was increased, the diameter of the fibers increased.


(a)


(b)

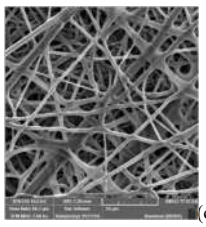

(c)

Fig. 1 The image of the electron microscope of the chitosan solution electrolytic network and the extract of 5% (a), 10%(b) , 15% (c)

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Paper code: 1246

Preparation and Evaluation of Electrospun Nanofiber Membrane Loaded with Green Tea Extract

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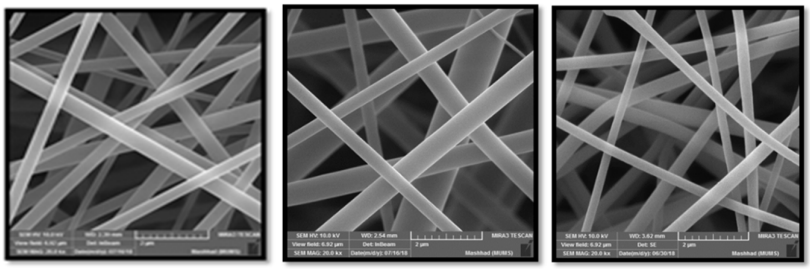
Electrospinning is a simple and inexpensive technique used for many purposes, such as tissue engineering, textiles, air and water treatment filter, solar cells, and producing really thin polymer fiber as drug delivery systems [1,2]. In this research, we prepared a nanofiber of zein polymer using electrospining method. Moreover, a modified electrospinning setup was used to successfully load Green Tea Extract (up to 24.5% w/w) in ultrathin electrospun zein fibres. Tea contains polyphenols that have effects like reducing inflammation and helping to fight cancer. Green tea is about 30 percent polyphenols by weight, including large amounts of a *catechin* called EGCG. Catechins are natural antioxidants that help prevent cell damage and provide other benefits [3]. Loading of plant material, through electrospinning, can accelerate their remedial potential to many folds. This process maximizes the therapeutic potential. The morphology of the nanofibers/green tee was characterized by scanning electron microscopy, Fourier transform infrared spectroscopy, and thermogravimetric analysis. As SEM images shown in Fig. 1, nanofibers were successfully fabricated by the electrospinning technique.



(A) (B) (C)

Fig. 1 Scanning electron microscopy (SEM) images of fiber electrospun solution: (A) green tea extract 5%, (B) green tea extract 7.5%, (C) green tea extract 10%

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Paper code: 1247

Fabrication and Study of *Nigella sativa*-Loaded Electrospun Nanofiber

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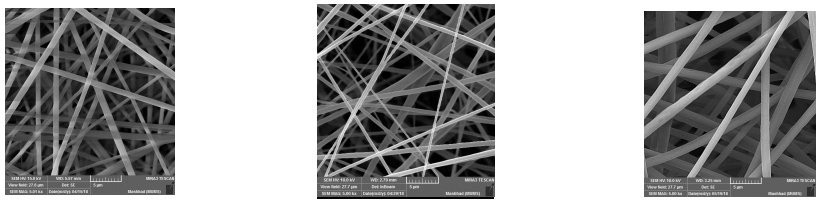
In this study, Zein and Nigella sativa solution was prepared with three different Nigella sativa concentrations of 5, 10, and 15 %w/v, and was electrospun. The voltage of electrospinning process at these three concentrations being 20kv; the distance between the tip of the needle and the collector in the three concentrations being 15cm; and the flow rate at the three levels being 4ml/h, were all constant. Results showed that changes in the concentration of Nigella sativa oil have a significant effect ($p \leq 0.05$) on fibre diametre; increasing the concentration of the Nigella sativa oil results into the increase of fibre diametre. Recently, biodegradable polymers have been widely used as drug carriers in the human body [1, 2]. These polymers have been used because they have very low, and near-to-zero, effects on human body; and one of their most important characteristics is that they are suitable carriers for drug delivery, and have direct response to physiological stimuli; and they are also non-official and economical [1, 3]. The purpose of this study is to produce microfibre of Zein protein and Nigella sativa oil with glacial acetic acid solvent. It will also investigate the effect of changing Nigella sativa oil concentration on the morphology and diametre of fibres.



a b c

Fig. 1 The imaje of the electron microscope of the zein solition electrolytic network and the extract of 5% (a), 10% (b), 15% (c)

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Development of Carbon Quantum Dot Decorated Multi-Walled Carbon Nanotubes Incorporated into the Recycled PET Nanocomposites for Dye Remediation

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Poly(ethylene terephthalate) (PET) is a thermoplastic polyester broadly used in various areas [1]. PET recycling is obviously a waste-management strategy which is receiving increasing attention that can decrease environmental influence and resource depletion. The great specific surface areas of multi-walled carbon nanotubes (MWNT)s, their hollow and layered structures, cause to they be an ideal sorbent [2, 3]. Conjugation of carbon quantum dots (CQD)s as capping agents on MWNTs surface not only prevents the formation of nanotubes aggregates but also can improve the removal efficacy of the contaminants. In this study, first the MWNTs surface was functionalized by CQDs. Then, nanocomposites (NC)s were prepared by incorporation of MWNT/CQDs into the recycled PET (r-PET) (Fig. 1A). The prepared NCs were further employed to eliminate methylene blue (MB) from aqueous media. MB sorption capacity values for all r-PET/MWNT/CQD NCs were not only higher than r-PET but also were higher than r-PET/MWNT NC 4 wt% (without CQD) (Fig. 1B).

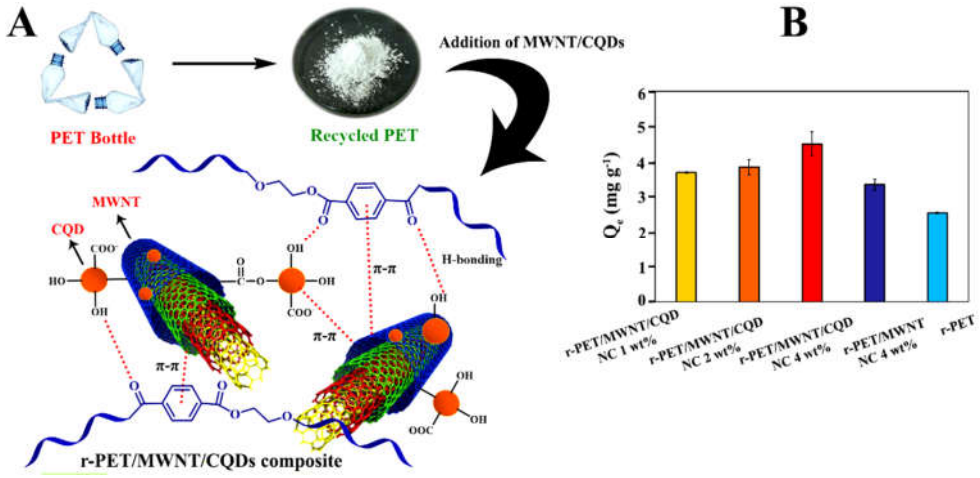

Fig. 1. (A) Schematic interaction between MWNT/CQD and r-PET matrix, (B) comparison between MB adsorption capacities by different samples

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Gold Nanoparticles: Synthesis and Application in Drug Delivery

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Inorganic nanoparticles and their combination with organic materials forming hybrid materials possess unique physical, chemical, optical and electrical properties which make them different and more applicable than large size materials. These types of platforms can be synthesized by different organic, inorganic or hybrid of organic and inorganic materials but among all these inorganic platforms are of most important for diagnosis and simultaneous therapy due to their easy modification, stability and high drug loading capacity [1]. Metal nanoparticles specifically gold nanoparticles have abundant use in the field of biotechnology and biomedicine because they have large surface bio conjugation with molecular probes [2]. In this study, we synthesized Au-peptide nanoparticles using organic reducing agents under microwave and ultrasound irradiation, and then, their anticancer effects were investigated. The resulting Au-nanoparticles were characterized using different techniques such as UV-Vis spectroscopy, Fourier transform infrared spectroscopy, X-ray diffraction, scanning electron microscopy, and transmission electron microscopy. The interaction of calf thymus DNA with Au-nanoparticles was studied by UV-Vis spectrophotometry at 300 and 310 K. $[L]_{1/2}$, ΔG^0, ΔS^0, and ΔH^0 values at 300 K were found to be 0.24352 mM, 26.729 (KJ/mol), 0.8574 (KJ/mol.k), and 286.435 (KJ/mol), and at 310 K, 0.33248 mM, 19.17 (KJ/mol), 0.8587 (KJ/mol), and 286.435 (KJ/mol), respectively. Kapp, n and g values were obtained 83.24, 6.74 and 4 at 310 K, respectively.

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Michael Addition Reactions in Dyeing of Protein Fibers with Quercetin

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The Michael reaction typically refers to the base catalyzed addition of a nucleophile (Michael donor) to an activated *α,β*-unsaturated carbonyl-containing compound (Michael acceptor). Base catalysts are often unnecessary in the case of amines, because of the strong nucleophilicity of the nitrogen atom, whereas weak bases aid in deprotonation of thiols [1]. Laccases are able to initiate nucleophilic amination of poly phenolic compounds with primary aromatic amines, resulting in the formation of the corresponding mono-aminated and di-aminated quinones [2]. The enzyme-generated quinones could react with proteins fibers [3]. Natural colorants are composed of polyphenolic compounds, so, they are good substrates for laccase to be converted to related quinones. Quercetin, a plant flavonol from the flavonoid group of polyphenols, is found in many fruits, vegetables and leaves. In this study a new idea was studied for making a covalent bond between quinones formed by laccase from quercetin, as a natural dye, and nucleophilic side chains. (Fig. 1). FTIR results and dye fixation measurements show the possibility of using this method to obtain colored wool with high wash fastness.

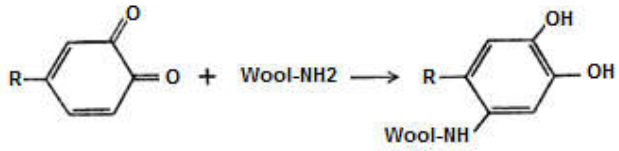

Fig.1 Tentative mechanism of Michael reaction of oxidized quercetin to amino group of wool

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Green Synthesis of Silver Nanoparticles using Grape Leaf, Stability and Antimicrobial Evaluation

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The chemical reduction of a silver salt by a reducing agent is the most common method for synthesis of silver nanoparticles (AgNPs). Chemical reducing agents may be associated with biological hazards or environmental toxicity. Therefore, there is growing interest to develop green methods for synthesis of AgNPs. Many reports are available on the biosynthesis of AgNPs using plants [1, 2]. Grape leaf is traditionally used as a cuisine, colorant in textile natural dyeing to obtain yellow shades and in indigenous medicine, grape leaves are used to stop bleeding, inflammation, and pain. Grape leaves contain high phenolic compounds [3]. In this study, the grape leaf extract solution was used to synthesize AgNPs. The tentative mechanism of AgNPs synthesis in the presence of polyphenols is illustrated in Figure 1. The formation of AgNPs was followed by UV–Vis absorption spectroscopy. The shape and size of biosynthesized AgNPs were considered by transmission electron microscopy (TEM). The stability of silver nanoparticles was investigated by dynamic light scattering (DLS) and UV-Vis spectroscopy. The antibacterial efficiency of AgNPs against *Escherichia coli* was investigated. In the presence of grape leaf extract; the nanoparticles showed stability at least for one week and exhibited excellent antibacterial activity.

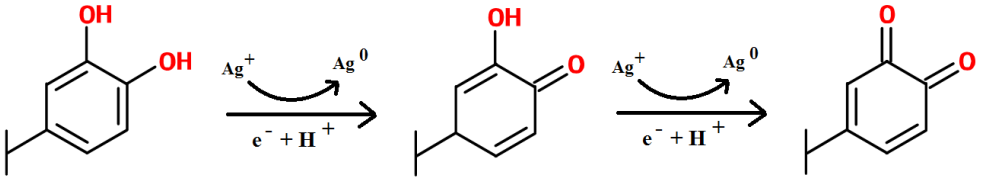

Fig. 1 Tentative mechanism of synthesis AgNPs by ortho-dihydroxy polyphenols

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Synthesis of Halloysite/Zein Nanocomposite for Controlled Drug Delivery of Phenobarbital Sodium

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Today, Halloysite nanotubes (HNTs) are used due to its high internal diameter, abundance, non-toxicity, high compatibility and availability in drug release systems. By adding a coat and synthesis a nanocomposite, the release rate of the drug can be further reduced. In this study, zein protein was used for coating and fabricate nanocomposites. Fabrication of nanocomposites was done via creating an electrostatic force between Halloysite and Zain via adjusting the pH via layer by layer synthesis. Synthesis of nanocomposite was assessed by FT-IR, Zeta potential, scanning electron microscopy, dynamic light scattering, X-ray diffraction, differential scanning calorimetry, and thermogravimetric analysis. Then, loading and release of the phenytoin sodium from pure nanotubes and nanocomposites was investigated using Ultraviolet-visible spectrophotometry. The results showed that the loading of the drug by the nanocomposite was twice as high as the loading of pure halloysite. The release rate of the drug also dropped dramatically, so that 50% of the drug loaded in halloysite was released in the first hour and the same amount of drug was released from the nanocomposite within 9 hours.

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Copper (II) acetate Intermolecular C (sp2)-H Amination of Directing Group with Electron-Rich Anilines

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N-(naphthalen-1-yl) picolinamide are ubiquitously found in numerous biologically active natural products, medicinally relevant scaffolds, pharmaceuticals, agrochemicals, dyes, and functionalized materials [1]. Conventionally, they are synthesized through a palladium- or copper-catalyzed Goldberg cross-coupling between aryl halides and amines [2]. In recent years, metal catalyzed C-H activation strategy provides a direct access to the functionalized amines obviating the need for aryl halides. In this vein, Pd, Ir, Rh catalysis have been explored with amines and highly energetic azides. To circumvent the metal poisoning issues with amines, the use of inexpensive first row transition metals such as manganese, iron, cobalt, nickel, and copper is emerging [3].Despite significant progress, copper-catalyzed/mediated C-H amination reactions with electron-rich anilines remains an unsolved problem due to catalyst deactivation and deleterious side reactions. Herein we report, a copper (II)-mediated C (sp2)-H amination of benzamides with electronically neutral or electron-rich anilines. A dramatic influence of Di-tert-butyl peroxide (DTBP), was observed on the reaction outcome (Fig. 1). The present protocol also demonstrates the synthesis of a number of non-steroidal anti-inflammatory drugs (NSAID's).

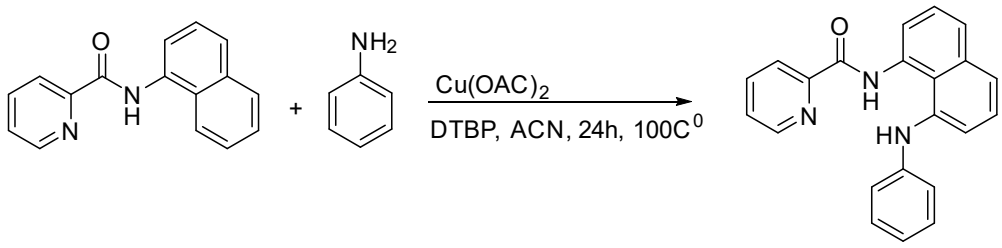

Fig. 1 synthesis Amination of Directing Group with Electron-Rich Anilines

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