Using 1-butyl-3-methylimidazolium bromide [bmim]Br as an efficient catalyst for One-Pot green synthesis of 4H-benzo[b]pyrans and 3,4-dihydropyrimidin-2-(1H) ones

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ILs are ionic compounds in which, at last the cation is an organic type cation. ILs contains only ionic species and sometime are known as molten salt, however while a molten salt is generally thought to refer to a high-melting, highly viscous and very corrosive medium, ionic liquids are already liquid at low temperatures (< 100℃) and have relatively low viscosity. The apparently somewhat arbitrary line drawn between molten salts and ILs at a melt temperature of 100℃ can be justified by the abrupt improvement in the range of applications for liquid salts below this temperature. Even though some examples are known in which high-temperature salt melts have been successfully used as reaction media for synthetic applications, only a liquid range below 100℃ can enable the versatile substitution of conventional, organic solvents by ionic liquid [1].

Among the heterocycles, functionally substituted 4H-chromenes have received considerable attention due to their spasmolytic, diuretic, anti-coagulant, anti-cancer and anti-anaphylactic activities[2]. 4H-benzo[b]pyrans are an important class of compounds which have received considerable attention in recent years due to their wide range of biological activities[3].

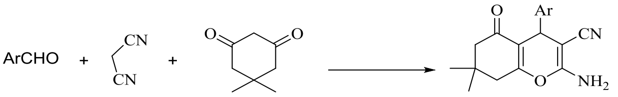

Figure 1. Scheme of the reaction.

Dihydropyrimidinones (DHPMs) as well as heterocyclic compound in the natural and synthetic organic chemistry due to their wide range of biological and therapeutic properties such as anti-viral anti-inflammatory, anti-tumor, and anti-bacterial activities [4].

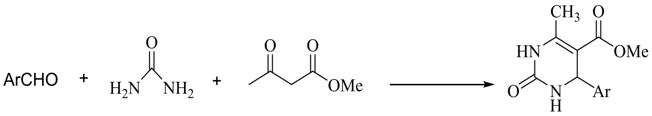

Figure 2. Scheme of the reaction.

A simple, efficient, and high yielding procedure for the preparation of 4H-benzo[b]pyrans and 3,4-dihydropyrimidin-2(1H)-ones is described using ionic liquid 1-butyl-3-methylimidazolium bromide [bmim]Br as a heterogeneous and efficient catalyst under ultrasonic and solvent-free conditions.

Simple methodologies, easy work-up procedure, easy preparation of the catalyst, excellent yields, and very short reaction times are among the other advantages of this study. Furthermore, this ionic liquid can be easily recovered.

References

[1] P. Wasserscheid, W. Keim, Angew. Chem. Int. Ed., 39, (2000) 3773-3789.
[2] N. Yu, J. M. Aramini, M. W. Germann and Z. Huang, Tetrahedron Lett., 41, (2000) 6993.
[3] S.S. Pourpanah, S.M. Habibi-Khorassani, M. Shahraki, Chin. J. Catal., 36, (2015) 757-763.

Efficient and Eco-Friendly Process for the Synthesis of Bis(1H-indol-3-yl)methanes Using Butylammonium Hydrogen Sulphate as an Ionic Liquid

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The synthesis of bis(indolyl)methanes has become the center of interest among world scientists due to their wide spectrum of pharmacological and biological applications. They have achieved a considerable importance as key moieties having extensive applications in medicinal and biological chemistrysuch as the inhibition of cancer cell growth through the induction of apoptosis and metastasis [1].These different pharmaceutical and biological applications have caused the development of a number of methods for the synthesis of bis(indolyl)methanes by the electrophilic substitution of indole with the various aldehydes in the presence of the different catalysts [2,3].

In recent years, ionic liquids as solvent or catalyst have attracted significant attention due to their peculiar properties including low vapour pressure, excellent thermal and chemical stability, tunable polarity, high ionic conductivity and immiscibility with certain organic solvents. In addition, the widespread range of possible cation and anion combinations represents the various applications and tunable interactions [4].

In this study, butylammonium hydrogen sulphate [(BA)(HSO_4)] was synthesizedas a ammonium-based ionic liquid*via* a simple chemical routein water. The [(BA)(HSO_4)] ionic liquid was successfully applied as an eco-friendly and recyclable catalyst for the synthesis of bis(indolyl)methane derivatives at room temperature under solvent-free conditions. Taking the environment and economy into consideration, the work presented here has the merits of environmental friendliness, high yields, simple work-up, easy operation and the avoidance of the organic solvents and inexpensive catalysts.

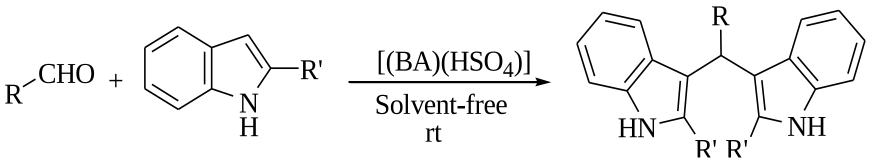

Figure 1. Synthesis of bis(indolyl)methane derivatives catalyzed by [(BA)(HSO_4)] ionic liquid.

References

[1] M. Shiri, M. A. Zolfigol, H. G. Kruger, Z. Tanbakouchian, Chemical Review 110(2010) 2250.
[2] D. Liang, W. Huang, L. Yuan, Y. Ma, J. Ma, N. Deman, Catalysis Communication 55(2014) 11.
[3] A. Mobaraki, B. Movassagh, B. Karimi, Applied Catalysis A: General 472 (2014)123.

Tris(hydroxymethyl)methane Ammonium Hydrogensulphate [(THA)(HSO_4)]: An Eco-friendly and Recyclable Catalyst for One-Pot , Three-Component Synthesis of 2-Amino-3-cyano-4H-pyran Derivatives in Water

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Ionic liquids have received significant interest in organic synthesis as catalyst because of their special properties such as low vapor pressure, excellent thermal and chemical stability, non flammability, tunable polarity, high ionic conductivity and immiscibility with certain organic solvents. Among the different ionic liquids, ammonium-based ionic liquids are considered to be the most promising and safer ionic liquids for further application in medical and pharmaceutical industries.Aliphatic ammonium-based ionic liquids are well known and have wonderful industrial uses due to their bioactivity and surface activity. Also, these ionic liquids are completely stabilized on exposure to air and water and easily prepared from cheap starting materials [1].

4*H*-Pyran and its derivatives represent the key building blocks of many natural products and constitute the core of valuable compounds exhibiting a wide range of pharmacological and biological activities such as anticancer, antimicrobial, antioxidant and antiproliferative properties [2]. In recent years, several methods have been reported for the One-Pot synthesis of 2-amino-3-cyano-4*H*-pyran scaffold *via* a three-component condensation of aldehydes and alkylmalonates with carbonyl compounds possessing a reactive α-methylene group in the presence of heterogenous and homogenous catalysts [3,4].

Tris(hydroxymethyl)methane ammonium hydrogensulphate [(THA)(HSO_4)] was synthesized as a novel ionic liquid and characterized by various techniques such as ^{1}H NMR, ^{13}C NMR, FT-IR, MS, TGA and elemental analysis. [(THA)(HSO_4)] ionic liquid was efficiently applied as an eco-friendly and recyclable catalyst for the One-Pot , three-component synthesis of 2-amino-3-cyano-4*H*-pyran derivatives in water. The most important advantages of this study are high yields, cleaner reaction profile, short reaction time, the avoidance of the organic solvents and easy work-up. In addition to the above-mentioned advantageous, the use of a recyclable nanocatalyst and water as a reaction medium are environmentally benign and cost-effective which makes our methodology proper for the industrial goals.

References

[1] C. Wang, L. Guo, H. Li, Y. Wang, J. Weng,L. Wu, Green Chemistry 8 (2006) 603.
[2] J. A. Makawana, M. P. Patel, R. G. Patel, Archiv der Pharmazie345 (2012) 314.
[3] D. Kumar, V.B. Reddy, G.B. Mishra, R.K. Rann, M.N. Nadagouda, R.S. Varma, Tetrahedron 63 (2007) 3093.

Nano-Fe_3O_4@SiO_2coated polyacrylicacid as an efficient catalyst for the synthesis of tetrahydrobenzo[*b*]pyran and 3,4-dihydropyrano[*c*]chromene derivatives

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Recently preparation and the use of nanoparticles (NPs) in organicsynthesis has become a subject of intense investigation. In particular, magnetic nanoparticles (MNPs) which offer advantages inclean and sustainable chemistry and also they can be nontoxic, readilyaccessible, and retrievable. Additionally, the activity and selectivity of magnetic nanocatalysts can be manipulated by its surfacemodification [1].Among these support materials, magnetic nanoparticles are verypopular when used for immobilization of active homogeneouscatalyst because their magnetic response causes simpleseparation of catalyst by using an external magnet. Howevermagnetic nanoparticles always tend to undergo agglomerationbecause of the magnetic dipole–dipole attractions betweenparticles; it was reported that formation of a passive coating ofinert materials such as polymers on the surfaces of iron oxidenanoparticles could help to prevent their aggregation insolvents and improve their chemical stability [2].

Herein we report a magnetically supported acidic polymeric on Fe_3O_4@SiO_2 nanoparticles (Fe_3O_4@ SiO_2-Guanidine-poly acrylic acid) was synthesized and evaluated as a recoverable catalyst for the One-Pot synthesis of tetrahydrobenzo[*b*]pyran and 3,4-dihydropyrano[*c*]chromene derivatives in high to excellent yield under ethanol/H_2O solvent conditions.

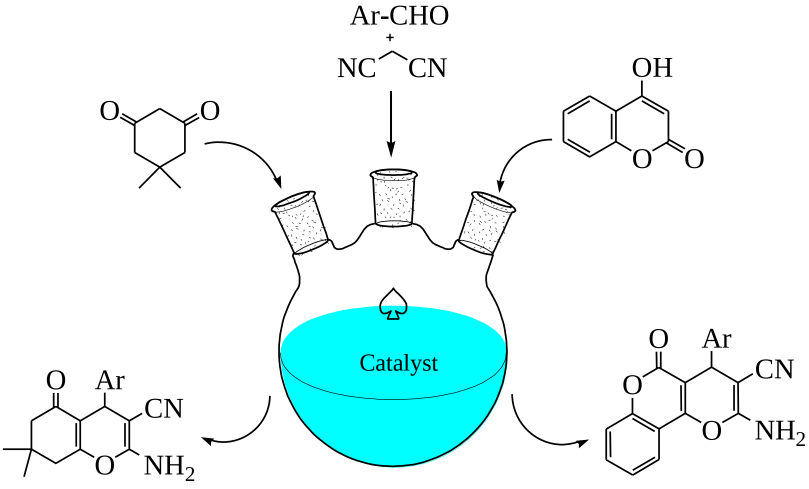

Figure 1. Scheme of the reaction.

References

[1] R.B.N. Baig, R.S. Varma, Chem. Commun. 49 (2013) 752.

[2] Yoon, H.; Ko, S.; Jang, J. Chem. Commun. 14 (2007) 1468.

Modification of Tragacanth as a Backbone to Prepare Biodegradable Superabsorbents: Graft Copolymerization via Free Radical Polymerization and ATRP

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Natural polymers are valuable materials because of their biocompatibility and biodegradability. They have been employed in various fields of applications in recent years [1]. Superabsorbents are polymeric networks with plenty of hydrophilic functional groups. These materials have high water absorption capacity with developed applications, especially for agricultural and horticultural purposes [2]. Tragacanth, as an abundant and low-cost biopolymer, is one of the most suitable candidates to employ in various fields.

In the present study, tragacanth was modifiedusing monochloroacetic acid to prepare sodium carboxymethyl tragacanth (CMT) as free radical initiator. Also tragacanth was modified with bromoacetyl bromide to prepare bromoacetyl tragacanth (BAT). The degree of substitution (DS) for both CMT and BAT was calculated in order to determine the active polymerization sites. Then graft copolymerization of vinyl monomers was carried out on the prepared CMT and BAT to prepare the final superabsorbents. Different analyses such as swelling ratio (SR), equilibrium swelling ratio (ESR) and water holding capacity (WH) in soil samples were studied on the prepared superabsorbents. Results showed acceptable efficiency for the prepared superabsorbents, especially for agricultural and horticultural purposes.

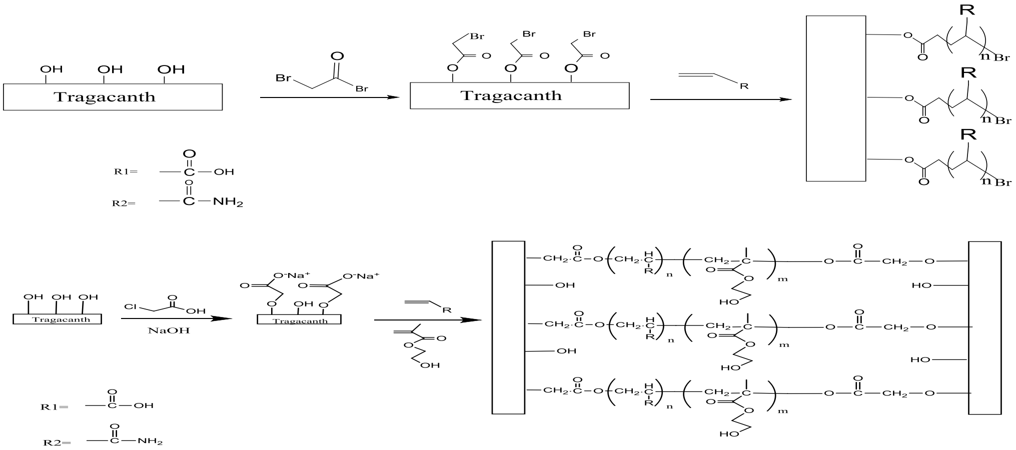

Figure 1. Scheme of the reaction.

References

[1] Xie, L., et al.Recovery of Ammonium onto Wheat Straw To Be Reused as a Slow-Release Fertilizer .Journal of agricultural and food chemistry, 2013. 61(14): p. 3382-3388.
[2] Feng, D.; Bai, B.; Ding , C; Wang , H.; Suo, Y., Synthesis and swelling Behaviours of Yeast-g-Poly(acrylic acid) superabsorbent co-Polymer. Industrial & Engineering chemistry Research 2014, 53, 12760-127690.
[3] Feng, D.; Bai, B.; Ding , C; Wang , H.; Suo, Y., Synthesis and swelling Behaviours of Yeast-g-Poly(acrylic acid) superabsorbent co-Polymer. Industrial & Engineering chemistry Research 2014, 53, 12760-127690.

Comparison of Essential oil Composition in Wild and Cultivated Populations of *Menthaaquatica L.* from Iran

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The genus *Mentha* (Lamiaceae) is one of the most significant sources of essential oil manufacture. Some members of this genus are also utilized as herbal teas and spices both in fresh and dried form due to their distinct scent [1]. *Menthaaquatica L.* is a perennial herb of the Lamiaceae family, common in Europe, North Africa, and West Asia, and was recently introduced to America, Australia and Madeira. It grows on the lagoons and lakes, but prefers calcareous soils. It is known for its analgesic, antipyretic, antiseptic, carminative, decongestant, antispasmodic, deodorant, diaphoretic,allergenic, digestive, diuretic, antiemetic, insecticides, sedative and vermifuge actions [2].In this investigation the essential oils of the wild and cultivated of *Menthaaquatica L.* were isolated and compared.

The characterization of essential oils was performed by means of gas chromatography-flame ionization detector (GC-FID) and gas chromatography-mass spectrometry (GC-MS) techniques. 43 components were characterized for cultivated plant with linalool (29.34%), linalool acetate (14.20%),α-terpineol (9.34%), E-caryophyllene (9.06%) and 1,8-cineole (6.87%) dominating constituents.46 constituents were identified for wild plant with linalool (48.00%), linalool acetate (20.47%),α-terpineol (7.45%) and 1,8- cineole (6.02%) as the major constituents.26 compounds were similarly identified in thesetwo EOs from each cultivated and wild *M aquatica L.*plant material which represented 97.84% and 98.96% of the total detectedconstituents in EOs of cultivated and wild plants, respectively.

References

[1] J. Gershenzon , M. Maffei, R.Croteau.Plant Physiol. 89(1987)1351.
[2] A. Monfared, M. R. Nabid , A. Rustaiyan. J. Essent. Oil Res. 14(2002) 51.

Extraction and Identification of Two Secondary Metabolites from*TeucriumstocksianumBoiss.*

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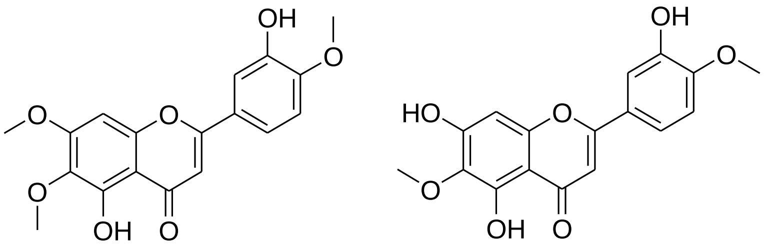
TeucriumstocksianumBoiss belongs to Lamiaceaefamily that havenumerous traditional uses as medicinal plant [1]. Reported activities for the Teucrium genus are anti-inflammatory, antibacterial, antifungal, antioxidant and antispasmodic.Moreover, the importance of the biological activities of the Teucrium species is evident as larvicidal, hypoglycemic, antispasmodic, antinocieceptive, hepatoprotective[2, 3]. Teucriumstocksianum Boiss. Growin gwild in south of Iran, Hormozgan: Hajiabad, Sirmand, Talmara, 800 m, was collected in April 2015 by M. A. Soltanipour. As a part of ongoing research program aimed at the isolation, structural elucidation and pharmacological evaluation of bioactive secondary metabolites from plants, we started the phytochemical analysis of TeucriumstocksianumBoiss. Our studies led to the isolation of two flavonoids(1 and 2 in Figure 1), together with several compounds, whose structures were secured by 1D and 2D-NMR spectroscopic studies, in particular homo-COSY and hetero-(HMQC and HMBC).



1 2

Figure1. Structure of secondary metabolites

References

[1] F. Naghibi, M. Mosaddegh, M.S.Motamed, A.Ghorbani. IJPR. 2(2005) 63.
[2] F. Mojab, K. Javidnia, D.Yazdani, A.Rustaiynan.J Med Plants. 2(2003) 49.
[3] N. A. A. Ali, M. Wurster, N. Arnold, U.Lindequist,L. Wessjohan. Rec. Nat. Prod. 2(2008)25.

A new nano Fe_3O_4-supported organocatalyst based on 3,4-dihydroxypyridine: An efficient heterogeneous nanocatalyst for One-Pot synthesis of pyrano[2,3-d]pyrimidines

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In the recent years, organocatalysis has attracted much attention as a powerful methodology in organic synthesis for the construction of new compounds. The application of organocatalytic systems for fine chemical synthesis provides some advantages such as lack of sensitivity to moisture and oxygen, ready availability, low cost, and low toxicity [1]. However, the capability and applicability of an organocatalyst in organic transformations can be improved if its recovery and reuse procedure become more and more facile [2]. So briefly the recycling capability of an organocatalyst has the following advantages: simplicity in the practical separation of the catalyst from the products and reaction mixture, economic impacts, avoiding wastes and potential for the application in large-scale operations[3].Among the used strategies, preparation of solid-supported organocatalysts are potentially highly useful method for the preparation of more efficient catalytic systems for the synthesis of fine chemicals under especially simple, mild and more environmentally benign conditions [4].

We have used Fe_3O_4 as a promising support for heterogenization of 3,4-dihydroxypyridine to make a new magnetically recoverable heterogeneous catalyst (Figure 1).Our experimental results reveal that pyridine-functionalized Fe_3O_4nano particles is an efficient base catalyst for the domino condensation of different aromatic aldehydes, Meldrum's acid and 5-methylpyrazol-3-amine under very mild reaction condition and in the presence of ethanol solvent. All reactions were completed in short times and all products were obtained in good to excellent yields. Also notably, the catalyst was reused for five times without significant degradation in catalytic activity and performance.

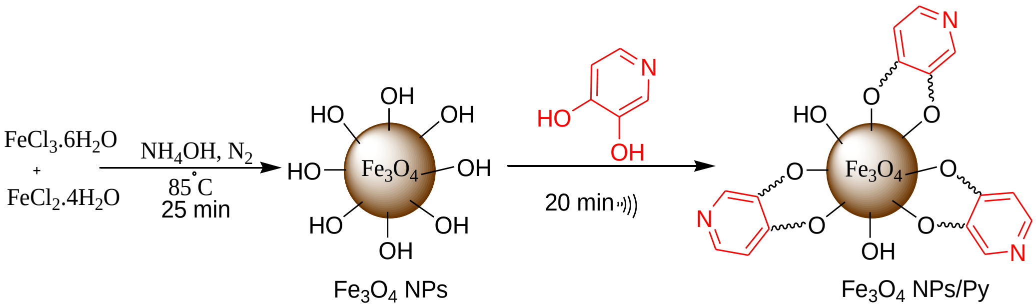

Figure 1. Preparation of Fe_3O_4/Py nanocatalyst

References

[1] B. List, Chem. Rev., 2007,107, 5413.
[2] J. Zhou, J. Wan, X. Ma, W. Wang, Org. Biomol. Chem. 2012, 10, 4179
[3] M.C. Varela, S.M. Dixon, K.S. Lam, N.E. Schore, Tetrahedron 2008, 64, 10087.
[4] A. Schatz, O. Reiser, W.J. Stark, Chem. Eur. J. 2010, 16, 8950.

Highly Efficient Method for the Synthesis of Chalcones, Catalyzed by Fe_3O_4 Magnetic Nanoparticles (MNPs) Under Solvent-Free Reaction Conditions

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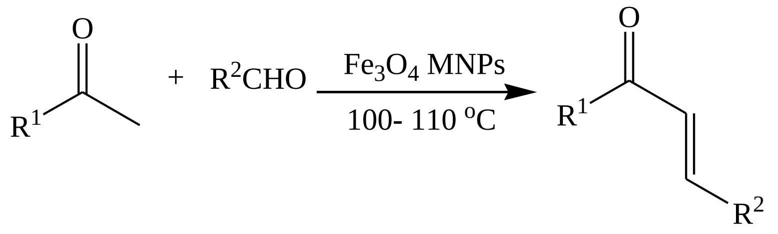
Chalcones are useful groups of natural products that are potentially important synthetic intermediates for preparation of flavonoids and a series of heterocyclic compounds [1].A number of methods based on heterogeneous catalysts such as $HClO_4/SiO_2$ [2], TiO_2 nanoparticles [3], and Fe_3O_4 MNPs [4] have been developed for the synthesis of chalcones, which usually required longer time, complex synthetic pathways and often expensive catalyst. Therefore, the search for new routes for the synthesis of chalcones has attracted considerable attention and the pursuance of more convenient and practical synthetic methods for these compounds still remains an active research area.

Herein we have developed a simple and efficient method for the synthesis of chalcones using Fe_3O_4 magnetic nanoparticles (MNPs) towards the cross aldol condensation reactions of 4-chloroacetophenone, benzalacetone, tetralone, acetone and 3-penatanone (as ketones having enolizable methyl and methylene groups) with substituted aromatic aldehydes under solvent-free conditions at 90–110 °C (Figure 1). The experimental procedure is very simple, the products are formed in high yields and the catalyst is easily separated by applying an external magnetic field.



R^1 = 4-ClC_6H_4; R^1 = CH_3; R^1 = C_6H_4-CH=CH; R^1COCH_3 = Tetralone

Figure 1. Synthesis of chalcones

References

[1] H. Hazarkhani, P. Kumar, K. S. Kondiram, K.S. Shafi, I.M. Gadwal, Synth. Commun.40 (2010) 2887.
[2] H.R. Shaterian, H. Yarahmadi, M. Ghashang, Tetrahedron, 64 (2008) 1263
[3] M. Rahimizadeh, Z. Bakhtiarpoor, H. Eshghi, M. Pordel, G. Rajabzadeh, Monatsh Chem, 140 (2009) 1465

Grind assisted nano magnetite catalyzed synthesis of 2-amino-4H-chromenes

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Chromene and its derivatives belong to a major class of natural heterocyclic compounds, which they occur widely in edible vegetables and fruits. They frequently expose a variety of biological and pharmacological activities. Based on the extensive researches, it has been observed that chromene derivatives include biological activities such as antioxidant, spamolytic, anti-HIV, anticancer, anti-anaphylactic, antibacterial activity antihypertensive, anti-tubulin, antiviral, activator of potassium channels and inhibition of phosphodiesterase IV or dihydrofolate reductase, etc [1-2].

Owing to the important applications of chromene derivatives, various synthetic methodologies for these compounds have been reported. However, many of these methods suffer from acidic media, unsatisfactory yields, longer reaction times, difficult work up, excessive use of reagents and catalyst. It is therefore, important to find more convenient methods for the preparation of these compounds.

In order to make the reaction simple and green and in continuation of our efforts for the synthesis of heterocyclic compounds [3], herein, Fe_3O_4 nanoparticles (MNPs) under grind condition has been successfully applied to perform the reaction of B-naphtol, malononitrile and arylaldehyde to provide a series of chromene derivatives in excellent yields and short reaction times.

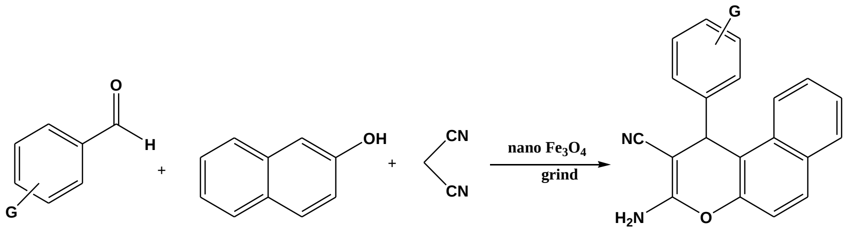

Figure 1. Scheme of the reaction.

References

[1] Z. Dua, W. Y. Siau, J. Wang. Tetrahedron Letters 52 (2011) 6137.
[2] L. Moafi, S. Ahadi, A. Bazgir. Tetrahedron Letters 51 (2010) 6270.
[3] L. Zare Fekri, M. Nikpassand, K. Hassanpour. Current Organic Synthesis 12 (2015) 76.

1, 4-Diazabicyclo[2.2.2]octanium diacetate catalyzed synthesis of chromenes

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Chromene and its derivatives belong to a major class of natural heterocyclic compounds, which they occur widely in edible vegetables and fruits. They frequently expose a variety of biological and pharmacological activities. Based on the extensive researches, it has been observed that chromene derivatives include biological activities such as antioxidant, spamolytic, anti-HIV, anticancer, anti-anaphylactic, antibacterial activity antihypertensive, anti-tubulin, antiviral, activator of potassium channels and inhibition of phosphodiesterase IV or dihydrofolate reductase, etc [1-2].

Several methods have been reported for the synthesis of 2-amino-4H-chromene derivatives using malononitrile, resorcinol and aldehyde. Various catalysts such as piperidine, cetyltrimethylammonium bromide (CTABr) , TFE , $Ca(OH)_2$, MgAl/HT and tungstic acid functionalized mesoporous SBA-15 have been used for these reactions. However, many of these methods suffer from acidic media, unsatisfactory yields, longer reaction times, difficult work up, excessive use of reagents and catalyst. It is therefore, important to find more convenient methods for the preparation of these compounds.

In order to make the reaction simple and green and in continuation of our efforts for the synthesis of heterocyclic compounds [3], herein, 1, 4-Diazabicyclo[2.2.2]octanium diacetatehas been successfully applied to perform the reaction of B-naphtol, malononitrile and arylaldehyde to provide a series of chromene derivatives in excellent yields and short reaction times.

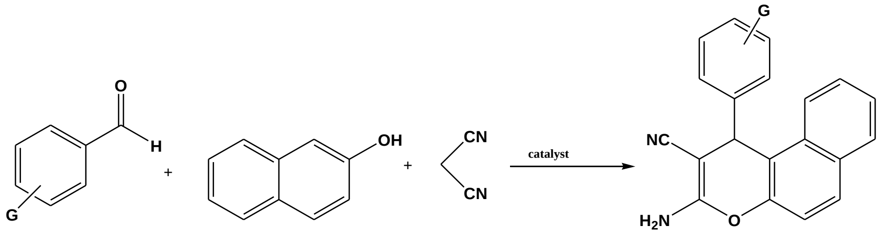

Figure 1. Scheme of the reaction.

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[1] T Z. Dua, W. Y. Siau, J. Wang. Tetrahedron Letters 52 (2011) 6137.
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[3] L. Zare Fekri, M. Nikpassand. Russian Journal of General Chemistry 84 (2014) 1825.

Synthesis of new oximes from octahydroxanthene compoundes based on 1,3-cyclohexanedione

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Oximes are important compounds due to the biological and pharmaceutical properties such as antimicrobial [1]and antitumor [2]. In this study, has been designed and synthesized the new series of oxime compounds. The route of synthesis of the mentioned compounds is shown in Figure 1. Reaction of 1,3-cyclohexanedione, aldehydes, and cyanogen bromide lead to the selective formation of octahydro-1H-xanthene-1,8(2H)-diones in moderate to good yields at room temperature under basic condition. Obtained octahydroxantene will be converted to oximes and thiosemicarbazone in the presence or hydroxylamine hydrochloride and thiosemicarbazide, respectively.

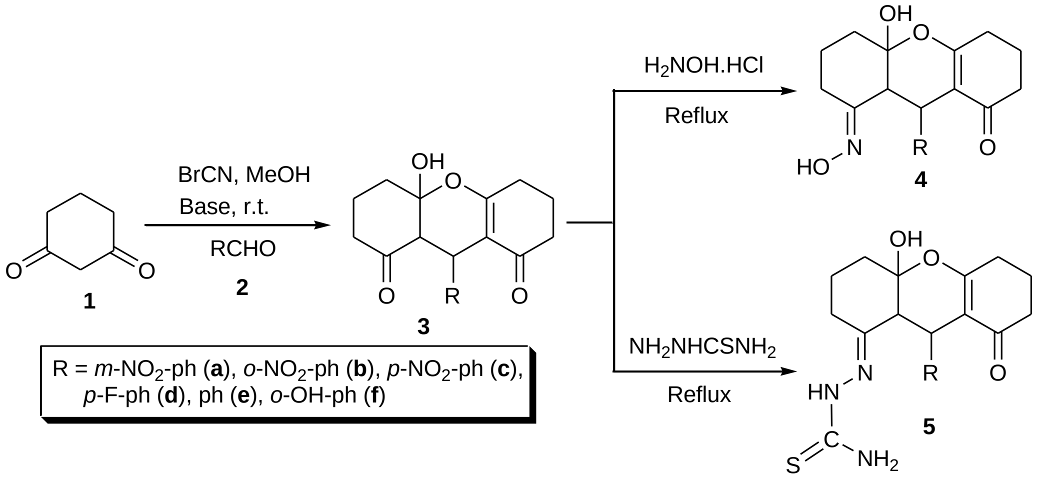

Figure 1. Scheme of the reaction.

References:

[1] (a) Li, H. Q.; Xiao, Z. P.; Yin, L.; Yan, T.; Lv, P. C.; Zhu, H. L. Eur. J. Med. Chem. 2009, 44, 2246. (b) Karakurt, A.; Sevim, D.; Özalp, M.; Özbey, S.; Kendi, E.; Stables, J. P. Eur. J. Med. Chem.2001, 36, 421.

[2] Wang, T. C.; Chen, I. L.; Lu, C. M.; Kuo, D. H.; Liao,C. H. Chem. Biodivers.2005, 2, 253.

Co_3O_4: An Efficient Heterogeneous Catalyst for Acetylation of Amines

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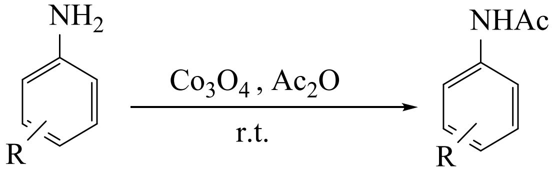
The selective protection of amines has attracted more attention for its fundamental importance and also for its role in multistep synthesis [1]. This important transformation is typically performed using acetic anhydride andformic acidin the presence of either basic or acidic catalysts. Numerous catalytic systems are available for acetylation and formylation of amines [2,3], but most of these have used homogeneous catalysts and non-recoverable, and they have the disadvantages of prolonged reaction time, low yields, harsh conditions, use of harmful organic solvents, tedious work-up procedures, excessive reagents or catalysts, and the use of explosive, moisture-sensitive, or expensive catalysts.

In this work, we have used Co_3O_4 as a heterogeneous catalyst for acetylation and formylation of amines in the presence of acetic anhydride andformic acidunder solvent-free conditions at room temperature.



R = Me, OH, OCH_3, NH_2, CH_2OH

Figure 1. Scheme of the reaction.

References

[1] J. R. Hanson Protecting Groups in Organic Synthesis. 1st Ed.Malden: Blackwell Science, 1999.
[2] P. Phukan.Tetrahedron Lett. 45 (2004) 4785.
[3] M. Moghadam, S. Tangestaninejad, V. Mirkhani, I. Mohamadpoor-Baltork, S. A. Taghavi.,J. Mol. Cat. A., 274 (2007)217.

Dramatic Rate Acceleration of Baylis-Hillman Reaction with Fe_3O_4 Nanoparticles and DBU in Solvent Free Medium

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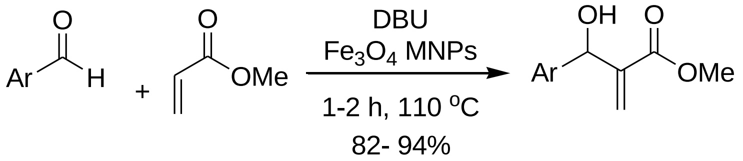
The Baylis-Hillman reaction, i.e., the coupling of aldehydes and activated vinyl compounds, is one of the most important carbon-carbon bond forming reactions in organic synthesis [1,2]. This reaction has attracted the attention of many synthetic organic chemists because the resulting β-hydroxy-α-methylene adducts can be transformed into a variety of natural and unnatural compounds [3]. However, the reaction suffers from poor reaction rates and many research groups have examined a variety of methods to accelerate the reaction. Various methods for the acceleration of Baylis-Hillman reaction have been developed with certain limitations.One of the most important methods is the salt effect using Lewis acid as co-catalyst [4].

In continuation of our interst for Baylis-Hilman adductsand mechanistic studies of this reaction,herein we wish to report our novel methodology for the acceleration of Baylis-Hillman reaction with magnetic iron oxide nanoparticles (MNPs) and DBU in a solvent free medium (Figure 1).



1 (a-h) **2** (a-h)

Ar = C_6H_5, 4-Py, 2-ClC_6H_4, 4-ClC_6H_4, 3-$NO_2C_6H_4$, 4-MeC_6H_4, 4-$MeOC_6H_4$, 4-$NMe_2C_6H_4$

Figure 1. Synthesis of Baylis-Hillman adducts.

References

[1] D. Basavaiah, A.J. Rao, T. Satyanarayana, T. Chem. Rev. 103 (2003)811.
[2] V. Singh, S. Batra, Tetrahedron, 64 (2008) 4511.
[3] R. Buchholz, H.M.R. Hoffmann,Helv. Chim. Acta,74 (1991) 1213.
[4] D. Basavaiah, K.V. Rao, R.J. Reddy,Chem. Soc. Rev., 36 (2007) 1581.

A New Route for the Synthesis of Unsaturated β-Lactam Derivatives from β-Hydroxy-α-Methylene Acrylates

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2-Azetidinones, commonly known as β-lactams, are well-known heterocyclic compounds among the organic and medicinal chemists [1]. The activity of the famous antibiotics such as penicillins, cephalosporins and carbapenems are attributed to the presence of 2-azetidinone ring in them [2]. Apart from clinical use, β-lactams can also serve as good synthons in the synthesis of many biologically active heterocycles [3]. A number of methods have thus been developed for their synthesis, however, these methods suffer from either limited scope of applicationor harsh experimental conditions. Therefore, the development of simple, economic, efficient and general methods is certainly highly desirable.

In continuation of our interest for the Baylis-Hillman adducts (β-hydroxy-α-methyleneacrylate adducts) and transformation of them into a variety of natural and unnatural compounds [4], herein we wish to report our results for the direct transformation of Baylis-Hillman adductsinto the correspondingα-methylene β-lactams and α-arylidene β-lactams using a new protocols (Figure 1).

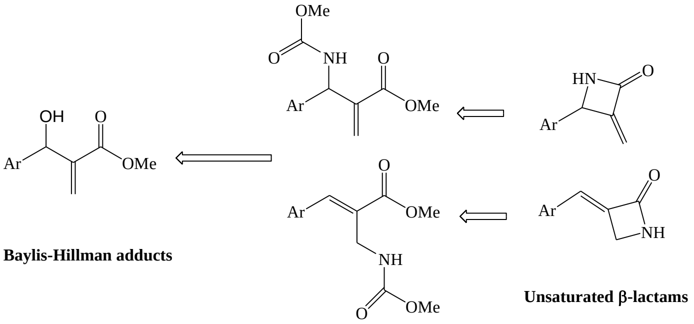

Figure 1. New routes for the synthesis of unsaturated β-lactamderivatives

References

[1] C.R. Pitts, T.Lectka,Chem. Rev.114 (2014) 7930.
[2] S. Coe, N. Pereira, R.M. Napier, P. Neve, J.V. Geden, G.J. Clarkson, D.J. Fox, M. Shipman, Org. Biomol. Chem., 13 (2015) 7655.
[3] W. Li, C. Liu, H. Zhang, K. Ye, G. Zhang, W. Zhang, Z. Duan, S. You, A. Lei, Angew. Chem., Int. Ed. 53 (2014) 2443.

Preparation and biodistribution assessment of ^{68}Ga-Bleomycin as a possible PET imaging

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Bleomycin is an anti-cancer ("antineoplastic" or "cytotoxic") chemotherapy drug which is classified as an antitumor antibiotic.Several radiolabeled Bleomycin derivatives have been developed for imaging and/or therapy of neoplastic tissues. The most important imaging compounds contain indium-111,[1] cobalt-57,[2] technetium-99m,[3] radioferricsalts[4] and rhodium-105 [5].The positron-emitting Ga(III) radioisotopes, $^{66}Ga^{3+}$and $^{68}Ga^{3+}$, have been proposed for applications inpositron emission tomography (PET) imaging.In this study, by applying a produced ^{68}Ge/^{68}Ga generator,a simple technique for the synthesis and quality control of ^{68}Ga-Bleomycin wasintroduced; followed by preliminary animal studies. $^{68}GaCl_3$ eluted from the generator was studied in terms of qualitycontrol factors including radiochemical purity (assessed by RTLC),chemical purity and radionuclide purity. This study reports the preparation and biodistribution assessment of Gallium-Bleomycin (^{68}Ga-BLM) complex as a radiopharmaceutical and optimization of its labeling conditions; pH, reaction time, temperature, concentration of Bleomycin and its biodistribution in normal mice. The biodistribution of the complex was compared with $^{68}Ga\text{-}Cl_3$ in 11 selected organs including blood, liver, lung, spleen, muscle, skin, heart, kidney, colon, colon content, and bladder at 4 selected times of 1, 2, 4, 24 hours after injection. The optimized pH condition was found 2 at temperature of 90ºC for reaction temperature of 30 minutes when 1 mg of bleomycin was mixedofabout2mCi of $^{68}Ga\text{-}Cl_3$.Radio thin layer chromatography showed an overall radiochemicalpurity of 90-94% at the optimized conditions with a specific activity of about 1.5mCi/m mole and radiochemical purity greater than 93% in 15 min.

References

[1] H. Umezawa, Antimicrobial Agents Chemother. 1965, 5 1079.
[2] H. Naganawa, Y. Muraoka, T. Takita, H. Umezawa, J. Antibiot., 1977, 15. 388.
[3] R. C. Brooks, P. Carnochan, J. K. Sasabowski, Nucl. Med. Biol., 1999, 26, 421.

Nef-isocyanide-perkow access to novel ketene dithioacetals

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Novel ketene dithioacetals have been synthesized *via*the condensation reaction of active methylene compounds with carbon disulfide in the presence of Et_3N in MeCN at room temperature. Phosphorylated hydroxyketenimines, synthesized *via* the reaction of ethyl chloroglyoxalate, cyclohexyl isocyanide and triethyl phosphide, were used for trapping of theketene dithioacetals to afford the push-pull olefinic product [1]. The phosphorylated hydroxyketenimines were generated in situ from a Nef-isocyanides-Perkow cascade reaction [2]. Various aspects of these transformations will be presented and discussed.

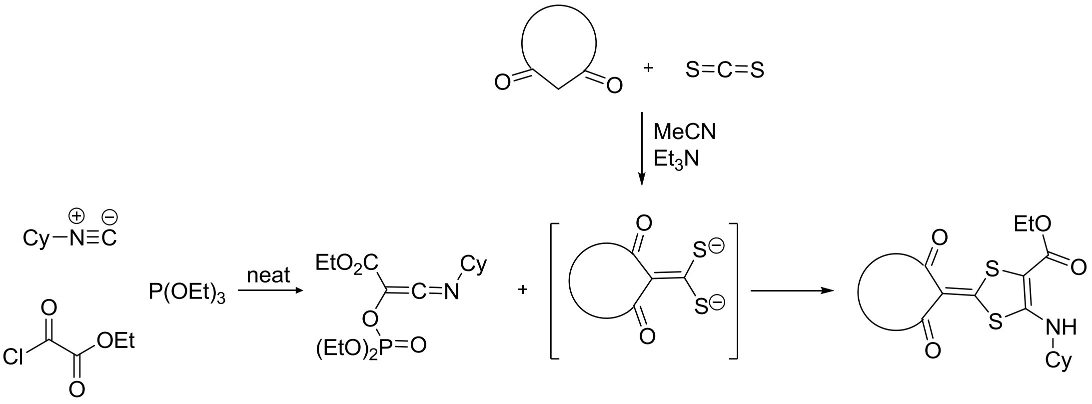

Figure 1. Synthesis of ketene dithioacetals and reaction with phosphorylated hydroxyketenimine

References

[1] I. Yavari, R.Hoseinpour, R. Pashazadeh. Helv. Chim. Acta 98 (2015) 374; I. Yavari, R. Hoseinpour, R. Pashazadeh. Tetrahedron 69 (2013) 2462.

[2] A. Habibi, A.Valizadeh. J. Sulfur Chem. 35 (2014) 362; D. Coffinier, L.El Kaim. Tetrahedron Lett. 52 (2011) 3023.

$FeCl_3$-catalized formation of indolizine derivatives *via* 1,3-dipolar cycloaddition between azomethineylides and chalcones

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The C-H bond activation by using iodine mediated *sp*^{3} C-H functionalization for the synthesis of alkyl azaarenepyridinium zwitterions showed.[1,2]$FeCl_3$-catalized 1,3-dipolar cycloaddition reaction of pyridinium-1-yl(quinolin-2-yl)methanides (prepared in situ from iodine catalyzed reaction of 2-methylquinoline and pyridine in the presence of base) with chalcones leading to a facile, One-Pot synthesis of aryl(2-aryl-3-(quinolin-2-yl)indolizin-1-yl)methanones in moderate to good yields.Various aspects of these transformations will be presented and discussed.

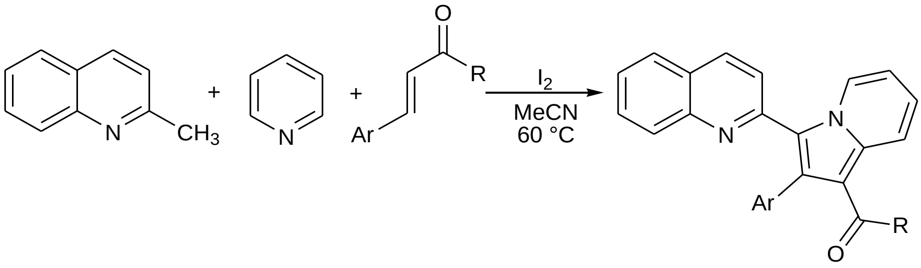

Figure 1. Synthesis of Indolizines

References

[1] I. Yavari, R. Hosseinpour, S.Skoulika. Synlett(2015) 380; I. Yavari, R. Hoseinpour,R. Pashazadeh.Synlett(2012) 1662
[2] I. Yavari, R. Hoseinpour, R. Pashazadeh, E. Ghanbari. Tetrahedron Lett. 54 (2013) 2785; I. Yavari,R. Pashazadeh, R. Hoseinpour. Helv. Chim. Acta95 (2012) 169.

Synthesis of triaryloxy-*s*-triazines in the reaction of phenols with BrCN

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1,3,5-Triazines are important products of modern organic chemistry. They are widely used as intermediates in dye chemistry, paint and varnish, and pharmaceutical industries, as herbicides and as monomers for the synthesis of thermostable polymers,and in several other branches of the national economy.The most promising method for the industrial synthesis of 1,3,5-triazines is the cyclotrimerisation of compounds containing a nitrogen-carbon triple bond,since this reaction usually occurs selectively to give high yields of the final products [1]. Among a wide variety of heterocycles that have been explored for developing pharmaceutically importantmolecules, such as organic compounds containing triazinering [2].Tri-substituted 1,3,5-triazines such as 2,4,6-tris(phenoxy)-1,3,5-triazine, are known as one of the oldest classes of organic compounds.These compounds have been used as subunits in the formation of supramolecular structures [3].In this research, unexpected novel cyclotrimerization of aryl cyanate gave 2,4,6-triaryloxy-l,3,5-triazines with excellent yield. No special catalyst is used in this reaction.

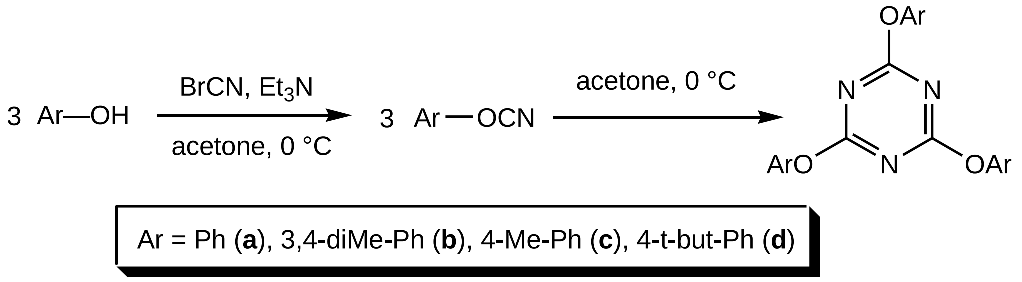

Figure 1. Scheme of the reaction.

References

[1] Russian Chemical Reviews 47(1978) 975.
[2] Y. Ninomiya, N. Shimma, H. Ishitsuka, Antiviral Res13(1990**)** 61.
[3] A. Dainyte, D.Gudeika, G.Buika, Mol. Cryst. Liq. Cryst.73(2014)590.

Synthesis of palladium nanoparticles supported on modified Merrifield resin as a novel heterogeneous catalyst for C-C cross coupling reactions

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Palladium-catalyzed cross-coupling reactions are one of the most important synthetic tools in modern organic synthesis. Variousresearch groups have dedicated efforts to the development of C-C coupling methods based on the well-established chemistry of Pd^0 and Pd^{II} species [1-5].

A new palladium catalyst based on modified Merrifield resin was synthesized. The structure of the catalyst was established by transmission electron microscopy (TEM), X-ray powder diffraction (XRD) and scanning electron microscopy (SEM). This study revealed that palladium is well-dispersed with typical diameter of nanometer.

The catalyst was employed in C-C reactions with aryl halides and produced promising results. The catalyst was recycled and used in five successive runs without loss of the catalytic activities.

References

[1] M. Mamaghani, F. Shirini, M. Sheykhan, M. Mohsenimehr, RSC Adv 5 (2015)44524–44529.
[2] R.J. Lundgren, M. Stradiotto, Chem-Eur. J. 18 (2012) 9758-9769.
[3] L. Yin, J. Liebscher, Chem. Soc. Rev 107 (2007) 133-173.

Synthesis of 2-hydroxy-1-(p-tolyl)ethan-1-one anddiethyl (2-oxo-2-(p-tolyl)ethyl) phosphate by reaction of arylglyoxalderivatives and trialkylphosphites.

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Recently we reportesd a three component reaction ofarylglyoxals, β-enaminones and triphenylphosphine to produce pyrroles [1]. The reactionbetween Pyrrole,arylglyoxal monohydrates and enaminoketones or enaminoesters in alcoholic media in the presence of $FeBr_3$ as a catalyst to produce 2,5-bis(1H-pyrrol-2-yl)-1H-pyrrole derivatives[2]. We also reported reaction ofarylglyoxalmonohydrates, malononitrile and trialkylphosphites to produce of polyfunctionalizedphosphonated furan derivatives [3]. In continuation of our previous works on the three-component reactions arylglyoxals[3] here we wish to report the result of our study on the reaction of arylglyoxals with trialkylphosphites. As shown in (figure 1) this reaction leads to products 3, 4. The structure of this productswere proved by ^{1}H-NMR, ^{13}C-NMR and IR spectral data and elemental analysis.

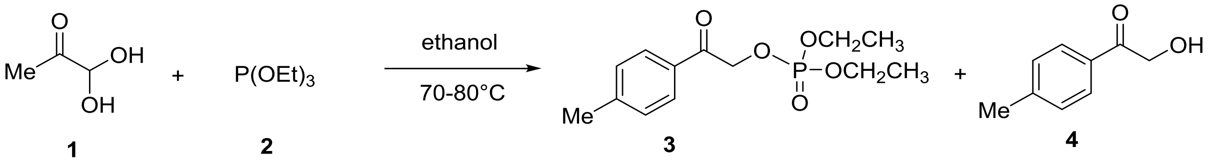

Figure 1. Scheme of the reaction.

References

[1] M. Masoudi, M. Anary-Abbasinejad,"A direct phosphine-mediated synthesis of polyfunction-alizedpyrroles from arylglyoxals and β-enaminones.", Tetrahedron Letter., 57.1 (2016) 103-104.

[2] M. Masoudi, M. Anary-Abbasinejad," Efficient synthesis of terpyrrole derivatives by a pseudo-five-component reaction between pyrrole, β-enaminocarbonyls and arylglyoxals", J. Iran. Chem. Soc., 39.3 (2015) 145-147.

[3] M.Anary-Abbasinejad, A.Falahati. "Synthesis of polyfunctionalized furans by three-component reaction between arylglyoxals, phosphites and malononitrile", J. Iran. Chem. Soc., 12.8 (2015) 1415-1418.

An Efficient Method for One-Pot Synthesis of 1,4-Dihydropyridines under Solvent-Free Conditions

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Dihydropyridine (DHP) derivatives are important class of organic compounds in view of its vast application in pharmaceuticals. These derivatives are widely known as calcium channel blockersand emerge as one of the most substantial classes of drugs for treatment of cardiovascular diseases including hypertension [1]. Many methods have been reported for the synthesis of 1,4-dihydropyridine derivatives in view of the biological importance associated with these compounds. However, many of them suffer from drawbacks such as unsatisfactory yields, long reaction time and pollution to the environment resulted from the use of organic solvent and/or acidic or basic promoters [2]. Thus, development of a simple, efficient, and versatile method for preparation of new derivatives of 1,4-dihydropyridine is a great challenge.The best known procedure for preparation of symmetrical 1,4-dihydropyridines is the classical Hantzch synthesis [3].

In the work presented here, an efficient one-step synthesis of 1,4-dihydropyridines in good to excellent yields via the $Al(OAc)_3$ catalyzed Hantzsch three-component reaction of an aldehyde, ethyl acetoacetate and ammonium acetate under solvent-free conditions at 80 ^{o}C and in room temperature is described and these different conditions are compared with each other. The present methodology offers several advantages such as simple procedure, excellent yields, and short reaction time. It would better to mention that catalyst can be easily separated from reaction mixture and reused severaltimes in subsequent reactions.

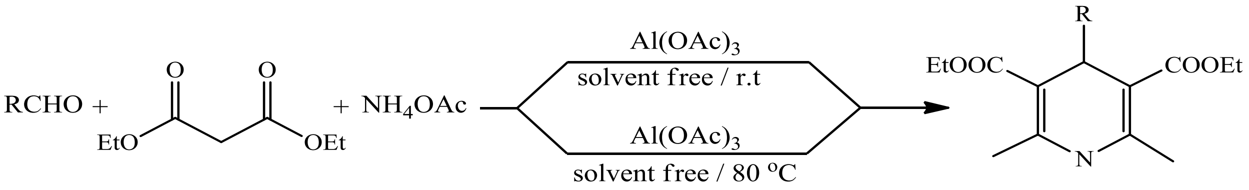

Figure 1. Scheme of the reaction.

References

[1] R. Budriesi, A. Bisi, P. Ioan. Bioorganic and Medicinal Chemistry 13 (2005) 3423.
[2] S.B. Sapkal, K.F. Shelke, B.B. Shingate, M.S. Shingare, Tetrahedron Letters 50(2009) 1754.
[3] J. J. Vanden Eynde, A. Mayence, Molecules 8 (2003) 381.

Synthesis of alkyl iodides from alcohols with silica iodide as a new heterogeneous regent

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Alkyl halides are versatile intermediates in organic synthesis, and their transformation to useful compoundsare well documented in the literature[1]. Amongst alkyl halides, alkyl iodides are used for ionic or radical carbon-carbon coupling reactions such as their application in substitution, elimination, coupling reactions, etc[2]. Iodination of alcohols is the most general protocol for the preparation of alkyl iodides and therefore this conversion is a frequently encountered transformation in organic synthesis [3]. Silica gel is used extensively as a support in organic chemistry. Modified silica supports for functional-group transformation are also of interest. One of the modified silica based materials is silica chloride, which has been reported as an efficient reagent in synthesis of many rang of organic compounds [4]. In this work, we prepared a new heterogeneous reagent SiO_2–I as simple, mild and high yield procedure for the iodination of allylic, allyl and benzylic alcohols.SiO_2-I wascharacterized by FT-IR, EDX and qualitative analysis.

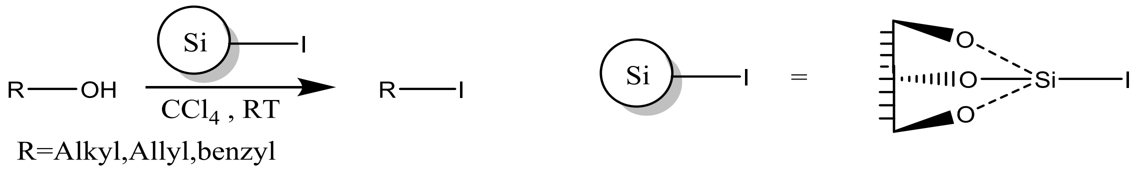

Figure 1. Scheme of the reaction.

References

[1] G. Anilkumar, H. Nambu, and Y. Kita, Org. Process Res. Dev., vol. 6, no. 2, pp. 190–191, Mar. 2002.
[2] M. D. Bhor, A. G. Panda, N. S. Nandurkar, and B. M. Bhanage, Tetrahedron Lett., vol. 49, no. 45, pp. 6475–6479, 2008.
[3] H. Firouzabadi, N. Iranpoor, and M. Jafarpour, Tetrahedron Lett., vol. 45, no. 40, pp. 7451–7454, Sep. 2004.

Preparation of stabilized ionic liquid on the SBA-15 and evaluating its catalytic property in oxidation of alcohols

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Selective oxidation of alcohols to carbonyl compounds is a fundamental synthetic transformation from both synthetic and industrial points of views, because corresponding carbonyl compounds are versatile intermediates of valuable compounds, such as pharmaceuticals, agricultural, and fine chemicals[1]. In the view of stringent environmental concerns, green chemistry, and specially atom efficiency, substantial amounts of researcheshave been recently dedicated to develop new and efficient catalytic protocols based on hydrogen peroxide as terminal oxidant[2].In this manner, transition metal-catalyzed oxidation of alcohols using hydrogen peroxide has been extensively investigated owing to the fact that hydrogen peroxide is a cheap and environmentally benign oxidant, which produces water as the only by-product.To achieve high efficiency and selectivity in the oxidation of alcohols, catalytic systems based on tungsten have been particularly received a great deal of attention[3].

This paper describes a simple procedure for the synthesis and application of SBA-15/Im/WO_4as a novel nano catalyst in oxidation of alcohols by 30% H_2O_2 as green oxidant under neutral aqueous reaction conditions. Furtheremore, in order to testify the recyclability of the catalyst, it is recovered and efficiency reused in 6 succeeding reaction cycles without any significant loss. The use of green solvent, very short reaction time with excellent yields.

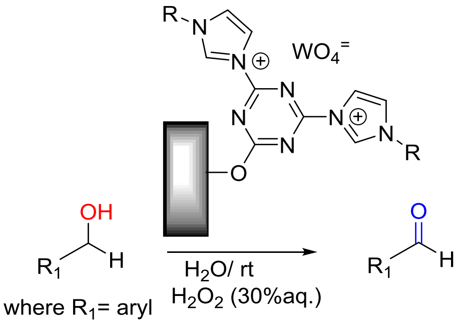

Figure 1. Scheme of the reaction.

References

[1] J. S. Carey, D. Laffan, C. Thomson, M. T. Williams, Org. Biomol. Chem. 2006, 4, 2337.
[2] Z. Wang, Y. Yang, X. Cao, M. Lu, J. Iran. Chem. Soc., 2015
[3] B. Karimi, F. B. Rostami, M. Khorasani, D. Elhamifar, H. Vali, Tetrahedron, 2014, 1.

Fabrication of super hydrophobic and self-cleaning nano-coating

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Many of today's technologies inspired from nature. Self-cleaning technology is one of them. The wings of butterflies and the leaves of cabbage and lotus as nature examples show self-cleaning behavior. Due to the wide spread range of applications, from window glass cleaning, solar panel cleaning and cements to textiles, this technology received a great attention during the late 20th century [1]. With increasing demand for hygienic, self-disinfecting, and contamination-free surfaces, a great deal of attentions has been attracted to developing efficient self-cleaning, protective surfaces and materials. Advances in nanotechnologies could make dirt-free surfaces a reality. This would improve the environment through reduced use of water, energy and petroleum-derived detergents [2,3]. Silica, titanium oxide, silver and calcium oxide nanoparticles are preferentially used for fabrication of super hydrophobic compounds [4].

Herein, we developed a new super-hydrophobic nanocomposite from PDMS and silica nanoparticles. The nanocomposite as a super hydrophobic material with contact angel bigger than 170 has a great attention to adhesion to different surfaces. The existence of nanoparticles was confirmed with TEM.

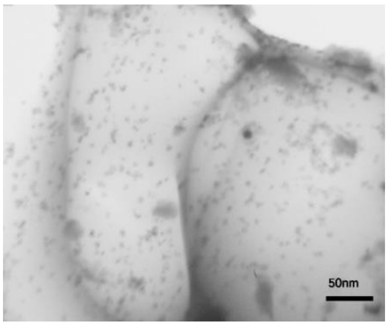

Figure 1. TEM image of nanocomposite

References

[1] V.A. Ganesh, H.K. Raut, A.S. Nair, S. Ramakrishna. Journal of Materials Chemistry (2011) 16304.

[2] P. Roach, N. Shirtcliffe, M. Newton, Soft Matter (2008) 224.

[3] D.J. Behnk, A. park, US Patent, 3913165, (1975).

Industrial preparation of Acamprosate Calcium

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Acamprosate Calcium, Calcium 3-(acetylamino)propane-1-sulfonate , with trade name of Campral is one of a limited number of pharmacological treatment option approved as an adjunct to psychosocial intervention to facilitate the maintenance of abstinence in alcohol dependent patioents [1].Chronic alcohol exposure is hypothesized to alter the normal balance between neuronal excitation and inhibition.In vitroandin vivostudies in animals have provided evidence to suggest Acamprosate may interact with glutamate and GABA neurotransmitter systems centrally, and has led to the hypothesis that Acamprosate restores this balance[2].

Acamprosatecalcium,is a synthetic compound with a chemical structure similar to that of the endogenous amino acid Homotaurine, which is a structural analogue of the amino acid neurotransmitter γ-aminobutyric acid and the amino acid neuromodulator Taurine.

Our process for the straightforwardsynthesis of Acamprosate calcium from 1,3-Propanesultone has been carried out under different reaction condition, and it's parameters has been studied.At last it synthesized corresponding USP (2013)[3,4]. This process is easy to scale up in industry.

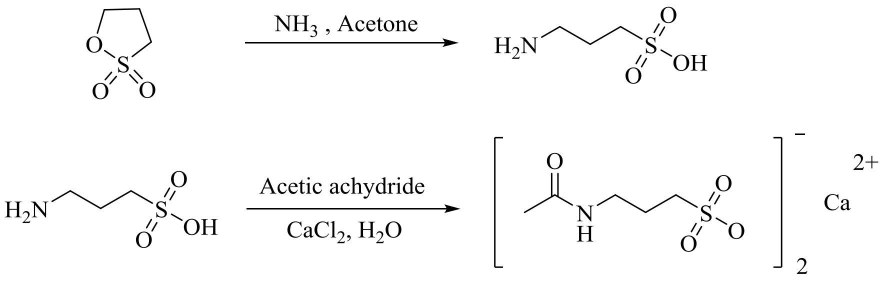

Figure 1. Scheme of the reaction.

References

[1] Plosker, G. L.Drugs, 75(July 2015)1255.
[2] B.J. Mason, A.M. Goodman, R.M Dixon, M.H. Hameed, Neuropsychopharmacology27 (2002) 596.
[3] X. Kong, D. Migneault, X. Wu, US. Pat. 7253306B2(2007).

Magnetic nanoparticles of iron (III) vanadate as a green versatile heterogeneous catalyst for selective oxidation of benzyl alcohols and indane

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Size and shaped-controlled synthesis of iron (III) vanadate (FeVO4) was achieved by the hydrothermal approach. Metal orthovanadates (MVO4) are an interesting class of compounds with diverse applications in various fields such as solar cells, gas sensors, cathode in lithium batteries and more importantly as catalysts [1].

The excellent catalytic activity of the prepared nano-rods of iron vanadate for the oxidation of benzylic alcohols by hint of a Fenton-like process [2] as well as its capability for oxidation of the benzylic sp^3 C-Hs was reported. In the presence of a well-known oxidant, urea hydrogen peroxide (UHP), oxidation have been perfrmed by leaving water behind at the end of reaction as that all ocates in category of green catalysts[3].

Technically, both of prepared nano-rods and nano-spheres were fully characterized by FT-IR, XRD, EDAX, ICP-AES, SEM and TEM. At a distinctive measurement,average diameter of ball- and bar-shaped nanostructures could be seen about 70 nm and 150 nm × 1.3 μm, respectivelv. In the presence of the catalyst, alcohols and methylene of a specific alkylarene, indane,chemo-selectively(100%) convert to the corresponding aldehydes/ketones and α-carbonylarene, respectively. Aftertotal monitoring the turn over number about 380 during ten consecutive runs was dramatically observed.

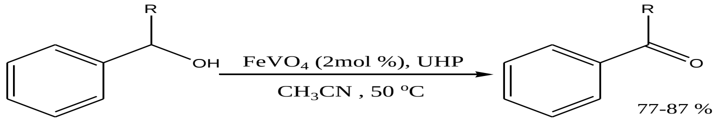

Figure 1. General scheme for chemoselective oxidation of benzyl alcohols

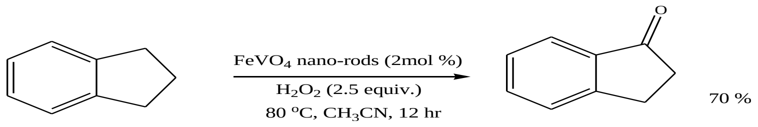

Figure2. Selective oxidation on the benzylic site ofindane system

References

[1] H.M. Zhang, J.B. Liu, H. Wang, W.X. Zhang and H. Yan, J. Nanopart. Res., 2008, 10,

[2] R. Z. Khaliullin, A.T. Bell and M. Head-Gordon, J. Phys. Chem. B, 2005, 109, 17984–17992.

[3] Y. M. A. Yamada, C. K. Jin and Y. Uozumi, Org. Lett., 2010, 12, 4540–4543.

Studies and antibacterial properties of a new synthesized complexe with a tridentate Schiff base ligand

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Antimicrobial activity of the tested samples was determinedusing a modified Kirby–Bauer disc diffusion method [1]. The antibacterialactivities were done by using gram +ve organisms (Staphylococcusaureus and Bacillus subtillis) and gram -ve organisms(Escherichia coli and Pseudomonas aeruginosa). These bacterialstrains were chosen as they are known human pathogens. Our studies showed that the metal complexes exhibit moderate antibacterial activity, and their antibacterial activity is higher than that of the ligand against both Gram positive and Gram negative bacteria. The studies on Schiff bases have been fast developed because of the wide variety and potential industrial, biological, analytical, medicinal, pharmaceutical and catalytical applications [2-5]. Moreover complexes of Schiff base ligands with some transition metals show significant biological activities, including antimicrobial, antibacterial and anticancer. In view of biological importance of Schiff base derived from the condensation of 2-amino phenol with 5-bromo salicyladehyde and its applications in various fields, in the present investigation we thought it worthwhile to synthesize the complexe. In the present work, we describe the synthesis of new metal complexes with 1-methyl-imidazole and a tridentate Schiff base ligand, obtained by the condensation of H_2L .

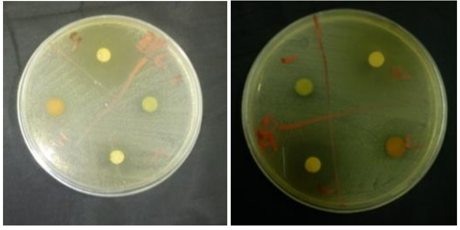

Figure 1.reaction of e.coli and stafilo on schif base complexes and H_2L.

References

[1] A.W. Bauer, W.M. Kirby, C. Sherris, M. Turck, Antibiotic susceptibility testingby a standardized single disk method, J. Am. Clin. Path. 45 (1966) 493.
[2] H. Hosseini-Monfared, N. Asghari-Lalami, A. Pazio, K. Wozniak, C. Janiak, norg. Chim. Acta 406 (2013) 241-250
[3] W.K. Dong, Y.X. Sun, Y.P. Zhang, L. Li, X.N. He, X.L. Tang, Inorg. Chim. Acta 362 (2009) 117–124.

Vitamine B_1 Functionalized γ-Fe_2O_3@SiO_2 :Organo catalysed Paal–Knorr Pyrrole Synthesis

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We supported vitamin B_1 (VB_1) on the magnetic surface to provide a hybrid organic-inorganic biocatalyst. This catalyst was evaluated in the synthesis of substituted pyrroles using condensation of 1, 4-diketone and primary amines and desired products were achieved in high yields. γ-Fe_2O_3@SiO_2@VB_1 showed a typical superparamagnetic behavior so we could separate this catalyst from the reaction vessel by external magnet. This biocompatible catalyst could be recovered 5 times without the significant loss of its activity. The amount of loaded vitamin B_1 on the surface was 0.02 mmol per gram of support. Cheap and minimal toxicity were reasons to use from VB_1 as a reusable organocatalyst.

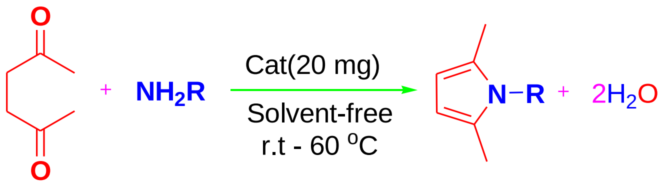

Figure 1: Synthesis of substituted pyrroles under optimized conditions

References

[1] T. Akiyama, Chem. Rev. 2007, 107, 5744.
[2] M.T. Reetz, B. List, S. Jaroch, H. Weinmann, Organocatalysis, Springer-Verlag,, Berlin Heidelberg, 2008.
[3] A. Rahmatpour, Appl. Organometal. Chem.2011, 25, 585.

Fingolimod interacted with the human serum albumin using hydrophobic forces

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Human serum albumin (HSA) has many physiological functions due to its high capacity as a carrier and as a reservoir for molecules such as fatty acids, nutrients and drugs. Fingolimod is the first oral therapy drug that approved by FDA for relapsing-remitting multiple sclerosis (RRMS) [1].

Interaction between human serum albumin (HSA) and Fingolimod has been investigated using spectroscopic methods. UV-vis spectrum of enhanced concentration of fingolimod was studied and the results showed an absorption enhancement in wavelength of 278 nm along with a shift from 278 to 275nm. According to the results the complex formation occurs and the change in HSA conformation following the complexation leads to maximum wavelength change. Fluorescence quenching titrationsin physiologic conditions (i.e pH 7.4), showed that tryptophan emission of HSA is quenched by the addition of enhanced concentrations of fingolimod which showed that fingolimod interacted with HSA and drug-HSA complexes, following the drug addition to the HSA solution. The results suggested well interaction between fingolimod and HSA. Accordingly the combined therapies should be administered with cautions to avoid unwanted variations in drug free fractions in blood. In additions the tendency of fingolimod to HSA could be regarded as a possible root for better drug delivery using albumin as a carrier in the future studies [2,3].

References

[1] Olsen H, Andersen A, Nordbø A, Kongsgaard UE, Børmer OP. Pharmaceutical-grade albumin: impaired drug-binding capacity in vitro. BMC Pharmacology and Toxicology. 2004;4(1):4.

[2] Safarnejad A, Shaghaghi M, Dehghan G, Soltani S. Binding of carvedilol to serum albumins investigated by multi-spectroscopic and molecular modeling methods. Journal of Luminescence. 2016;176:149-58.

[3] Jokubaitis VG, Li V, Kalincik T, Izquierdo G, Hodgkinson S, Alroughani R, et al. Fingolimod after natalizumab and the risk of short-term relapse. Neurology. 2014;82(14):1204-11.

Use of starch–sulfuric acid and steam as a bio and recyclable system for Hantzsch reaction

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In recent years, much attention has been paid to the synthesis of 1,4-dihydropyridines (1,4-DHPs) due to their relevant biological activity [1]. The classicalmethods for the synthesis of 1,4-DHPs is the Hantzsch multicomponent synthesis between an aldehyde, a 1,3-dicarbonyl compound and a source of ammonia, for example, ammonium acetate or an amine in the presence of different acid–basic catalysts[2].Recently, the direction of science and technology has been shifting toward more eco-friendly, natural product resources and reusable catalysts. Natural biopolymers are attractive candidates in the search for solid support catalysts [3].

Starch–sulfuric acidwas prepared by reaction between starchand chlorosulfonic acid. This catalyst has been used for some multicomponent reactions [4].Nowwe report an efficient and convenient procedure for the One-Pot synthesis of ethyl acetoacetate, aromatic aldehydes and ammonium acetate, by using heterogeneous catalyst starch–sulfuric acidunder solvent-free and steam conditions to produce the 1,4- dihydropyridine derivatives in excellent yields (Figure 1).

Steam conditions improved the Hantzsch reaction and the yields of 1,4-dihydropyridines under steam conditions are similar to or higher than those described in the literatures. In conclusion, we have demonstrated for the first time a novel synthetic protocol enabling access to Hantzsch 1,4-DHPs in good to excellent yields in short reaction times at room temperature. We believe that the present improved modification is a convenient and attractive alternative to the existing methods for the synthesis of 1,4-DHPs.

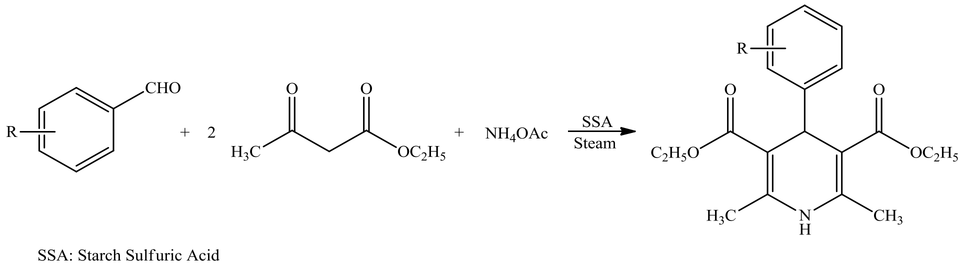

Figure 1. Steam mediated synthesis of 1,4-DHPs

References

[1] V. Estévez, M. Villacampa, J.C. Menéndez. Chemical Society Reviews39 (2010) 4402.
[2] M.B. Gawande, R.K. Pandey, R.V. Jayaram, Catalysis Science & Technol. 2 (2012) 1113.
[3] A. Buleon, P. Colonna, V. Planchot, S. Ball, International Journal of Biological Macromolecules 23 (1998) 85.

β-Cyclodextrin Polymer Functionalized Magnetic Nanoparticle as a Novel Nano-inhibitor System in Flexible PVC

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The migration of phthalate plasticizers poses a serious threat to public health and the environment, because some of the phthalate series such as dioctyl phthalate (DOP) are suspectedas endocrine disruptor and potential health risks may arise from its chronic exposure. Thus, aneffective and practical approach is required for reducing DOP migration from plasticized PVC (P-PVC) [1,2].

In this study, we have synthesized a novel nano-inhibitor system, poly β-cyclodextrin conjugated magnetic nanoparticle (MNP-PCD) and explored its application in the efficient reduction of DOP migration from the P-PVC [3]. Migration tests of the flexible PVC were carried out according to the Organization for Standardization (ISO) 3826:1993(E) method, and the quantity of migrated DOP was then measured by using Gas chromatography (GC) and ultraviolet-visible (UV-vis) spectroscopy. From this result, it is observed that the synthesized novel nano-inhibitor system offers efficient interaction of poly β-cyclodextrin with DOP and effectively reduces the DOP migration from P-PVC (reduction efficiency was found to be 55 ~ 65%) without resulting in any serious changes in mechanical properties of plasticized PVC.

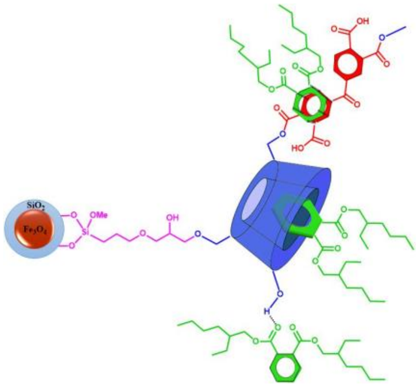

Figure 1. Scheme of the reaction.

References

[1] Federica Chiellini , Marcella Ferri, Andrea Morellia, Lucia Dipaola, Giuseppe Latini. Progress in Polymer Science 38 (2013) 1067– 1088.

[2] Byong Yong Yu, Ah Reum Lee, Seung-Yeop Kwak. European Polymer Journal 48 (2012) 885–895.

[3] Hiroyuki Kono, Taichi Nakamura. Reactive & Functional Polymers 73 (2013) 1096–1102.

Synthesis, characterization of new azomethine compounds based on aminophenolmoiety and evaluation of their antibacterial properties

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Schiff base which contain an azomethine group attract much interest in synthetic chemistry. Schiff base imports in elucidating the mechanism of transformation reactions in biological systems due to presence of imine (-N=CH-) group[1]. AzoSchiff bases are used as substrate in the preparation of a number of industrial and biologically active compounds via closure, cycloaddition and replacement reactions. Moreover,azomethineare also known to have biological activities such as antibacterial [2], antifungal and antitumoractivities [3].

In the present investigation, a series of newly azo Schiff bases containing aminophenol derivatives synthesized for evaluating of their possible antibacterial activity.New compounds were synthesized from 2-hydroxy-5(pyridine-4-yl-diazenyl)benzaldehyde and *n*-aminophenol in absolute ethanol.The structures of thenewly synthesized compounds have been confirmed on the basis (IR, ^{1}HNMR, and ^{13}CNMR spectroscopy).Antibacterial activityof synthesized compounds against*Bacillus cereus*, *Staphylococcus aureus*, *Escherichia coli* and *Klebsiella pneumonia*was studied by disc diffusion method.The results indicated that some of the prepared compounds had antibacterial activities against Gram-positive bacteria (S. aureus and B. cereuss), but they were slightly active against Gram-negative bacteria (E. coli and K. pneumonia).

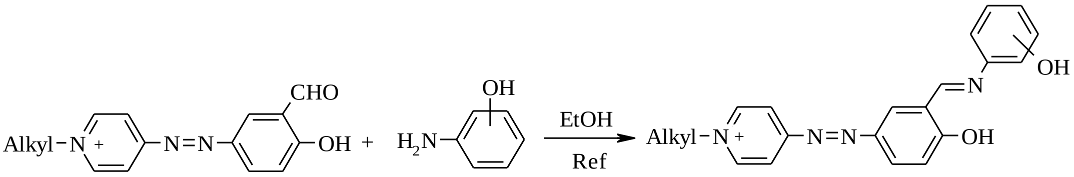

Figure 1. Scheme of the reaction.

References

[1] A.Kakanejadifard, FaridehAzarbani, AbedinZabardasti, AzamRezayat, MotalebGhasemian, SaharKakanejadifard, SpectrochemicaActa A. 114(2013) 404.
[2] S.M.Karthikeyan, J. D. Prasad, B. Poojary. Bioorg.Med. Chem, 14(2006) 14,7482.
[3] M.Ghasemian, A.Kakanejadifard, F.Azarbani, A.Zabardasti, ,S.Kakanejadifard,SpectrochimicaActa A. 124 (2014) 153.

Preparation of Novel Molecular Imprinted Polymer Nanoparticles for the Cancer Drug Delivery

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The aim of the engineered drug delivery systems for cancer treatment is increasing the efficacy of chemotherapeutic agents while minimizing the interactions with healthy sites in the body [1]. This goal can be achieved by modifying their bio-distribution and controlling the rate at which the agent is released [2]. In this regard, different materials such as porous silica, carbon nanotube, calcium phosphate cement and various polymers have been intensively investigated in drugdelivery systems [3].

Herein, we would like to report preparation of the NIPAAM-functionalized MNPs (NIPAAM@Fe_3O_4)[4]addition of the DOX medicine to NIPAAM@Fe_3O_4, and preparation of the related polymer for delivery of DOX with the pH and thermosensitive properties.

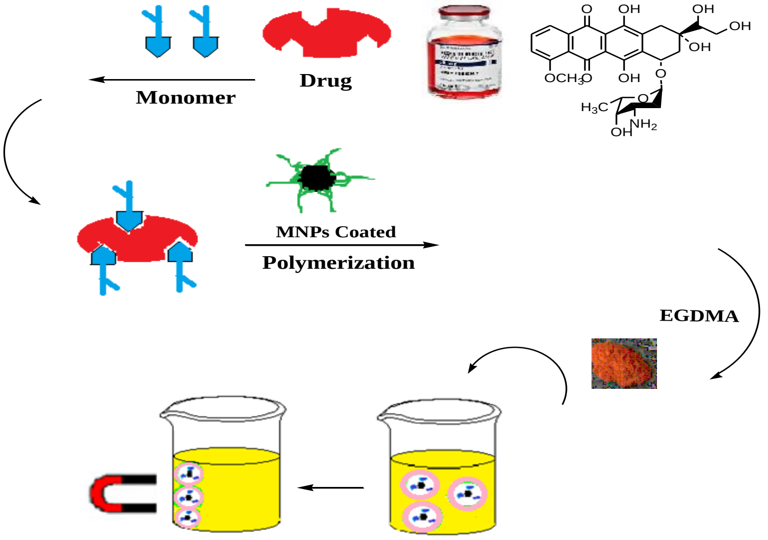

Figure 1. Synthesis of molecularimprinted nanoparticle polymer

References

[1] E.V. Batrakova, A.V. Kabanov,J.Controled Release, 130 (2008) 98.
[2] Z. Wei, J.G. Hao, S. Yuan, Y.J. Li, W. Juan, X.Y. Sha X.L.Fang, Int. J.Pharm.376 (2009) 176.
[3] C.S. Yong, J.S. Choi, Q.Z. Quan, J.D. Rhee, C.K. Kim, S.J. Lim, K.M. Kim, P.S. Oh, G. Choi,Int. J.Pharm.226 (2001) 195.

Convenient One-Pot Synthesis of Spirooxindole Derivatives Containing a 1,3,4-Thiadiazine Scaffold

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Heterocycles containing the spirooxindole scaffold has been found to display antitumor, antimicrobial, antifungal and antimalarial activities. Moreover, the spirooxindole motif is a core structure of various natural products, such as spirotryprostatin, strychnofoline and cyclopiamine. Molecules containing the 1,3,4-thiadiazineskeleton are frequently found in biologically activecompounds that display excellent antifungal, antimicrobial, anti-inflammatory, cardiovascular, anti-HIV, antidiabetic and antidepressant activities. Generally, 1,3,4-thiadiazine derivatives are preparedthrough cyclocondensation of amino thiols with bifunctionalreagents such as α-halo ketones [1].On the other hand,various methods have been reported in the literature for the synthesis of spirooxindoles [2], but the synthesis ofmolecules containing both spirooxindole and 1,3,4-thiadiazinemoieties has not been reported. In a continuation of our efforts toward the synthesis ofspirooxindole derivatives [3], we report the One-Pot threecomponentreaction of isatin derivatives1, 2-aryl-2-oxoethylthiocyanates 2, and hydrazonoyl chlorides 3 in thepresence of Et_3N in refluxing EtOAc to afford the corresponding4′*H*-spiro[indole-3,5′-[1,3,4]thiadiazin]-2(1*H*)-ones 4 in high yield (figure 1).

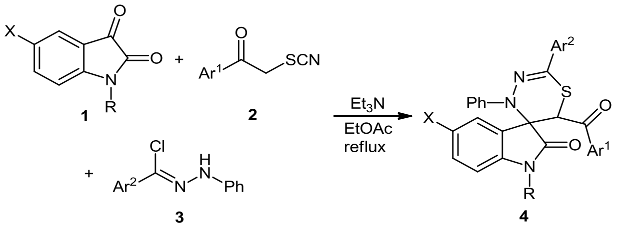

Figure 1. Synthesis of 4′H-spiro[indole-3,5′-[1,3,4]thiadiazin]-2(1H)-ones

References

[1] (a) Mohareb, R. M.; Shams, H. Z.; Elkholy, Y. M.Phosphorus,Sulfur Silicon Relat. Elem. 1992, 72, 93.(b) Jira, T.; Pfeiffer, W. D.;Lachmann, K.; Epperlein, U. Pharmazie1994, 49, 401. (c) Jira, T.;Stelzer, A.; Pfeiffer, W. D.; Schopplich, C.; Siegert, S.;Kindermann, M. Pharmazie1997, 52, 831.

[2] (a) Vidhya Lakshmi, N.; Tamilisai, R.; Perumal, P. T. TetrahedronLett. 2011, 52, 5301. (b) Esmaeili, A.; Amini-Ghalandarabad, S.; Mesbah, F.; Tasmimi, M.;Izadyar, M.; Fakhari, A.; Salimi, A. Tetrahedron Lett2015, 71, 2458.

[3] (a) Alizadeh, A.; Mokhtari, J. Tetrahedron Lett2011, 67, 3519. (b) Alizadeh, A.; Moafi, L. Helv. Chim. Acta2015, 98, 546.

Evaluation of 5-fluorouracil imprinted polymer for controlled drug delivery

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Since the seminal work of Polyakov in the 1930s, using silica matrices, the idea of a molecularly imprinted polymer has evolved to include a massive array of organic polymers and polymer formats[1]. MIP has several applicants in various areas such as biosensors, membrane separation, solid-phase micro extraction, molecular recognition and drug delivery system (DDS). In molecular imprinting, the target molecule (or a derivative thereof) acts as the template around which interacting and cross-linking monomers are arranged and co-polymerized to form a cast-like shell. Initially, the monomers form a complex with the template through covalent or noncovalent interactions. After polymerization, the template is removed, and binding sites are exposed that are complementary to the template in size, shape, and position of the functional groups. In essence, a molecular "memory" is imprinted on the polymer, which is now capable of selectively rebinding the template [2]. This work use 5-florouracil as template which is anticancer drug and use as chemotherapeutic agent, Meta acrylic (MAA) acid as Functional monomer,trimethylolpropane trimethacrylate (TRIM) as cross-linker and 2,2'-Azobis(2-methylpropionitrile) (AIBN) as initiator in Dimethyl sulfoxide (DMSO) as solvent. Results from Fourier Transform Infrared Spectroscopy (FTIR), Thermogravimetric Analysis (TGA), Scanning Electron microscopy (SEM) show that this imprinted sorbent exhibits good recognition and high affinity for 5-florouracil. Selectivity of molecularly imprinted polymers (MIP) was evaluated by comparing several substances with similar molecular structures to that of 5-florouracil. The results show the ability of MIP polymers to control 5-florouracil releases.

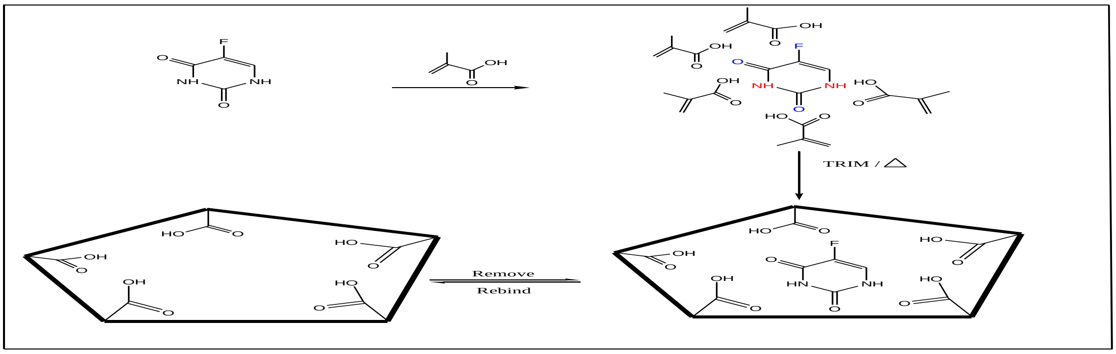

Figure 1 . Synthesis of 5-fluorouracil Molecular imprinted polymer

References

[1] Alexander, C.; Andersson, H. S.; Andersson, L. I.; Ansell, R. J.; Kirsch, N.; Nicholls, I. A.; O'Mahony, J.; Whitcombe, M. J., Molecular imprinting science and technology: a survey of the literature for the years up to and including 2003. *Journal of molecular recognition : JMR* 2006,*19* (2), 106-80.

[2] Cunliffe, D.; Kirby, A.; Alexander, C., Molecularly imprinted drug delivery systems. Advanced drug delivery reviews 2005, 57 (12), 1836-53.

$CoFe_2O_4$@ Nano-hydroxyapatite (n-HA) nanocomposite loaded with amoxicillinand streptomycin antibiotics as drug carrier

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Magnetite nanoparticles (MNPs) are among the most highly applied particles. The wide range of MNPs utilization are consisted of various fields such as catalysis, separation, and drug delivery [1]. In order to be used for biomedical purposes, magnetic nanoparticles mustbe pre-coated with substances that ensure their stability, biodegradability and non-toxicity in a physiological medium [2]. Nano-hydroxyapatite (n-HA) has been considered as an idealinorganic drug carrier due to its high surface area to volume ratio,high surface activity, good biocompatibility, and strong ability toabsorb a variety of chemical species [3].

In this study, amoxicillin (AMX)and streptomycin (STR) antibiotics were supported on a nancomposite consisted of cobalt ferrite nanomagnetic core coated with hydroxyapatite (HA). After obtaining and characterization of the $CoFe_2O_4$@HA@AMX and $CoFe_2O_4$@HA@STR nanocomposites, their bactericidal activity were studied against some gram-positive and gram-negative bacteria using diffusion disc method. The step by step preparation of $CoFe_2O_4$@HA@drugnanocomposites is shown in the following figure.

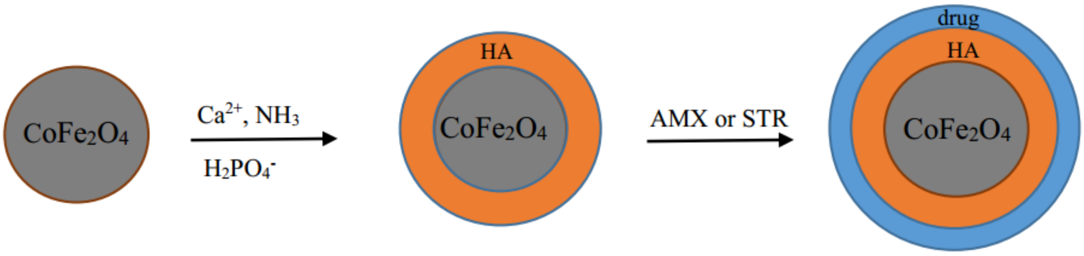

Figure 1. *Scheme of the reaction.*

These antibacterial composites showed an improvement in antibacterial effect of the drugs andadditinall, they can be easily removed from solution by magnetic decantation after treatment to avoid contamination of the aquasystems.

References

[1] F.Farjadian,at al, International Journal of Pharmaceutics504 (2016) 110-116.
[2] A. S. Timin, at al, Materials Science and Engineering: C 64 (2016) 20–28.
[3] S. Jafari, at al, Colloids and Surfaces B: Biointerfaces140 (2016) 223-232.

Antibacterial activity of streptomycin intercalated magnetic zinc–aluminium–carbonate LDH nanocomposite

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Layered double hydroxides (LDHs), also known as hydrotalcite-like compounds or anionic clays, have been investigated as potential materials for adsorbents, ion-exchangers, pharmaceutics, mechanical properties, UV photostability, and so on [1]. Indeed, intense research interests have focused on creating novel magnetic LDHs to control drug release at defined target cells of tissues.The intercalation processes are carried out following different routes (direct synthesis, co-precipitation, and anion exchange) [2].

In this study, streptomycin was intercalated into a nanocomposite consisted of cobalt ferrite magnetic core coated with zinc-aluminium layered double hydroxide (LDH). After obtaining and characterization of the resultednanocomposite by various techniques, its antibacterial activity was studied against some gram-positive and gram-negative bacteria using diffusion disc method. The step by step preparation of $CoFe_2O_4$@ZnAl-Str-LDH nanocomposite is shown below.

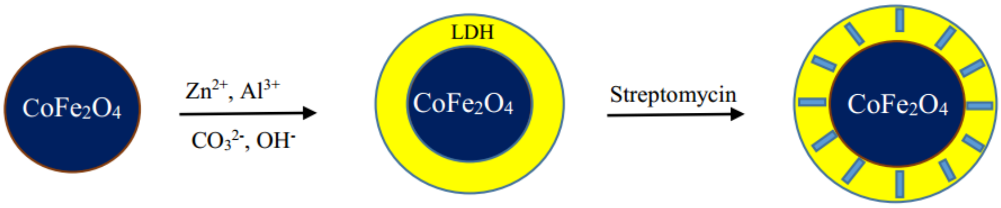

Figure 1. *Scheme of the reaction.*

The as-preparednanocomposite showed an improvement in the antibacterial activity of streptomycin indicating the presence of synergistic effect. This antibacterial agent can be easily removed from disinfected solution by magnetic decantation to avoid any contamination to the environment.

References

[1] S. Xu, at al, Applied Clay Science 114 (2015) 112–119.
[2] Y.Kuthati, at al, Applied Clay Science 112–113 (2015) 100–116.

Synthesis of Magnetite Nanocomposite with Ability to Remove Pb^{2+} ions from Aqueous Solutions

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Contamination resulted by toxic metal ions has been a major environmental problem since the development of industry. Pb^{2+} is one of the most toxic metal ions, which can accumulate in human body and cause serious damages to the hematopoietic and cardiovascular systems [1]. There are many chemical and physical processes to remove heavy metal ions from water. Of these, adsorption is one of the most promising technologies due to its high removal efficiency, simplicity and availability of low-cost adsorbents which can be found locally [2].Encapsulation of magnetic nanoparticles (MNPs) in polymeric structures prevents direct contact of magnetic substance with the environment and leads to its improved colloidal and chemical stability and reduces its toxicity for removal of heavy metal ions. Modification of the nanoparticle surface develops its applications in a wide variety of fields such as adsorption purposes [3]. Magnetic-core and polymer-shell configuration synergistically combines the multiple advantages of MNPs and the polymer.

In the present study, a novel magnetic nanoadsorbent was synthesized by grafting of poly(acrylamide) onto the surface ofmodified Fe3O4 nanoparticles. For this purpose firstly the nanoparticle surface was modified through silylation reaction with 3-aminopropyl triethoxysilane (APTES).Then The terminal amino groups were then reacted with glycidyl methacrylate (GMA) to generate the vinyl-containing moieties on the nanoparticle surface. Finally, acrylamide (AAm) was polymerized on the surface of vinyl-containing nanoparticles to prepare the final nanoadsorbent. The adsorbent was characterized by Fourier transform infrared (FT-IR) spectroscopy, X-ray diffraction (XRD) and vibrating sample magnetometry (VSM).The synthesized nanoadsorbent exhibited high adsorption affinity for Pb^{2+} in aqueous media.

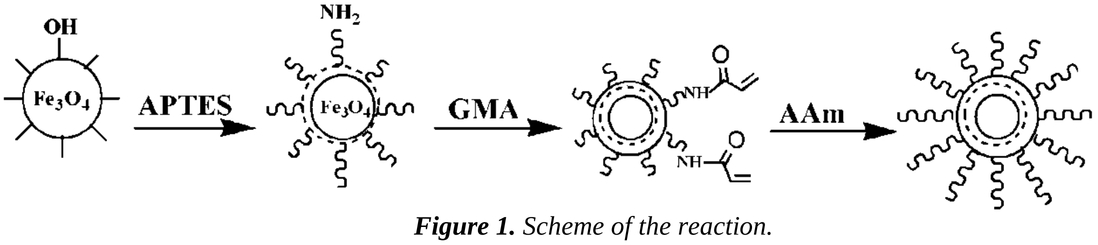

Figure 1. *Scheme of the reaction.*

References

[1] Li, Zhili, Yan Kong, and Yuanyuan Ge."Synthesisof porous lignin xanthate resin for Pb^{+2} removal from aqueoussolution." Chemical Engineering Journal 270 (2015): 229-234.

[2] Nguyen, Thuy Chung, et al. "Simultaneous adsorption of Cd, Cr, Cu, Pb, and Zn by an iron-coated Australian zeolite in batch and fixed-bed column studies." Chemical Engineering Journal 270 (2015):393-404.

[3] Horák, Daniel, et al. "Monodisperse magnetic composite poly (glycidyl methacrylate)/La 0.75 Sr 0.25 MnO 3 microspheres by the dispersion polymerization." Polymer 51.14 (2010): 3116-3122.

Synthesis and Characterization of a New Polyamide Network for Use as Cu^{2+} Adsorbent from Aqueous Media

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Water contamination with toxic ions has become a great environmental problem. Among toxic metal ions, copper is a micronutrient element and play an important role in the bone formation together with certain proteins and enzymes. But, it is considered a hazardous pollutant when it cannot be maintained at an appropriate physiological concentration. Cu^{2+} ions have been introduced from several industrial wastewaters. Therefore a simple, reliable, selective and sensitive method for Cu^{2+} monitoring and removal is important for environmental safety and health [1]. Various methods and technologies have been developed and reported for effective removal of Cu^{2+} from aqueous solutions. Among these methods, adsorption with a chelating resin containing amino and carboxyl groups has attracted considerable research interest in recent years due to advantages of achieving high efficiency, good selectivity, reusability and relatively low cost [2]. There are several groups of chelating agents that contain carboxylate functional groups bound to one or more nitrogen atoms and have the ability to sequester metal ions. Therefore, surface functionalization with these high affinity binding groups has received considerable research interests in the recent years [3].

In this work, firstly 2, 6-dimethyl-3, 5-pyridinedicarboxhydrazide (DMPDCH) was synthesized using the Hantzsch pyridine synthesis followed by reacting with hydrazineaccording to Figure 1. Then a novel polyamide network was prepared by condensation polymerization of the DMPDCH with citric acid (CA). The prepared poly (DMPDCH-*co*-CA) was used as chelating agent to remove Cu^{2+} from aqueous solutions. Different parameters were investigated to obtain optimized condition. Results showed acceptable efficiency for the prepared resin. The structural characterization of the resin was studied using FT-IR, TGA and SEM analyses.

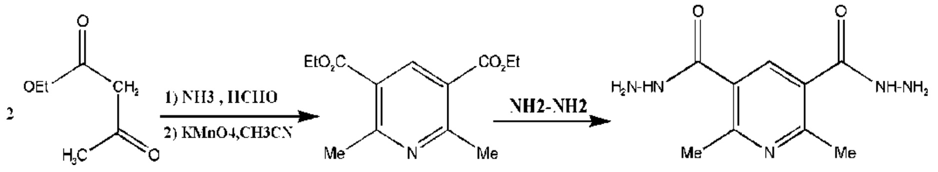

Figure 1. *Scheme of the reaction.*

References

[1] Awual, Md Rabiul. "A novel facial composite adsorbent for enhanced copper (II) detection and removal from wastewater." Chemical Engineering Journal 266 (2015): 368-375.

[2] Repo, Eveliina, et al. "Aminopolycarboxylic acid functionalized adsorbents for heavy metals removal from water." Water research 47.14 (2013): 4812-4832.

[3] Emik, Serkan. "Preparation and characterization of an IPN type chelating resin containing amino and carboxyl groups for removal of Cu (II) from aqueous solutions." Reactive and Functional Polymers 75 (2014): 63-74.

Synthesis of arylhydrazonesusing stable diazonium salts and dimedone,malononitrileor ethylacetoacetate under mild conditions

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Diazonium salts are useful synthetic building blocks in organic synthesis because these compounds can be linked to methine or aromatic sp^2-hybridized C-atoms. The diazotization and diazo coupling reactions are usually carried out with protonation of nitrous acid under strongly acidic conditions, and azo coupling carried out at low temperature in the presence of nucleophilic coupling components [1]. Although satisfactory yields of products are usually obtained, the diazotization and diazo coupling reactions are complicated by numerous competing reactions. For example, reaction temperatures above 10 °C generally promote phenol formation in aqueous media, and subsequent coupling of the phenol with undecomposed diazonium salts produces azophenols. Moreover, because of this instability, subsequent reactions with diazoniumsalts must be carried out under the same conditions that these saltsare formed. Thus, aryldiazonium salts with higher stability andversatility that can be easily made and stored under solid stateconditions with explosion-proof properties are desired andnecessary.In continuation of our studies on the application of stable diazonium salts [2,3], herein, we wish to report a convenient and rapid method for the synthesis of some arylhydrazonesusing aryl diazonium silica sulfates in the presence of dimedone, malononitrile and ethyl acetoacetate under mild conditions. The use of inexpensive materials, simple and clean work-up, short reaction times and good yields are advantages of this method.

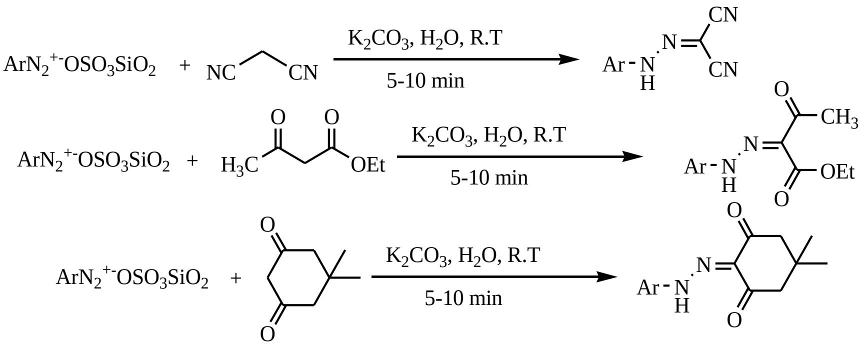

Figure 1. Scheme of the reaction.

Refrences

[1] H. Zollinger. Diazo chemistry I, aromatic and heteroaromatic compounds. Weinheim: Wiley VCH; 1994.
[2] A. Zarei, A.R. Hajipour, L. KHazdooz, F. Mirjalili, A. NajafiCHermahini. Dyes Pigments 81(2009)240.
[3] A. Zarei, A.R. Hajipour, L. KHazdooz, F. Rafiee, G.Azizi, A. Abrishami. Tetrahedron Lett53 (2012) 406.

Immobilization of Palladium Complex in Mesoporous Silica MCM-41: an efficient and reusable catalytic system for C-C coupling reaction

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Among the various types of mesoporous silica, MCM-41 shows a highly ordered hexagonal array of one dimensional mesopores with pore diameter of 20–100 A°, high surface area (>1000 $m^2.g^{-1}$), structural and high thermal stability (ca. 900 °C), which their surface can be functionalized [1].. This compound has been used as support in the preparation of catalysts for organic transformations [2,3]. In the current study, we try to report the synthesis of immobilized palladium S-methylisothiourea complex on MCM-41 (Pd(0)-SMT-MCM-41) its catalytic properties in the C-C cross coupling reactions. This catalyst was characterized by TGA/DTA, XRD, SEM/EDX, Fourier FT-IR, and TEM. Thus, this catalytic system was offered, simplicity of operation, heterogeneous nature, excellent yields, short reaction times, simple work up in cross-coupling reactions for the formation ofcarbon–carbon bonds using of aryl halides with Ph3SnCl. Finally, the catalyst was recovered and reused for several times without significant loss of their catalytic activity.

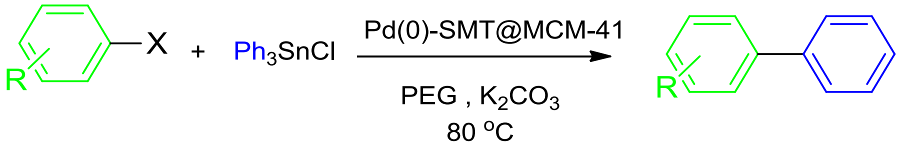

Figure 1. Synthesis of biphenyle using Pd(0)-SMT@MCM-41 with Aryl hildes and Sodium Tetraphenylborate.

References

[1] K. Dhara, K. Sarkar, D. Srimani, S. Kumar. Saha, P. Chattopadhyay, A. Bhaumik. Dalton Transactions 39 (2010) 6395.
[2] M. Abdollahi-Alibeik, M. Pouriayevali. Reaction Kinetics, Mechanisms and Catalysis 104 (2011) 235.
[3] S. Ajaikumar, A. Pandurangan, Journal ofMolecularCatalysis A:Chemical 286 (2008) 21.

Palladium complex grafted onto MCM-41 as efficient, heterogeneous and reusable nanocatalyst for the Suzuki reaction

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In general, various supports have been employed to fabricate heterogeneous Pd catalysts such as carbon [1], ionic liquids [2], polymers [3], molecular sieves (SBA-15 and MCM-41) [4,5], and and etc. In this study, mesoporous MCM-41 has been considered as a very good support for Pd complex. The reason for the use of mesoporous MCM-41 as a good support is that it possess thermal, mechanical and chemical stability. It also has extremely high surface area (1000 m^2g^{-1}), and large channels from 1.5 to 10 nm, ordered in a hexagonal array and large pore volume, which allows for the easy diffusion of substrates to the active sites. A (Palladium S-methylisothiourea) complex supported on functionalized MCM-41 was prepared by a post-grafting method and considered as efficient catalyst for the C-C cross coupling reactions between various aryl halides and sodium tetraphenylborate. Also this catalyst shows good reactivity towards amination of aryl halides.The nanocatalyst was characterized by Analysis (TGA), (XRD), (SEM/EDS), Fourier Transform (FTIR), (ICP) and (TEM)techniques It was also found the catalyst is active, stable and reusable (figure 1).

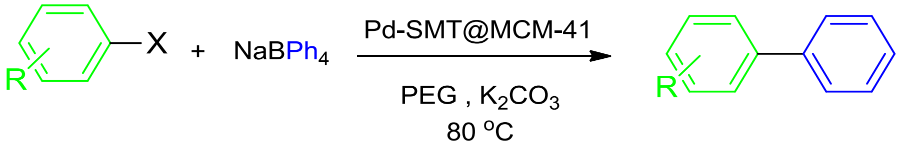

Figure 1. Formation of C-C bond in peresence Pd-MPA@MCM-41.

References

[1] L. Zhang, C. Feng, S. Gao, Z. Wang, C. Wang. Catalysis Communication 61 (2015) 21.

[2] S. Ghosh, R. Dey, S. Ahammed, B. C. Ranu. Clean Technologies and Environmental Policy 16 (2014) 767.

[3] Z. Dong, Z. Ye. Applied Catalysis A: General 489 (2015) 61.

Chemically binding carboxylic acid of L-valine amino acid onto α-MnO_2 nanorods, preparation of PVA/α-MnO_2-L-valine nanocomposite films and study their properties

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Manganese dioxide (MnO_2) is one of the most attractive inorganic materials because of its structural flexibility, ecological and economical compatibility, excellent chemical and the high surface area. Hence, MnO_2 finds application in many fields such as molecular/ion sieves and removal of heavy metal ions [1]. The α-MnO_2nanorods were prepared by a hydrothermal method [2]. The surface of α-MnO_2nanorods was modified chemically with L-valine amino acid by solvothermal strategy. Then poly(vinyl alcohol)/α-MnO_2-L-valinenanocomposites (NCs) containing 1, 3 and 5 wt% of modified α-MnO_2nanorodswere prepared through ultrasound-assisted technique and characterized.Following, effects of α-MnO_2-L-valine nanorods on the properties of NCs such as mechanical and thermal properties were studied. Finally, adsorption behavior of NC 3 wt% was investigated as an adsorbent for sorption of Pb(II) ions. It showed good adsorption potential for the removal of Pb(II)in aqueous solution.

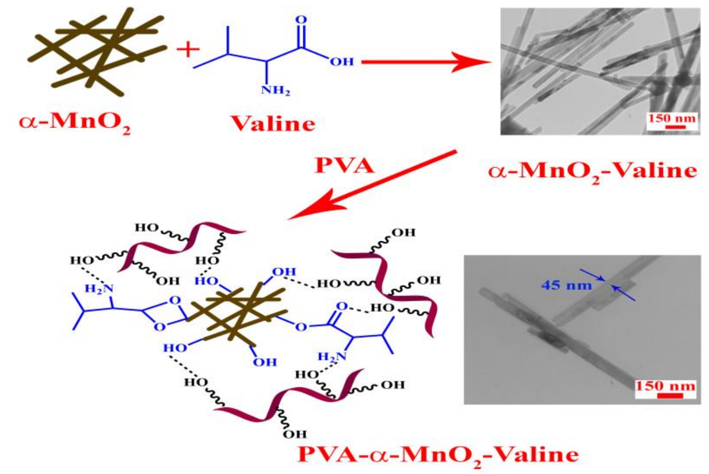

Figure 1. Preparation of PVA/α-MnO_2-L-valine NCs.

References

[1] Z. Song, W. Liu, M. Zhao, Y. Zhang, G. Liu, C. Yu, J. Qiu, J. Alloys Compd. 2013, 560, 151.

[2] Y. Li , H. Xie, J. Wang, L. Chen, Materials Letters. 2011,65, 403–405.

Efficient synthesis of 5-substituted tetrazoles catalyzed by Ni-S-methylisothiourea complex supported on boehmite nanoparticles

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Tetrazoles, being an interesting class of nitrogen-rich heterocycles, wide range of applications as drugs in pharmaceuticals, in coordination chemistry, in synthetic organic chemistry, in catalysis technology, in medicinal chemistry, in the photographic industry, in organometallic chemistry and in various materials science applications including propellants. Also, tetrazoles and their derivatives have been reported as analgesic, antiviral, anti-inflammatory, anti-proliferative, antibacterial, potential anti HIV drug candidate, antifungal, herbicidal and anticancer agents. Therefore, recently, many catalysts have attracted increasing interest in the context for synthesis of tetrazole derivatives [1, 2]. In order to combine the advantages of both homogeneous and heterogeneous catalysis, immobilization of homogeneous catalysts on heterogeneous nanomaterials have been widely used as efficient and reusable catalysts for synthesis of tetrazole derivatives. But, some of nanomaterial are expensive or unstable. Also, synthesis of other nanoparticles require inert atmosphere or high temperature for calcination or preparation [3]. While, boehmite nanoparticles is not air or moisture sensitive, and can be prepared in water at room temperature. Boehmite nanoparticles have several advantages such as non-toxicity, stability, high specific surface area, ease of surface modification due to many hydroxyl groups on its surface, inexpensive and easily and readily available. Several methods have been reported for synthesis of boehmite nanoparticles; but, most of them have focused on the effect of temperature, ultrasonic waves, time and Al/OH molar ratio on morphologies, chemical and physical properties of the prepared particles. Meanwhile, nanoboehmite has been rarely used as support for catalyst [4]. Therefore herein a Nickel S-methylisothiourea complex immobilized on boehmite nanoparticles (Ni-SMTU@boehmite) has been reported as organometal nanocatalyst for the synthesis of 5-substituted 1*H*-tetrazole derivatives using nitriles and sodium azide in PEG-400.

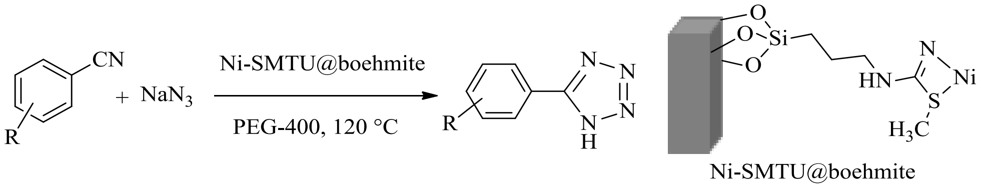

Figure 1. Scheme of the reaction.

References

[1] A. Khalafi-Nezhad, S. Mohammadi, RSC Advances3 (2013) 4362.
[2] F. Abrishami, M. Ebrahimikia, F. Rafiee, Applied Organometallic Chemistry29 (2015) 730.
[3] M. Hajjami, B. Tahmasbi, RSC Advances 5 (2015) 59194.

Synthesis and characterization of Ni-SMTU@Boehmite and its catalytic application in the oxidation of sulfides and oxidative coupling of thiols

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Nanoparticles due to their high surface area and facile recovery, have recently emerged as catalyst supports. One of the novel nanomaterial supports is boehmite. Boehmite has important applications in the preparation of catalysts in petrochemical. Boehmite is structure consists of double sheets of octahedral with aluminum ions at their centers and the sheets themselves are composed of octahedral chains and has a cubic orthorhombic structure [1]. Boehmite is also used as adsorbent, catalyst, cosmetic products and coatings, due to its unique properties such as good thermal stability, high specific surface area and mesoporous properties. A major advantage of boehmite nanoparticles is availability on a large industrial scale [2]. Therefore, several methods have been described for preparation of boehmite nanoparticles. But, most of them have focused on the morphologies, chemical and physical properties of the prepared particles; meanwhile, there is little literatures on the modification of nanoboehmite surface as heterogeneous support [3]. Hence, an attempt has been made to modify of boehmite nanoparticles in this work. In order to regard of this issue, nickel S-methylisothiourea complex has been immobilized on boehmite nanoparticles and further applied as an excellent nano organometal catalyst for the selective oxidation of sulfides to sulfoxides and oxidative coupling of thiols to corresponding disulfides. Because oxidation of sulfides and oxidative coupling of thiols are useful in the synthesis of new molecules, as well as for various medical, chemical, biological, materials, and nanotechnological applications [3, 4].

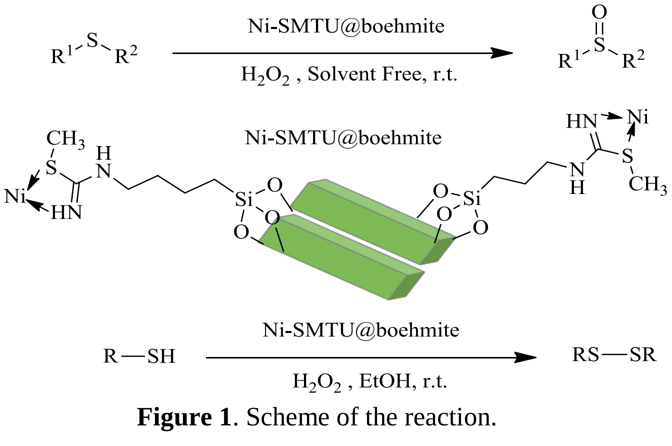

Figure 1. Scheme of the reaction.

References

[1] A. Ghorbani-Choghamarani, B. Tahmasbi, P. Moradi, RSC Advances6 (2016) 43205.
[2] M. Mirzaee, B. Bahramian, A. Amoli, Applied Organometallic Chemistry 29 (2015) 593.
[3] A. Ghorbani-Choghamarani, B. Tahmasbi, F. Arghand, S. Faryadi, RSC Advances 5 (2015) 92174.

Synthesis and characterization of new Pd-complex supported on boehmite nanoparticles and their application for C-C bond formation

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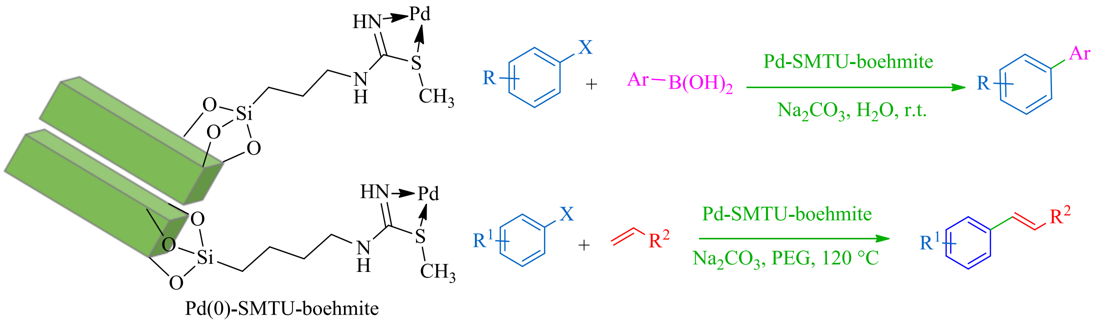
Boehmite is an aluminum oxide hydroxide (γ-AlOOH) particles, which the surface of boehmite nanoparticles covered with hydroxyl groups. Boehmite is structure consists of double sheets of octahedral with aluminum ions at their centers and the sheets themselves are composed of octahedral chains and has a cubic orthorhombic structure. Also, boehmite nanoparticles was not moisture-or air sensitive, and was synthesized in H_2O at room temperature without inert atmosphere using available materials. Boehmite has excellent properties such as chemical resistance, good mechanical strength, good conductivity, high hardness, low cost, high abrasive and corrosion resistance, excellent biocompatibility, relatively and controllable synthesis [1]. Numerous methods have been reported for the preparation of boehmite nanoparticles such as hydrothermal (HS), sol–gel, and hydrolysis of aluminum. Despite several studies on morphology, properties and preparation of boehmite, there are few reports on the modification of nano boehmite surface that have been reported as heterogeneous catalyst [2]. Therefore in this work, palladium S-methylthio urea complex has been supported on boehmite nanoparticles and applied as an excellent and reusable nano organometallic catalyst for the C-C coupling reactions, because cross-coupling reactions were used as a powerful method in modern synthetic organic chemistry for the preparation of natural products, advanced materials, agrochemicals, pharmaceuticals, herbicides, biologically active compounds, polymers, UV screens, preparation of hydrocarbons and liquid crystal materials [3, 4].



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References

[1] M. Mirzaee, B. Bahramian, A. Amoli, Applied Organometallic Chemistry 29 (2015) 593.
[2] A. Ghorbani-Choghamarani, B. Tahmasbi, F. Arghand, S. Faryadi, RSC Advances 5 (2015) 92174.
[3] A. Ghorbani-Choghamarani, H. Rabiei, Tetrahedron Letters 57 (2016) 159.

Pd-S-methylisothiourea complex supported on boehmite nanoparticles: as efficient synthesis of 5-substituted tetrazoles

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In the last decades, supporting of homogeneous catalysts on various heterogeneous solids has been studied as recyclable catalysts. However, many supports such as TiO_2 NPs, MCM-41, SBA-15, iron oxide, carbon nanotubes, heteropolyacids, graphene oxide, ionic liquids, molecular sieve or some polymers have been used as heterogeneous catalysts or as support for homogeneous catalysts, which most of them is expensive, requires inert atmosphere or high temperature for calcination and a lot of time and tedious condition to prepare [1]. While synthesis of boehmite was not moisture or air sensitive, also boehmite was synthesized in H_2O at room temperature using available materials. Nanoboehmite have several attractive features such as stability, non-toxicity, high dispersion of the active phases, high specific surface area, ease of surface modification, readily and easily available, and favorable biocompatibility. Although boehmite nanoparticles has been rarely employed as heterogeneous support [2]. Therefore herein a moisture- and air stable Pd-SMTU@boehmite has been reported as new organometallic catalyst for the synthesis of tetrazole derivatives. Because tetrazoles are important heterocyclic compounds, containing several applications in organic synthesis, material science, coordination chemistry, and medicinal chemistry. For example, Valsartan and Losartan are two typical examples of the extensive application of these compounds in drugs. Also tetrazoles and their derivatives have been reported as antiviral, antibacterial, anti-inflammatory herbicidal, potential anti HIV drug candidate, anti-proliferative, analgesic, and antitumor agents [3, 4]. Thus the synthesis of these heterocycles has become an area of great interest.

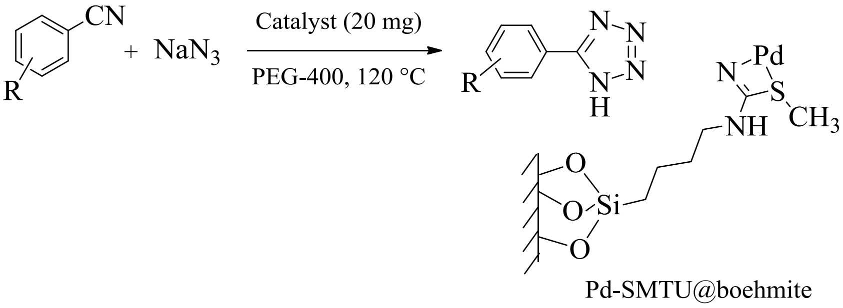

Figure 1. Scheme of the reaction.

References
[1] M. Hajjami, B. Tahmasbi, RSC Advances5 (2015) 59194.
[2] A. Ghorbani-Choghamarani, B. Tahmasbi, F. Arghand, S. Faryadi, RSC Advances 5 (2015) 92174.
[3] F. Dehghani, A.R. Sardarian, M. Esmaeilpour, Journal of Organometallic Chemistry 743 (2013) 87.

Deep eutectic solvent (ChCl/Urea) as a green catalyst for reductive amination of aldehydes and ketones

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Using the non-toxic and environmentally friendly reagents is one of the goals of green chemistry. One of the main components of mostorganic reactions is catalyst. The use of green and non-toxic catalyst is an important issue in a chemical reaction and of particular interested to researchers.Employment of heterogeneous or heterogenized homogeneous catalytic systems, utilization of organic compounds, organocatalysts, and designing the catalytic systems based on environmentally friendly compounds such as ionic liquids are among the attempts that have beenmade in recent years to bring the catalysts closer to the aims of green chemistry. Recently, deep eutectic solvents (DESs) have emerged.

DESs are peers of the conventional ionic liquids (ILs)and as they have low vapor pressure and low flammability [1]. Themain difference between these two families of compounds is that ILsare neither biodegradable nor cost-effective but DESs are biodegradable,non-toxic, inexpensive, and easily prepared.

Due to their presence in natural products, pharmaceutical, and many biologically active molecules, as well as their role as intermediates in the synthesis of fine chemicals and dyes, amine structure has become an important component in chemistry[2] Despite the development of several synthetic methods for the preparing of these compounds in recent years[3] the direct reductive amination of carbonyl compounds is still the powerful tool for this purpose. In this study, we are going to report the synthesis of secondary amines by reductive amination of aldehydes/ketones in the presence of DES (ChCl/Urea) as catalyst and $NaBH_4$ as a reducing agent in MeOH (Figure 1).

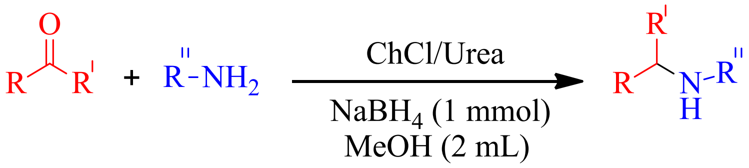

Figure 1. ChCl/Urea catalyzed reductive amination of aromatic aldehydes/ketones with amines

References

[1] Francisco, A.V.D. Bruinhorst, M.C. Kroon, Angew. Chem. Int. Ed.2013, 52, 3074.
[2] A.P. Abbott, T.J. Bell, S. Handa, B. Stoddart, Green Chem.2005, 7, 705.
[3] G. Jiang, J. Chen, J.S. Huang, C.M. Che, Org. Lett.2009, 11, 4568.

The One-Pot Synthesis of Pyrimidine Derivatives by Using NanoSilica Boron Sulfuric Acid as an Efficient Catalystunder Solvent-Free Conditions

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In recent decades, One-Pot multicomponent reactions are known as important and environmentally benign processes in synthetic chemistry because they decrease the number of steps and reduce energy consumption and waste production [1].Pyrimidine and its derivatives constitute an important class of natural and synthetic products that possess significant biological and pharmaceutical properties [2]In particular, functionalized pyrimidinessuch as fused pyrimidinones with an arylidene part are essential heterocyclic motifs in antitumor agents. Regarding the importance of arylideneheterobicyclicpyrimidinonesand the great need for environmentally benign chemical productions, the development of suitable green synthetic methods for these compounds has attracted considerable interest.

Recently, more attention has been paid to the application of solid acids in organic synthesis because of many advantages such as their easy handling and separation, reducing reactor corrosion problems and environmentally safe disposal [3]. So, herein we report a new, convenient, mild, andefficient procedure for One-Pot , three-component synthesis of pyrimidine derivativesin the presencenanosilica boron sulfuric acid (NSBSA) as an effective solid acid catalyst under solvent-freeconditions.

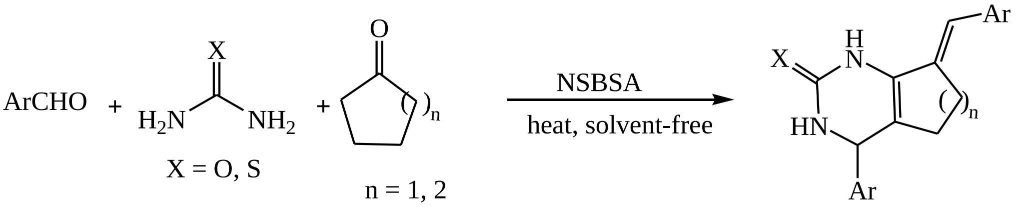

Figure 1. Scheme of the reaction.

References

[1] D. J. Ramon; M. Yus.AngewandteChemie 117 (2005) 1628.

[2] H. I.El-Subbagh, S. M. Abu-Zaid, M. A. Mahran, F. A. Badria, A. M. Al-Obaid.Journal of Medicinal Chemistry43 (2000) 2915.

[3] Z. Li, A. Zhu, X. Mao, X. Sun, X. Gong.Journal of Brazilian Chemical Society, 19(2008), 1622.

Synthesis of 1,2,3-triazoles Catalyzed by Cu-Supported SiO_2

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1,2,3-Triazoles are typical nitrogen-containing heterocyclic molecules that have attracted increasing interest due to their wide range of applications. The 1,2,3-triazole unit is present in several classes of compounds that display different biological activities [1]. Additionally, these components have gained special attention in the drug discovery because several drug molecules contain 1,2,3-triazole group such as Tazobactam, Cephalosporin and Cefatrizine[2].Different methods are available for the synthesis of 1,2,3- triazoles. The most attractive involves the thermal 1,3-dipolar cycloaddition of azides with alkynes, discovered by Huisgen and popularized independently by Sharpless and Meldal [3].

In this method, we have reported synthesis of 1,2,3-triazoles by catalyzed SiO_2/2-Aminothiophenol/CuI. The reaction proceeds by mixing the α-bromoketone, sodium azide, alkyne and the catalyzed in aqueous media to afford the desired products in excellent yield. The heterogeneous catalytic system showed highly efficiency, performing the multicomponent Huisgen reaction in a green approach based on recoverability, recyclability and avoidance of wastes.

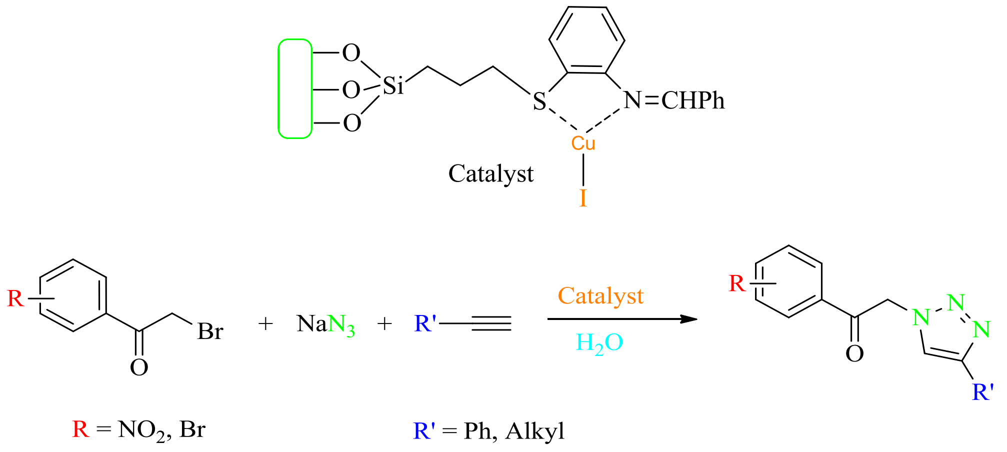

Figure 1. Click reaction catalyzed by CuI-Silica

References

[1] A. R. Katritzky, A. F. Pozharskii. In Handbook of Heterocyclic Chemistry, Second Edition; Pergamon: Oxford, (2000).
[2] E.M. Guantai, K. Ncokazi, T.J. Egan, J. Gut, P.J. Rosenthal, P.J. Smith, K. Chibale, Bioorg. Med. Chem. (2010) 8243–8256
[3] R. Huisgen, Angew. Chem., 1963, 75, 604.

PVC/α-MnO_2-KH550 nanocomposites: Studies on Morphology, thermal, mechanical and Pb(II) adsorption properties

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It is accepted that the poly(vinyl chloride) (PVC) has low thermal stability and is brittle. To improve these limitations and achieve desired properties, nano-fillers should be uniformly distributed in polymer matrix [1,2]. α-MnO_2nanorods have been synthesized through a simple method without the presence of catalysts and templates. The prepared nanorods were employed as fillers to retrofit and increase the mechanical strength, thermal stability and adsorption properties of PVC as one of the most important thermoplastics. To prevent accumulation and increase compatibility of α-MnO_2 with the organic PVC matrix, the nanorods were modified with γ-aminopropyltriethoxysilane (KH550). Nanocomposites (NCs) were prepared with different amounts of modified α-MnO_2nanorods (1, 3 and 5 wt%)(Figure 1). The results indicated that PVC/α-MnO_2-KH550 NCs exhibit better thermal stability, tensile and self-extinguishing properties than pure PVC in three weight percentages. The obtained results of adsorption revealed that the NC films could be used for the removal of Pb(II) ions from aqueous medium.

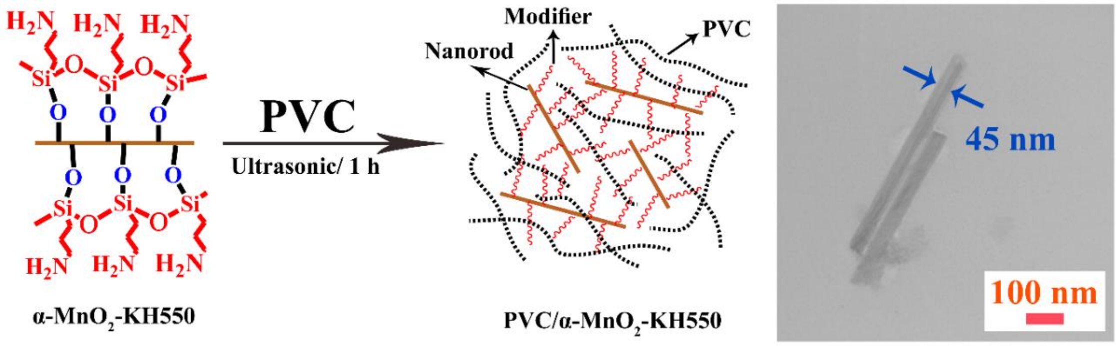

Figure 1. Reaction sequence for the preparation ofPVC/α-MnO_2-KH550 NCs

References

[1] S. Albeniz, M. a. Vicente, R. Trujillano, S. a. Korili, A. Gil, Appl. Clay Sci. 99 (2014) 72–82.

[2] K. Sterky, H. Jacobsen, I. Jakubowicz, N. Yarahmadi, T. Hjertberg, Eur. Polym. J. 46 (2010) 1203.

Green Method of Preparing High Surface Area Boehmite

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High surface area boehmiteAlO(OH) are widely used in the industry of adsorbents, catalysts and catalyst carriers [1]. Various synthesis methods are possible for boehmite. It can be prepared by the sol-gel process using aluminum alkoxides [2]. However, the synthetic route used industrially involves the precipitation of aluminum salts, which may be followed by a period of ripening in hydrothermal conditions [3].

At the present investigation, a green, inexpensive and straightforward method for the synthesis of high surface area boehmite has been described. Our studies showed that walnut shell powder as an agricultural wastecan be used as the hard template and aluminium nitrate as source of alumina in aqueous media to synthesis boehmite and characterized using powder X-ray diffraction, thermal analysis and N_2 adsorption/desorption. Synthesized mesoporous-boehmite has high specific surface area (304 m^2/g), narrow pore size diameter (3.32 nm) and high pore volume (70 cm^3/g). The presence of walnut shell in the precursors of boehmite is critical for the formation of high surface area mesoporous structure.

Furthermore, γ-alumina supported vanadium, molybdenum and tungsten catalyst obtained from calcination of hard-templatedboehmite was prepared by impregnation method, and its catalytic performance in the oxidation of alcohols was also investigated.

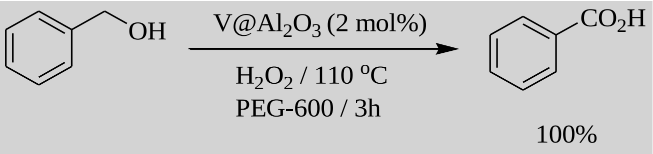

Figure 1. Scheme of the reaction.

References

[1] a) C. Misra, Aluminium oxide, hydrated, in Kirk-Othmer Encyclopedia of Chemical Technology, J. Wiley, New York, 4th edn., 1994, vol. 2, p. 317. b) A. Pearson, Aluminium oxide, activated, in Kirk-Othmer Encyclopedia of Chemical Technology, J. Wiley, New York, 4th edn., 1994, vol. 2, p. 291.
[2] a) P. Alphonse, M. Courty, Thermochim. Acta. 425 (2005) 75. b) X. Bokhimi, A. Morales, J.S. Valente, J.
Phys. Chem. C. 111 (2007) 103.
[3] a) S. Musić , D. Dragčević , S. Popović, N. Vdović, Mater. Sci. Eng. B. 52 (1998) 145. b) Y. Mathieu, B.
Lebeau, V. Valtchev, Langmuir23 (2007) 9435.

Epoxidation of Cyclooctene Catalyzed by 12-Molybdophosphoric Acid and 12-Molybdosilicate Acid Supported on Polyaniline as Heterogeneous Catalysts

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Heteropolyacids due to high variations in charge, size and chemical nature, have unique features. Some of these features include thermal resistance, high acidity, solubility and redox noted Properties. Thermal resistance of heteropolyacids is of great importance especially in cases where they are used as a heterogeneous catalyst [1].

Epoxidation of alkenes is one of the most important chemical processes, the products of this reaction are used as a precursor for the synthesis of many chemicals and pharmaceuticals as well as for the production of many valuable materials including epoxy resins, paints and surfactants [2].

Polyaniline (PANI) is one of the oldest artificial conductive polymers that its high electrical conductivity has attracted a lot of attention. Easy synthesis and high surface area are its other features that can be noted. PANI was prepared by dissolvingdistilled aniline and ammoniumproxydisolfatin 1MHClaccording to the reported procedures [3].

HPAs($H_3[PMo_{12}O_{40}]$and $H_4[SiMo_{12}O_{40}]$) also were prepared according to the reported procedures [1] and then they were supported on PANI by refluxing in ethanolfor 3 hours.

In this work, the epoxidation of cyclo-octene as a model reaction have been investigated with$H_3[PMo_{12}O_{40}]$and $H_4[SiMo_{12}O_{40}]$supported on PANI. The various parameters such as type of solvent (1,2-dicholoroethane , chloroform, carbon tetrachloride, acetonitrile and methanol), type ofoxidant (hydrogen peroxide, t-butyl-hydro-peroxide and hydrogen peroxide/urea), amount ofoxidant (0.1, 0.2, 0.3 and 0.4ml t-butyl-hydro-peroxide) and amount of catalyst (5, 10, 15 and 20 mg) were optimized for this reaction. The progress ofthese reactionswas analyzedusinggas chromatography (GC) during 30-180 minutes.The optimum conditions were found carbon tetrachlorideas a solvent, 1mmol TBHP as oxidant, 20 mg catalyst for 0.5 mmolcyclo-octene at reflux temperature. At these conditions, $H_3[PMo_{12}O_{40}]$and $H_4[SiMo_{12}O_{40}]$reached near complete conversion during 90minutes.

References

[1] Kozhevnicov I. V, Catalysts for Fine Chemical Synthesis , John Wiley and Sons, University of Liverpool, UK, 2002.
[2] Mizuno N, Yamaguchi K, Kamata K. Coordination chemistry reviews. 2005 Sep 30;249(17):1944-56.
[3] Huang J, Kaner RB. A ge. Journal of the American Chemical Society. 2004 Jan 28;126(3):851-5.

Synthesis of iodinated copolymers for medical purposes

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Radiopaque materials have been used for variety of medical applications such as embolization process, preparation of implant, prosthesis and drug delivery; because they positioned by X-radiography easily[1,2].Usual polymers have low electron density and low specific gravity, why so they are made of atoms such as carbon, hydrogen, oxygen and nitrogen; so these polymers are radiolucent to X-ray. Using heavy elements in the structure of polymers is a conventional method for preparation of radiopaque biomaterial. But, covalent binding of iodine atom to monomers or performed polymers has been achieved great attention. Iodinated moieties, is the most widely radiopacifying agents used for synthesis of radiopaque polymers [3].

In this work methyl methacrylate and acrylic acid were copolymerized and the copolymer was modified through reaction of carboxylic acid groups onthe main chain with4-iodophenyl isocyanate and 3,4,5-triiodophenyl isocyanate. Iodinated moieties were used as radiopacyfying agents; sothe modifiedcopolymers exhibited excellentradiopacity, whereas non-modified copolymer has no significant X-ray visibility. X-radiography was carried out on the iodinated copolymersand MTT assay was used for biocompatibility studies.

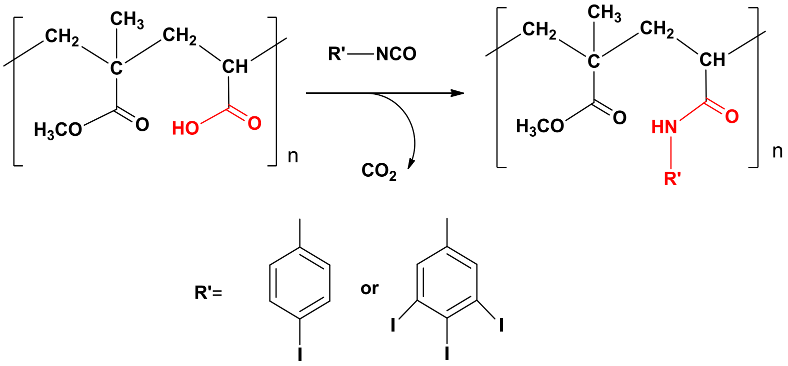

Figure 1. Synthesis and miodination of P(MMA-co-AA)

References

[1] S. Kiran, R. Joseph,Journal of Biomedical Materials Research Part A 103 (2015) 2214.
[2] G. Agusti, O. Jordan, G. Andersen, É. Doelker, Y. Chevalier, Journal of Applied Polymer Science (2015) 132.
[3] H. Lusic, MW Grinstaff, Chemical reviews 66 (2012) 113.

Preparation of radiopaque nanocomposites by using iodinated polymers

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Graphene and its derivatives such as graphene oxide(GO),has attracted great attention because of amazing thermal, mechanical and electrical properties.Graphene, a monolayer of sp^2-hybridized carbon atoms, has been employed in many fields, especially in the synthesis of nanocomposites[1,2]. In this work radiopaque polymers/(GO)nanocomposites were prepared via solution method. Radiopaque materials have been used for various medical applications such as embolization process, preparation of implant, prosthesis, and drug delivery. These polymers have been synthesized via various method such as blending of polymers with heavy elements or their salts; but covalent binding of iodine to monomers or performed polymers have been considered[3].

Radiopaque copolymers was synthesized via modification of P(MMA-co-AA) by mono- and triiodophenylisocyanate. In order to preparation of nanocomposites, various ratios of GO (5, 10 and 20%) were used. The radiopaque copolymers were dissolved in acetone and also different amount of GO was dispersed in acetone via ultrasonic homogenizer. Then GO and polymer solutions were mixed and stirred for 24-48 h. After that, the solvent was evaporated and the final products were dried in vaccum. The obtained composites were characterized by using scanning electron microscopy (SEM)and X-ray diffraction (XRD).Also thermal properties of the nanocomposites were investigated.Radiopacity of copolymers and nanocomposites were explored by using X-radiography.

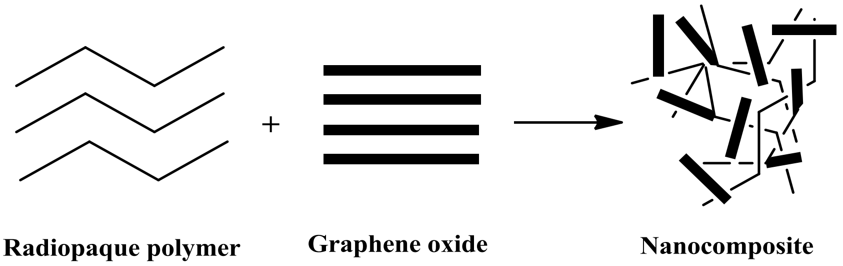

Figure 1. Preparation of nanocomposite with different percent of grapheme oxide

References

[1] J. R. Potts, S. H. Lee, T. M. Alam, J. An, M. D. Stoller, R. D. Piner, R. S. Ruoff, Journal of carbon 49 (2011) 2615.
[2] T. Kuilla, S. Bhadra, D. Yao, N. H. Kim, S. Bose, J. H. Lee. Journal of Progress in Polymer Science 35 (2010) 1350.
[3] S. Kiran, R. Joseph, Journal of Biomedical Materials Research Part A 103 (2015) 2214.

Study of supramolecular effect of tolanophanesin wacker-type oxidation

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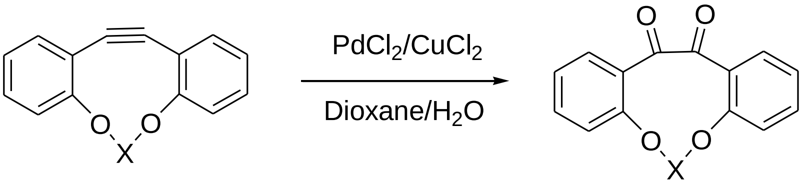
1,2-diketones are an important class of compounds which employed in synthesis of organic compoundssuch as imidazoles, quinoxalines, chiral 1,2diols. Several methods have been developed for synthesis of 1,2-diketones.wacker-type oxidation of alkynes catalyzed by $PdBr_2/CuBr_2$ was reported. The Pd-catalyzed Wacker oxidation is a well-known method for converting alkynes to carbonyl compounds [1]. Because of practical and environmental concerns, this transformation has recently received much attention. In continuous of our work on stilbenophanes [2-3], we now report our studyonoxidationtolanophanes**1**underwacker reaction.We first synthesized and characterized the diketones**2**. We also found thatthe Wacker oxidation of two defined tolanophaneswith different alkyl chain lengths gave the corresponding cyclic diketones in different rate. We concluded that the oxidation rate of tolanophanesshow the importance of supramolecular effect in elucidation of the reaction mechanism.



1
X= $(CH_2)_n$
n= 3,4

2
X= $(CH_2)_n$
n= 3,4

Figure 1. The Wacker oxidation of tolanophanes**1**.

References

[1] Wei, R.; Yuanzhi, X.;Shun, J.;Yong, Z.;Xiaobing, W.;Jing, Z. Org. Lett. 2009, 11, 1841-1844.
[2] Darabi, H. R.;Mirzakhani, M.;Aghapoor, K.;Jadidi, K.;Faraji, L,;Sakhaee, N. Journal of Organometallic Chemistry,2013,740, 131-134.
[3] Darabi, H. R.;Mirzakhani, M.; Aghapoor, K. Journal of Organometallic Chemistry,2015, 786, 10-13.

Triethanolammonium lactate: An efficient and reusable catalyst for the preparation of dihydropyrano[c]chromene derivatives

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Coumarin and some of its hydroxylated derivatives containing a benzene ring fused with a c-pyrone ring possess important chemical reactivity and are naturally occurring compounds, which exhibit antibacterial, antioxidant, anticancer, and antiallergy activities. They are frequently used as intermediates in the production of dyes and herbicides. Derivatives of 4-hydroxycoumarin have been used successfully as potent warfarin-type anticoagulents (i.e., bromadiolone, brodifacoum, flocoumafen, thioflocoumafen) with low toxicity[1].Ascompared to the first-generation multidosewarfarintypeanticoagulants, these compounds are more potentin rodents and require reduced feeding periods andbaits [2].

A task-specific ionic liquid with a Bronsted acid (Triethanolammonium lactate) were used as an efficient and reusable catalyst for the One-Pot three-component condensation of 4-hydroxycoumarin, aldehydes, and malononitrile (or ethyl cyanoacetate) to approach to dihydropyrano[c]chromene derivatives under solvent-free condensation reaction.

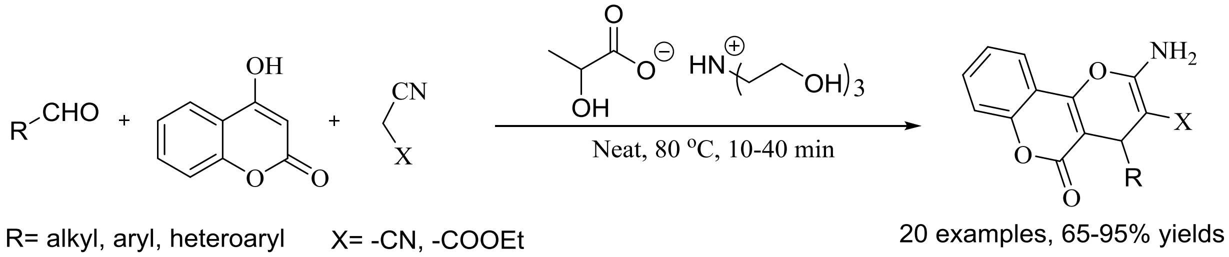

Figure 1. Three-component condensation of 4-hydroxycoumarin, aldehydes, and malononitrile(or ethyl cyanoacetate)

The products and ionic liquid could be conveniently separated from the reaction mixture, indicating that the whole process was performed as a green chemical transformation.

References

[1] Jung, J.C.; Lee, J.H.; Oh, S.; Lee, J.G.; Park, O.S.;Bioorg. Med. Chem. Lett.2004, 14, 5527-5531.
[2] Dubock, A. C.;Plant Protect. Bull.1980, 22, 223-238.

Efficient synthesis of 2,3-dihydroquinazolin-4(1H)-ones using (Fe_3O_4@SiO_2-NH) a reusable catalyst

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(Fe_3O_4@SiO_2-NH-) was found to nanocatalyst efficiently a One-Pot three-component cyclocondensation of isatoic anhydride and primary amines or ethylene amine with aromatic aldehydes under solvent free conditions to afford the corresponding mono- and disubstituted 2,3-dihydroquinazolin-4(1H)-ones in good yields. The adventure of these catalytic condensation reactions represent green chemical processes, high yields, short reaction time and eco-friendly catalyst.

One of the most important organic compounds are quinazolinones. Quinazoline and their derivatives have been reported to possess varied pharmacological properties including antitumor, anti-cancer, diuretic activities, anticonvulsant, anti-inflammatory, antimalarial and antihypertensive [1].For these reasons, much attention has been paid to the synthesis and biological evaluation of quinazoline derivatives. Several methods have been reported for the synthesis of 2,3-dihydroquinazolinone derivatives through One-Pot condensation of isatoic anhydride and amines with aldehydes [2-4].

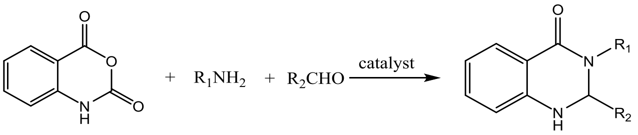

Figure 1.synthesis of 2,3-dihydroquinazolin-4(1H)-ones

Nanocatalysis is recently developing field and is most important component of “sustainable technology and organic transformations” applicable to almost all types’ catalytic organic transformations. Among nanocatalysts, several forms such as magnetic nanocatalysts, nano mixed metal oxides, core-shell nanocatalysts, nano-supported catalysts, graphene-based nanocatalysts have been employed in catalytic applications [5].

References

[1] M. Srivastav, M. D. Salahuddin, S. Shantakumar.E-Journal of Chemistry, 6(4), (2009), 1055
[2] M. Baghbanzadeh, P. Salehi, M. Dabiri, G. Kozehgarya. Synthesis, (2006), 344
[3] M. Dabiri, P. Salehi,; S. Otokesh, M. Baghbanzadeh, G. Kozehgarya, A. A. Mohammadi, Tetrahedron Lett 46, (2005), 6123

Choline peroxydisulfate: triple role player in direct synthesis of 14-Aryl-14*H*-dibenzo[a,j]xanthenes and 1,8-dioxo-octahydroxanthenes from benzyl alcohols under solvent-free conditions

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Xanthenes and their derivatives have attracted substantial research interest due to their various biological activities and antibacterial, antioxidant, anticancer, antimalarial, and anti-inflammatory properties. Furthermore, some of these compounds have been widely used as lecodyes6 and pH-sensitive fluorescent materials for visualization of biomolecules and are utilized in laser technologies [1].Tandem catalytic processes can replace multi-step syntheses with efficient catalytic reactions that can have significant impact on the manufacture of fine chemicals and pharmaceutical intermediates [2].

14-Aryl-14*H*-dibenzo[a,j]xanthenes and 1,8-dioxo-octahydroxanthenes were synthesized directly from benzyl alcohols via a tandem catalytic process using Choline peroxydisulfate (ChPS). The synthesis proceeds through two steps: an oxidation of the benzyl alcohols to benzaldehydes followed by condensation with 2-naphthol or dimedone to form products. Choline bisulphate (ChBS) reduced species is generated in-situ from ChPS, which catalyses formation of desired products in shorter reaction time, with good to excellent yields

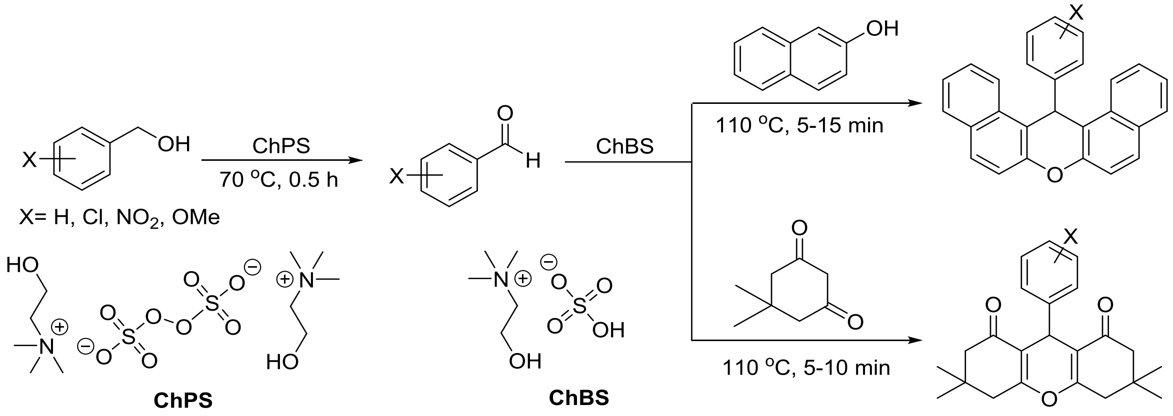

Figure 1. Tandem synthesis of xanthenes from benzyl alcohols in the presence of ChPS

References

[1] He, X.; Tao, J.; Hu, X.; Wang, H.; Shang, Y.; J. Org. Chem.2016, 81, 2062-2069.

[2] Sheldon, R. A.; Pure Appl. Chem.2000, 72, 1233-1246.

Modification of physiochemical properties in polycaprolactone based nanocomposites by the incorporation of PVA-modified ZnO nanoparticles

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Nowadays attentions were drawn over development of biodegradable polymers to reduce the use of fossil fuels [1]. Polycaprolactone (PCL) is a hydrophobic, biodegradable aliphatic polyester with crystallinity about 50% that can be synthesized from crude oil via the ring opening polymerization of caprolactone monomers [2]. Inorganic-organic hybrid nanocomposites (NCs) have attracted more attention because they combine rigidity and high stability of inorganic nano-fillers with flexibility, ductility, dielectric and easy processability of organic matrix [3].

In this paper, nanocomposite films of polycaprolactone (PCL)/ZnO-PVA were prepared by casting/solvent evaporation method. For this purpose, ZnO nanoparticles (NPs) were first modified with poly(vinyl alcohol) (PVA), at room temperature by ultrasound irradiation method. Then, PCL/ZnO-PVA NCs were obtained by addition of various weight percentages (2, 4 and 6 wt%) of ZnO-PVA into the PCL matrix, under vigorous stirring and subsequent ultrasonic irradiation (Figure 1). The structural characterization of the NC films was carried out using transmission electron microscopy (Figure 2) and X-ray diffraction. It was found that relative changes in the peaks were observed, as the concentration of filler was increased. In addition, embedding the NPs into PCL exhibited a reduction in thermal stability of NCs as compared to the pure PCL. Tensile tests for the prepared films with different NP loadings showed that the tensile strength of the NCs have significantly improved compared with pure PCL.

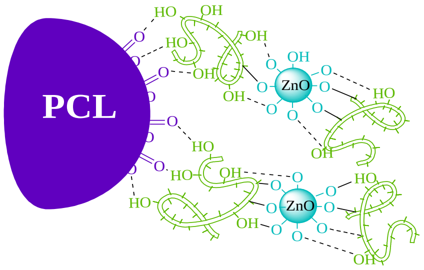

Figure 1

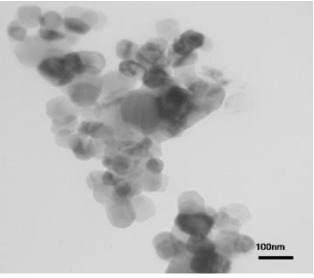

Figure 2

Refrences

[1] J. Zhang, E. Manias, C. A. Wilkie, Journal of Nanoscience and Nanotechnology 8 (2008) 1597.
[2] K. Takashi, H. H. Richard, Z. Xing, R. M. Briber, Polymer 45 (2004) 881.
[3] J. Gao, Y. Du, C. Dong, Polymer Composites 31 (2010) 1822-1827.

Synthesis of *N*-phenylacetamideand arylcarboxyamideby using aryl diazonium silica sulfates under mild conditions

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Aromatic diazonium salts have been prepared and studied for years. These salts are important building blocks in classical and modern organic synthesis, and interest in these versatile and reactive species remains high [1]. Although diazonium salts have wide applications in the synthesis of various compounds, these salts have a serious drawback in their intrinsic instability and explosive potential. Therefore, these compounds are usually synthesized at around 10 °C, and to avoid their decomposition, they are handled below 0 °C [2].Thus, aryldiazonium salts with higher stability and versatility that can be easily made and stored under solid state conditions with explosion-proof properties are desired and necessary. In continuation of our studies on the application of stable diazonium salts [3,4],herein, we wish to report an efficient, fast and straightforward procedure for the synthesis of *N*-phenylacetamide and arylcarboxyamide using aryl diazonium silica sulfates in the presence of acetonitrile orisocyanides. Using the present method, different kinds of aryl diazonium silica sulfates, containing electron withdrawing groups as well as electron donating groups, were rapidly converted to the corresponding of *N*-phenylacetamide and arylcarboxyamide in good yield. Simple and clean work-up, and good yields were the advantages of this method.

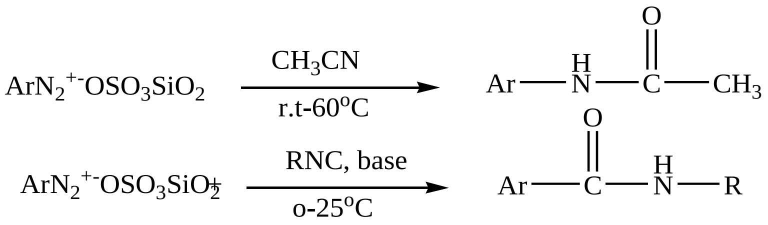

Figure 1. scheme of reaction

References

[1] A. Roglans, A. Pla-Quintana, M. Moreno-Manas. Chem. Rev. 106 (2006) 4622.
[2] H. Zollinger. Diazo Chemistry I; VCH: Weinheim, 1994.
[3] A. Zarei, A.R. Hajipour, L. KHazdooz, F. Mirjalili, A. NajafiCHermahini. Dyes Pigments 81(2009)240.

Synergistic effect of diacid-modified ZnO as nanofiller, for enhancing the properties of polycaprolactone-based nanocomposites

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Polycaprolactone (PCL) is a semi-crystalline, hydrophobic, biocompatible and biodegradable polymer that has extensively been used in packaging materials and biomedical applications [1]. However, PCL has some drawbacks including slow crystallization rate and low stiffness that limited its practical application. These drawbacks can be overcome by incorporation of nanofillers such as metal oxide nanoparticles (NPs), which improve the physical properties and extend its practical use [2].

We prepared nanocomposites (NCs) based on polycaprolactone and diacid based on bioactive amino acid (N-trimellitylimido-L-alanine) (DA)-modified ZnO, using ultrasound irradiation. First, the surface modification of NPs was accomplished using ultrasound irradiation, in order to increasing the compatibility and dispersity in the polymer matrix. Then PCL composite films containing different amounts of modified NPs were achieved through solvent casting method by the use of dichloromethane as a solvent. Transmission electron microscopy images (Figure 1) verified the presence of NPs in the polymer matrix. The films were characterizedby Fourier transform infrared spectroscopy, X-ray diffraction andthermogravimetricanalysis. The nature of interaction between PCL and the NPs was determined by Fourier transform infrared spectroscopy.

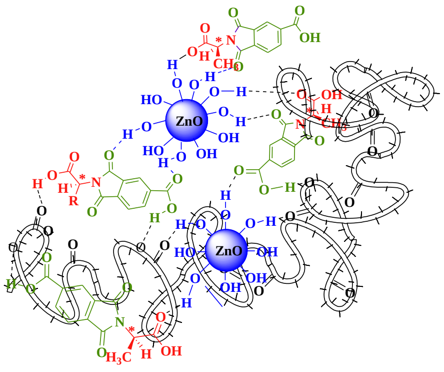

Figure 1

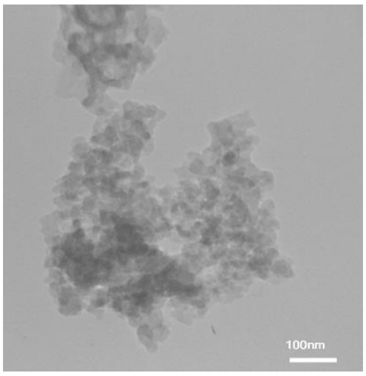

Figure2

References

[1] H.J. Lim, H. Lee, K.H. Kim, J. Huh, C. Ahn, J.W. Kim, Colloid and Polymer Science 291 (2013) 1817-1827.
[2] D. Ju, L. Han, F. Li, S. Chen, L. Dong,International Journal of Biological Macromolecules 67 (2014) 343-350.

Synthesis and structure of a new dithiazolopyridine as a novel fluorescent sensor of cyanide ion

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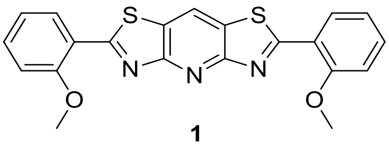
Recently, we reported the synthesis and characterization of the dithiazolopyridine**1** and studied its optical properties upon coordination to Cu^{2+} to give complex Cu^{2+} [1]. We found that Cu^{2+} displays high sensitivity, well reversibility and rapid response (<1 min) for recognizing CN^-in THF.



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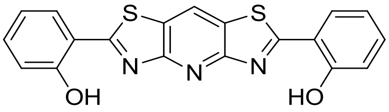

2

Herein, the synthesis and characterization of dithiazolopyridine2 is reported. In contrast to compound 1, probe 2 detected directly the cyanide ions without using of its metal complexes [Figure 1]. The practical application of the 2 for the detection of CN^- ions was realized by using solution coated silica strips (TLC plates).

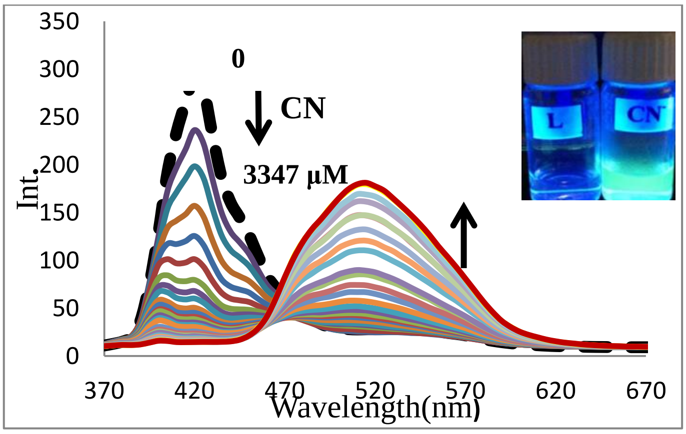

Figure 1.compound**2** detected directly CN^-

Reference

[1] H. R. Darabi, et al.,Tetrahedron Letters 57 (2016) 256–259.
[2] Xu, Z.; Chen, X.; Kim, H. N.; Yoon, J. Chem. Soc. Rev. 2010, 39, 127.
[3] H. R. Darabi, et al.,Tetrahedron Letters 57 (2016) 256–259

A Simple, Green and One-Pot Four-component Synthesis of Polycyclic Dihydropyridine Derivatives

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1,4-Dihydropyridines (1,4-DHPs) are important class of compounds in the field of drugs and pharmaceuticals [1]. The DHP moiety is common to numerous bioactive compounds. Recently, several modifications for this classical method have been reported for the facile and efficient synthesis of important dihydropyridine derivatives [2].Improvements in such syntheses have been sought continuously. Melamine-formaldehyderesin supported H^+[MFRH] works under heterogeneous conditions. It is an inexpensive and non-hazardous solid acid catalyst. It can easily be handled and removed from the reaction mixtures by simple filteration [3].

In this communication, we describe a simple but effective modification of the Hantzschreaction that produces high yields of the desired dihydropyridines while preserving the original One-Pot strategy. The reaction of dimedone, barbitoric acid, aromatic aldehydes, and ammonium acetate in the presence of [MFRH] as a mild acid catalyst resulted in the formation of polycyclicdihydropyrimidinones (Figure 1).

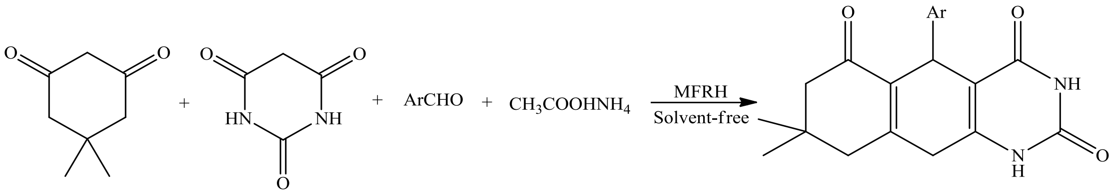

Figure 1. Synthesis of polycyclic dihydropyridines over [MFRH]

In conclusion, the present method demonstrates an operationally simple and clean procedure for the synthesis of polycyclic dihydropyridines using a catalytic amount of melamine-formaldehyderesin supported H^+. In addition, low cost, recyclability, low toxicity, high acidity andmoisture compatibility of the catalyst, excellent yields of products within short reaction time make this methodology a valid contribution to the existing processes in the field of 1,4-Dihydropyridine synthesis.

References

[1] G.M. Reddy, M. Shiradkar, A.K. Chakravarthy, Current Organic Chemistry 11 (2007) 484.
[2] A. Debache, R. Boulcina, A. Belfaitah, S. Rhouati, B. Carboni, Synlett, (2008) 509.
[3] R. Rezaei , R. Khalifeh , M. Rajabzadeh , L. Dorosty, M. M. Doroodmand,Heterocyclic. Communications, 19 (2013) 57.

Mesoporous Silica-coated Fe_3O_4 Magnetic Nanoparticles as an Efficient and Recyclable Nanocatalyst for Synthesis of Diversified Indolyl 4*H*-chromenes

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Mesoporous silica-coated magnetic nanoparticles (Fe_3O_4@MSNs) is found to be an efficient recyclable organocatalyst for selective synthesis of indolyl 4*H*-chromenes derivatives [1].Easy reaction conditions coupled with simple work-ups, makes this methodology a superior option for synthesis of diversified indolyl 4*H*-chromenes [2].

The versatility ofFe_3O_4@MSNs catalyst is studied for the synthesisof indol-3-yl-4*H*-chromene derivatives from the reactionbetween salicylaldehyde, active methylene compounds, and substituted indoles [3].

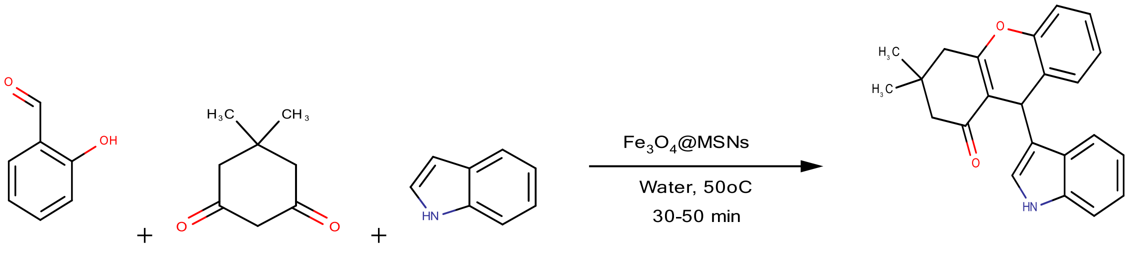

Figure 1. General scheme for the synthesis of indolyl 4H-chromenes derivatives.

Reference

[1] J. Yang, F. Zhang, W. Li, D. Gu, D. Shen, J. Fan, W. X. Zhang, D. Zhao, Chemical Communications 50(2014) 713.

[2] Z. Nasresfahani, M. Z. Kassaee, M. Nejati-Shendi, E. Eidia, Q. Taheri, RSC Advances 6 (2016) 32183.

[3] S. D. Dindulkar, D. Jeong, E. Cho, D. Kimb,S. Jung, Green Chemistry(2016) in press: 10.1039/c6gc00137h.

Synthesis, characterization and catalytic properties of $MoO_2(acac)_2$ immobilized on nanostructured polyaniline

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Preparation and characterization of catalysts are highlighted in this study.In particular,nonosized materials offer an awarding challenge with the respect of elucidation reaction pathways on structured catalytic surfaces,leading eventually to significant improvements in catalyst performance[1].

Polyaniline is one of the most versatile conducting polymers which have been extensively investigated due to its remarkable properties,such as tunable electrical conductivity ,inexpensive monomer,facile synthesisand good environmentalstability [2].

In the present study,PANInanoparticles were synthesized by polymerization techniques using Ammonium persulfate as oxidizing agent.For the synthesis of a heterogeneous catalyst polyaniline/Mo,complex $MoO_2(acac)_2$ was loaded onto the surface of the modified polyaniline nanoparticles.This catalyst was as an efficient catalyst for epoxidation of cis-cyclooctene and wide variety of alkenes,including aromatic and aliphatic terminal ones using *tert*-butylhydroperoxide(TBHP) as oxidant.This new heterogeneouscatalyst could easily be recovered and reused four consecutive with no loss of activity.

The new catalyst was characterized by FT-IR,CHNS,ICP, TGA and FE-SEM.

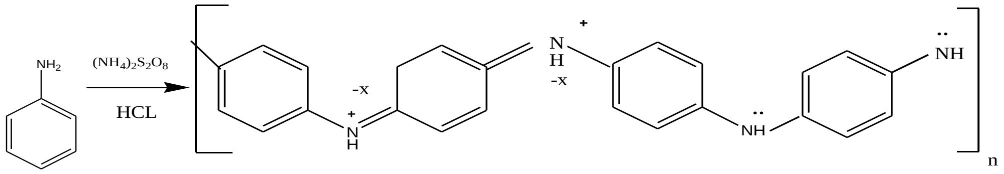

Figure 1. Scheme of the reaction.

Refrences

[1] M. Moshref-Javadi, M. Moghadam, I. Mohammadpoor-Baltork,S. Tangestaninejad, V. Mirkhani, H. Kargar, M. Nawaz-Tahir, Polyhedron 2014, 72, 19.
[2] Tran, H. D., D'Arcy, J. M., Wang, Y., Beltramo, P. J., Strong,V. A., &Kaner, R. B. (2011). The oxidation of aniline to produce "polyaniline": a process yielding many different nanoscale structures. Journal of Materials Chemistry, 21,3534–3550.

Synthesis characterization and anti-bacterial properties of $MoO_2(acac)_2$ immobilized on nanostructured polyaniline

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The metallic nanoparticlesare considered as the most promising compounds as they contain remarkable antibacterial properties due to their large surface area to volume ratio.There are many interest for researchers in this area due to the growing microbial resistance against metal ions, antibiotics and the development of resistant strains [1].Among the all novel metal nanoparticles, silver nanoparticles are the arch products from the field ofnanotechnology which have gained boundless interests because of theirunique properties such as antibacterial and antifungal activity as well as their catalytic properties [2].

In the present study,PANI/Ag nanocomposites with Ag concentration were synthesized by polymerization techniques using Ammonium persulfate as an oxidising agent.For the synthesis of PANI/Ag nanoparticles, silver ions were loaded onto the surface of the modified polyaniline and reduced to silver nanoparticles by addition $NaBH_4$. For the synthesis of PANI/Mo, complex $MoO_2(acac)_2$ was loaded onto the surface of modified polyaniline nanoparticles.Antimicrobial effects of PANI/Ag and PANI/Mo sampleswere tested against Bacillus subtilisand Pseudomonas syringeato evaluate their antibacterial activity and also against Fusariumgraminearum and Rhizoctoniasolanifor assessment of their antifungal activity. The obtained biological results showed that,bothnanocomposite have shown excellent antibacterial and antifungal activity against abovementioned organisms.

The structure and properties of PANI/Ag and PANI/Mo nonocompositeswere assessed by XRD,FT-IR,ICP, CHNS and TGA.

References

[1] Khalil KA, Fouad H, Elasaranagawy T, Almajhdi FN. Preparation and characterization of electrospun PLGA/silver composite nanofibers for biomedical applications. Int J ElectrochemSci 2013;8:3493-93.
[2] Ahmad A, Mukherjee P, Senapati S, Mndal D, Khan MI, Kumar R, Sastry M. Extracellular biosynthesis of silver nanoparticles using the fungus FusariumoxysporumColloids Surf B: Biointerefaces 2003;28:313-8.

One-Pot Three-Component Synthesis of 1,2,3-Triazoles using PVC-Supported 1,2,3-Triazole-Copper(0) as a Novel Heterogeneous Catalyst

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Heterogeneous catalysis, especially involving metal nanoparticles, offers several advantages over the homogeneous counterpart such as easy recovery, easy recycling, and enhanced stability of the catalyst. Some heterogeneous catalytic systems have recently been developed including copper nanoparticles on activated multi-walled carbon nanotubes [1] and copper(I)-modified zeolites [2].

In this work, we prepared the novel PVC-supported triazole-copper(0) nanoparticle catalyst from PVC, sodium azide, phenyl acetylene, and copper(II) sulfateunder the reduction conditions. The catalyst was characterized by the FT-IR, ICP, and XRD analysis techniques.

Thecatalyst was screened for the synthesis of 1,2,3-triazoles by thecopper-catalyzed click reaction. The multi-component reactions ofaryl iodides, terminal alkynes, and sodium azide in the presence of the catalyst produced 1,4-disubstituted 1,2,3-triazoles via the Ullman-Click reactions. This method offers several advantages including excellent product yields, an environmentally friendly procedure, short reaction times, and a simple work-up procedure, which make it a useful process for the synthesis of 1,2,3-triazoles(Figure 1).

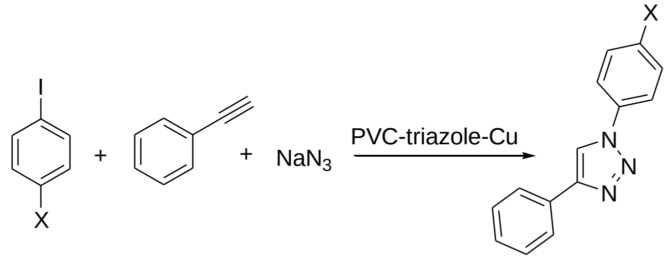

Figure 1. Synthesis of 1,4-diaryl-substituted 1,2,3-triazoles using PVC-supported 1,2,3-triazole-copper(0) catalyst.

References

[1] H. Sharghi, M. H. Beyzavi, A. Safavi, M. M. Doroodmand, R. Khalifeh. Advanced Synthesis & Catalysis351 (2009) 2391.
[2] T. Boningari, A. Olmos, B. M. Reddy, J. Sommer, P. Pale, European Journal of Organic Chemistry (2010) 6338.

Novel Multi-Component Synthesis of Pyranopyrazoles from Pyrazolones, Phenylacetylene, and Aldehydes

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Multi-component reactions (MCRs) have emerged as a powerful tool for the construction of novel and complexmolecular structures due to their advantages over the conventional multi-step synthesis.The major advantagesof MCRs include lower costs, shorter reaction times, high atom-economy, and energy savings by avoiding thetime-consuming and expensive purification processes [1]. Pyranopyrazoles are an interesting class of heterocyclic compounds. They have been used as fungicidal, bactericidal,and anti-cancer agents. They have also been reported as pharmaceutical ingredients and biodegradable agrochemicals [2].

In this paper, novel multi-component syntheses of pyranopyrazoles from pyrazolones, phenyl acetylene, and aldehydes in the presence of TFA/HOAcarereported. The structures of the products obtainedwere determined by the^{1}H NMR, ^{13}C NMR, FT-IR, and mass spectroscopic techniques. After determining the optimumreaction conditions, new pyranopyrazolederivatives were synthesized.

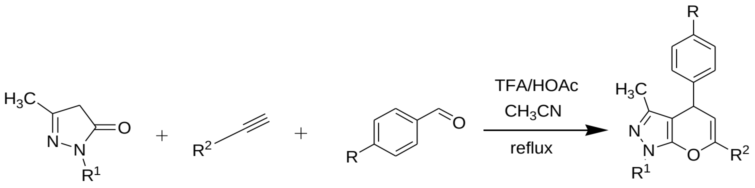

Figure1. Novel multi-component synthesis of pyranopyrazoles from pyrazolones, phenylacetylene, and aldehydes.

References

[1] M. Abd El Aleem, A. A. El-Remaily. Tetrahedron 70 (2014) 2971.
[2] A. R. Moosavi-Zare, M. A. Zolfigol, R. Salehi-Moratab, E.Noroozizadeh. Journal of Molecular Catalysis A415 (2016) 144.

Synthesis, characterization and structural study of a new rigid cyclophane

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Cyclophanes play an important role in "host–guest" chemistry andsupramolecular assembly. Stilbenophanes, cyclophanes containing stilbene moieties,are interesting classes of macrocyclic hosts, whichcan be used as platforms for the design of supramolecularsystems.
In continuation of our investigation on stilbenophanes[1–2], herein, we report the synthesis, structure of a new stilbenophaneand its complexationbehavior. The stilbenophane**2**was synthesised based onthe intramolecularMcMurry coupling of the corresponding**1**. Its structure was confirmed by NMR, Mass spectroscopy.

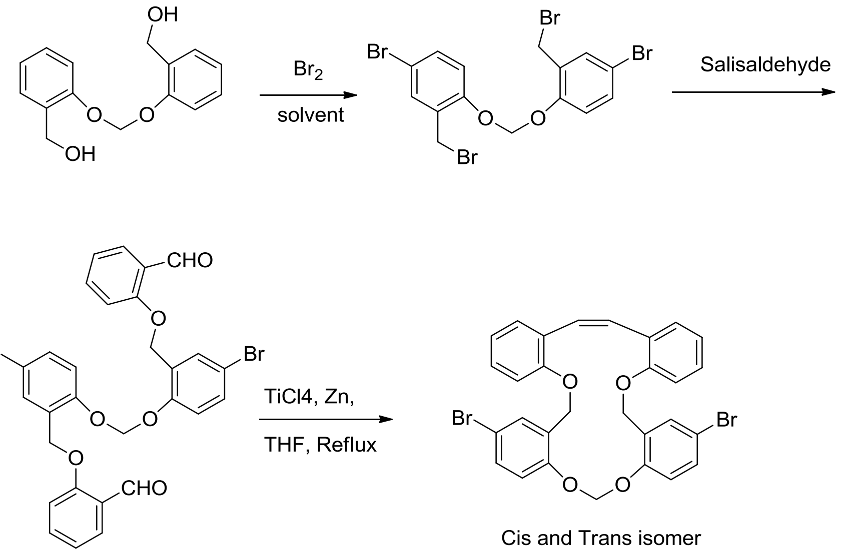

Figure 1. Scheme of the reaction.

[1] Darabi, H.R.; AzimzadehArani, M.; Motamedi, A.; Firouzi,R.; Herges, R.; Mohebbi, A.R.; Nasseri, S.; Nather, C.Supramol. Chem.2009, 21, 632.
[2] Darabi,H.R.; Jadidi, K.; Mohebbi, A.R.; Faraji, L.;Aghapoor, K.; Shahbazian, S.; Azimzadeh Arani, M.; Nasseri, S.M. Supramol. Chem. 2008, 20, 373.

Nano-gama-Al_2O_3.$SbCl_5$; an efficient and heterogeneous solid acid for the synthesis of azo dyes based on 2-naphthol at room temperature

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In recent decades, organic color chemistry is undergoing very exciting development as a result of the opportunities presented by dye applications in high technology fields: electronic devices, linear and nonlinear optics, reprography and sensors. In pharmaceutical, azo compounds are well known for antifungal, antiviral activity and some are useful as chemotherapeutic agents polymer [1]. Commonly, they are prepared by diazotization, a procedurein which a primary aromatic amine is treated with a source of nitrous acid. In spite of all precautions the formation of dark decomposition products due to the existence of nitrous acid and its aromatic amine is unavoidable, thus lowering the yield and also making the product difficult to isolate [2].

Antimony pentachloride ($SbCl_5$), a thin, colored and fuming liquid, is used in industry and organic synthesis. Since Antimony pentachloride is a liquid with a high specific gravity which fumes in air and reacts with moisture to form HCl, its handling and usability in the liquid form is laborious, the supported form is indeed preferable. It has been claimed that the supported $SbCl_5$ is a solid superacid [3].

Herein, we wish to report a convenient method for diazotizationand diazo coupling reactions by using nano-*gama*-Al_2O_3.$SbCl_5$ at room temperature by grinding (scheme 1).

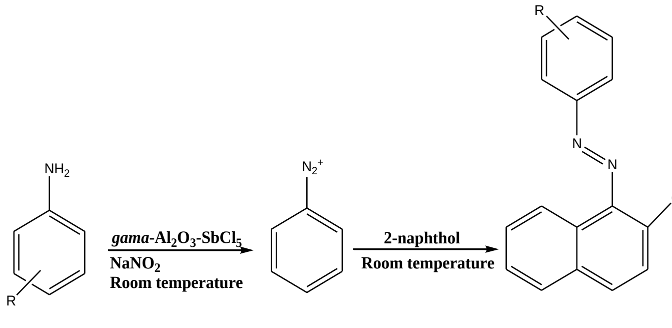

Figure 1. Scheme of the reaction.

References

[1] A. Bamoniri, A.R. Pourali, S.M.R. Nazifi.Iranian Journal of Catalysis 4 (2014) 261.
[2] K.J. Cai, H.Q. He, Y.W. Chang, W.M. Xu. Green and Sustainable Chemistry 4 (2014) 111.
[3] B. Sadeghi, B.F. Mirjalili, S. Bidaki, M. Ghasemkhani. Journal of the Iranian Chemical Society 8 (2011) 648.

PVC-supported phenylene diamine-copper(0) nanoparticles as an efficient catalyst for synthesis of 1,2,3-triazoles

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The challenges of the 21st century require scientific and technological achievements that must be developed under sustainable and environmentally benign practices. In this vein, click chemistry and green chemistry walk hand in hand on a pathway of rigorous principles that help to safeguard the health of our planet against negligent and uncontrolled production [1].Cu(I)-catalyzed terminal alkyne–azide cycloaddition (CuAAC) has recently emerged as a powerful 'click' reaction, known for its exquisite selectivity and high yields [2].

In this work, we prepared a newPVC-supported phenylene diamine-copper(0) nanoparticlecatalyst, and used it for the synthesis of 1,2,3-triazoles by copper-catalyzed alkyne–azide cycloaddition (CuAAC).The catalyst was prepared from PVC, 1,2-phenylene diamine,and copper(II) acetate under the reduction conditions.This new functionalized polymer was fully characterized with different methods such as the ICP, XRD, and elemental analysistechniques. 1,2,3-triazoles were synthesizedvia the multi-component reaction ofan azide, an alkyne, and anorganic halidein the presence of the catalystat 60^{0}C.This method offers several advantages including excellent yields, an environmentally friendly procedure, short reaction times, and a simple work-up procedure, which make it a useful process for the synthesis of 1,2,3-triazoles.

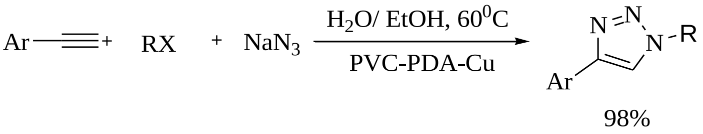

Figure 1. 1,3-dipolar azide-alkyne cycloaddition reaction catalyzed by Cu(0)nanoparticles on PVC surface.

References

[1] F. Alonso, Y. Moglie, G. Radivoy. Accounts of Chemical Research9 (2015) 2516.
[2] M. Meldal, C.W. Tornøe, Chemical Reviews108 (2008) 2952.

Synthesis of Novel 1,2,3-Triazole-based Fluorinated 1,2,4-Triazoles by Copper(0)-Catalyzed Click Reaction

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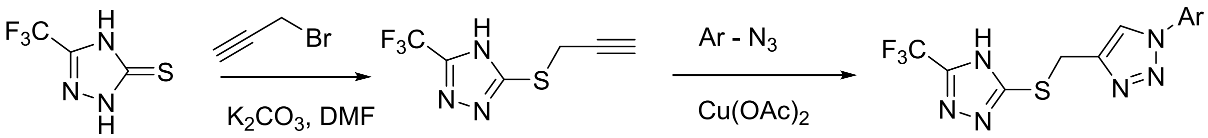
The copper(I)-catalyzed 1,2,3-triazoleformation reaction between azides and terminal alkynes has become the gold standard of 'click chemistry' due to its reliability, specificity, and bio-compatibility [1]. The chemistry of triazoles and their fused heterocyclic derivatives has received considerable attention due to their synthetic and effective biological importance. A large number of 1,2,4-triazole derivatives have attracted much attention due to their interesting biological activities such asthe anti-inflammatory, anti-malarial, anti-fungal, and anti-cancer ones [2-3]. In this work, we synthesized 3-(prop-2-yn-1-ylthio)-5-(trifluoromethyl)-4H-1,2,4-triazole 2 from 5-(trifluoromethyl)-2,4-dihydro-3H-1,2,4-triazole-3-thione 1 and 3-bromoprop-1-yne in the presence of K_2CO_3. Then the click reaction of 2 with aromatic azides in the presence of $Cu(OAc)_2$ and sodium ascorbate in DMF,as solvent,led to the formation of the desired 1,2,3-triazole compounds in good yields. The structuresof the compounds obtained were characterized by theIR, NMR, and elemental analysistechniques.



1 2 3

Figure 1. Synthesis of 1,2,3-triazole-based1,2,4-triazoles.

References

[1] A.K. Feldman, B.Colasson, V.V. Fokin, Organic Letters 6(2004) 3897.
[2] B.L. Wang, L.Y. Zhang, Y.Z. Zhan, Y. Zhang, X. Zhang, L.Z. Wang, Z.M. Li, Journal of Fluorine Chemistry 184 (2016) 36.
[3] S.G. Küçükgüzel, P.Ç. ıkla-Süzgün, European Journal of Medicinal Chemistry(2014) 1.

Chemoselective reaction of 4,6-diaminopyrimidine-2(1H)-thione with halo-heteroaryl compounds in solid phase

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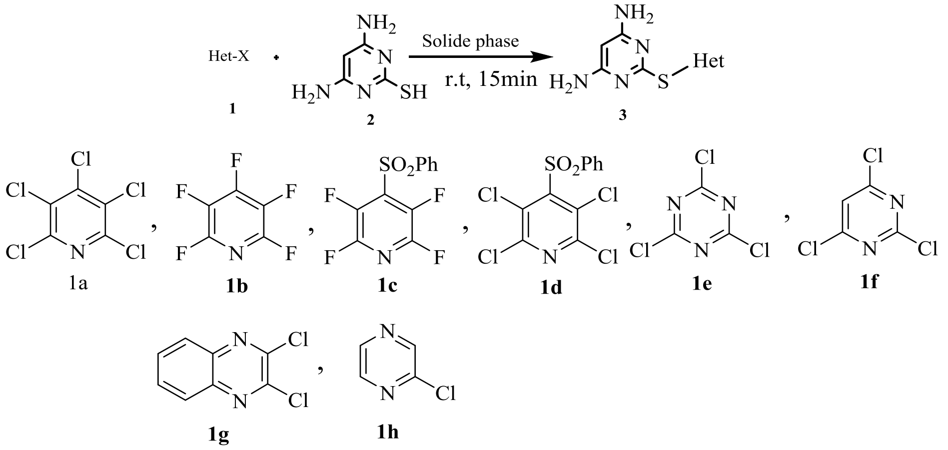
Heterocyclic compounds have increasing important in the pharmaceutical industry and the most of important life-science products are contain heterocyclic structures [1].

Perhalogenated pyridines have a broad chemistry that arising from replacement of halogen atom by various nucleophiles via aromatic nucleophilic substitution reaction.Halogen substituents atdifferent positions of heteroaromatic systemsring indicate different reactivity tonucleophiles, for example reaction of various nucleophiles with pentachloropyridine [2] and pentafluoropyridine [3]reported in detail.Regiochemistryof nucleophilicsubstitution reactions is depend on the nature of nucleophile, reaction condition, and solvent [4].Herein we wish to report the solid phase synthesis of some substituted diheteroaryl sulfide from reaction of some fluooro- and chloro-heteroaromatic 1 compounds in porcelain mortar with of 4,6-diaminopyrimidine-2(1H)-thione2 for 15 min at room temperature. The structure of compounds were confirmed with ^{1}H-NMR,^{13}C-NMR and^{19}F-NMR spectroscopy.



Scheme 1- substrate and reaction from 1 and 2

In conclusion, we have shown that some substituted diheteroaryl sulfide could be synthesised from chemoselectiv reaction of 4,6-diaminopyrimidine-2(1H)-thione*via* S nucleophile site with some fluooro- and chloro-heteroaromatic compounds.

Refrences

[1] Pozharskii, A. F.; Soldantenkov, A. T.; Katritzky, A. R. Heterocycles in Life and Society; John Wiley and Sons: New York, NY, 1997.

[2] H. Suschitzky, Polychloroaromatic Compounds, Plenum press London and New York, 1974.

[3] Amii, H., Uneyama, K., 2009. Chem. Rev. 109, 2119–2183.

Synthesis of 1,3-Diphenyl-1*H*-pyrazole-5-carbonitrile via Multicomponent Reaction

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Pyrazole is amongst the most important structural units found in many different natural and synthetic products that exhibit a wide range of biological activities [1]. Thepyrazole core is a privileged heterocyclic scaffold, and is a constituent of agro-chemicals, and polymeric materials, besides its use as a unique ligand. Although pyrazoles are rarely found in natural products, they represent an important motif of man-made biologically active compounds such as celecoxib, fipronil, lonazolac, viagra, and many others. In continuance of our interest in the 1,3-dipolar cycloaddition reactions [2,3] we describe our endeavor toward the synthesis of 1,3-diphenyl pyrazoles on the basis of the 1,3-dipolar cycloaddition protocol. Therefore a straightforward, operationally simple and high yielding protocol for the synthesis of pyrazole derivatives, from easily available starting materials is always needed. Presented in this article are the results of One-Pot , three-component coupling of, 4-oxo-4*H*-chromene-3-carbaldehyde, hydroxylamine hydrochloride and hydrazonoyl chlorides **1** to yield 1,3,4-trisubstituted pyrazoles **2**.We describe a straight forward strategy for the regioselective synthesis of pyrazoles in good to excellent yields in EtOH as solvent at room temperature (Figure 1).

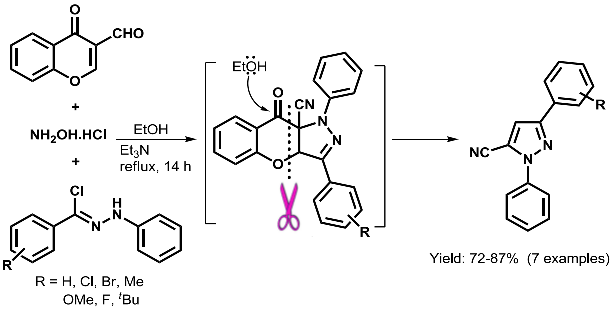

Figure 2. Synthesis of 1,3-diphenyl-1*H*-pyrazole-5-carbonitrile *via*three-component reaction

References

[1] (a) Fischer D. S.; Allan, G. M.; Bubert, C.; Vicker, N.; Smith, A.; Tutill, H. J.; Purohit, A.; Wood, L.; Packham, G.; Mahon, M. F.; Reed, M. J.; Potter, B. V. J. Med. Chem. 2005, 48, 5749; (b) Yang, Y. S.; Li, Q. S.; Sun, S.; Zhang, Y. B.; Wang, X. L.; Zhang, F.; Tang, J. F.; Zhu, H. L. Bioorg. Med. Chem.2012, 20, 6048.

[2] Alizadeh, A.; Moafi, L.; Ghanbaripour, R.; Hosseinabadi, M.; Zhu, Z.; Kubicki, M. Tetrahedron2015, 71, 3495.

[3] Alizadeh, A.; Ghanbaripour, R.; Zhu, L. G. Synlett 2013, 24, 2124.

One-Pot Synthesis of New 2,3-Disubstituted Thiazolo[4,5-b]quinoxalines through Pd-Catalyzed Coupling Reaction/Hetero-Annulation

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The Sonogashira cross-coupling reaction of terminal acetylenes with aryl or vinyl halides has been evidenced to be a powerful method for the creation of substituted alkynes, which has been widely applied in the synthesis of heterocyclic compounds [1]. The thiazoloquinoxaline ring system dramatically increases a variety of biological properties such as the anti-bacterial, anti-viral, and anti-amoebic activities [2-3].In this work, we synthesized a number of 3-benzyl-2-(4-styryl)-2,3-dihydrothiazolo[4,5-b]quinoxaline3 derivatives from the Sonogashira coupling reaction of 2-chloro-3-(prop-2-ynylthio)quinoxaline 1 with various aryl iodides followed by hydroamination and the subsequent cyclization of the resulting 2-chloro-3-((3-(4-nitrophenyl)prop-2-yn-1-yl)thio) quinoxaline2in a One-Pot procedure. Theproducts obtained were characterized by the spectroscopic data and screened for anti-bacterial activity.

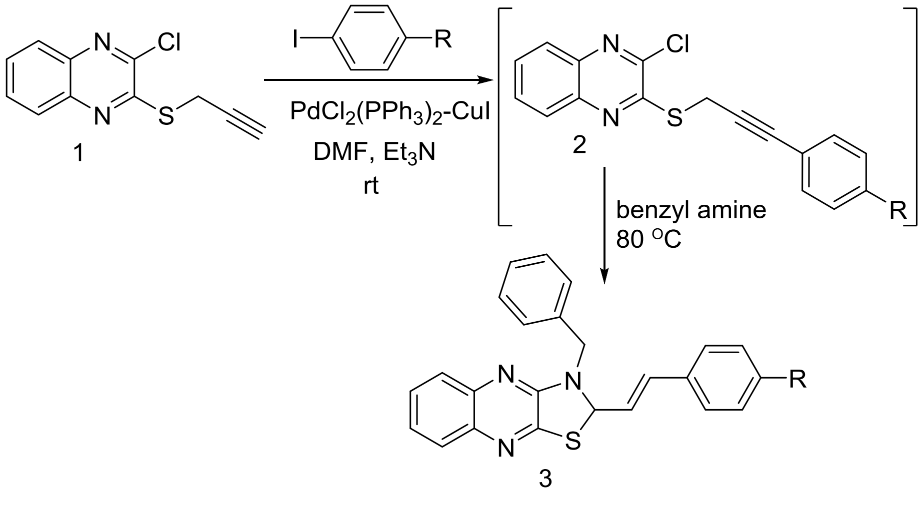

Figure 1. Synthesis of thiazolo quinoxaline derivatives

References
[1] S. A. Khan, K. Saleem, Z. Khan, European Journal of Medicinal Chemistry 42 (2007) 103.
[2] S. A. Khan, European Journal of Medicinal Chemistry 43 (2008) 2040.
[3] J.T. Guan, G.A. Yu, L. Chen, T.Q. Weng, J.J. Yuan , S.H. Liu, Applied Organometallic Chemistry23 (2009) 75.

Synthesis of New 3-Substituted Thieno[2,3-b]quinoxalines by Sonogashira Coupling and Intramolecular Heck Reactions

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Quinoxalines are of interest sincesome natural compounds bearing the quinoxaline unit exhibit high biological activitiessuch as the anti-microbial, anti-inflammatory and anti-cancer ones [1-3].Palladium-catalyzed coupling reactions have become a powerful tool in organic synthesis.In this work, we present a procedure for the synthesis of some new thieno[2,3-b]quinoxalines **3**viathe Sonogashira coupling followed by an interamolecular Heck reaction.Treatment of 2-chloro-3-(prop-2-yn-1-ylthio)quinoxaline**1**with various aryl iodides in the presence of Pd-Cu catalyst afforded 2-(3-arylprop-2-ynylthio)-3-chloroquinoxalines **2** in good-to-high yields. The resulting compoundsunderwent cyclization to 3-substituted thieno[2,3-b]quinoxalines**3**under the Heck reaction conditions(Figure 1).The products obtained were characterized by theIR, ^{1}H NMR, ^{13}C NMR, and mass spectroscopic techniques. Alsothese quinoxaline derivatives were evaluated for anti-microbial activity against the microorganisms such as *Escherichia coli*(Gram negative bacteria) and *Bacillus subtilis* (Gram positive bacteria).

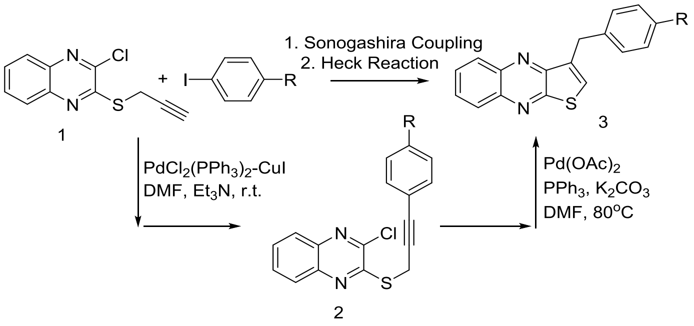

Figure 1. Synthesis of new3-substitutedthieno[2,3- b]quinoxalines.

References

[1] A.Y. Ponomareva, D.G. Beresnev, N.A. Itsikson, O.N. Chupakhin, G.L. Rusinov, Mendeleev Communications16 (2006),16.
[2] Burguete, D. Hadjipavlou-Litina, E. Pontiki, R. Villar, E. Vicente, B. Solano, S. Ancizu, S. Pe´rez-Silanes, I. Aldanaa, A. Monge, Bioorganic & Medicinal Chemistry Letters17 (2007), 6439.
[3] M. Waly, S. Elgogary, A. Lashien, A. Farag, Journal of Heterocyclic Chemistry52 (2015), 411.

Survey reactivity of some 1,3- dicarbonyl with pentachloropyridine

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Perhalogenated aromatic and heteroaromatic compounds are important starting materials for the synthesis of other heterocyclic [1].Pentachloropyridine reacted with bulky nucleophiles at 2-position of pyridine ring and with small nucleophiles at 4-position of pyridine ring [2].

In this work we investigated the reaction of pentachloropyridinewith anion derived from1,3- dicarbonylcompounds in the presence of potassium carbonate in DMSO as solvent.Our study indicated that the initial substitution occurs atthe 4-position of pyridine ring followed by cyclization at the 3-position of pyridine ring(Figure 1). The structure of compounds was confirmedby ^{1}H-NMR and ^{13}C-NMR spectroscopy data.

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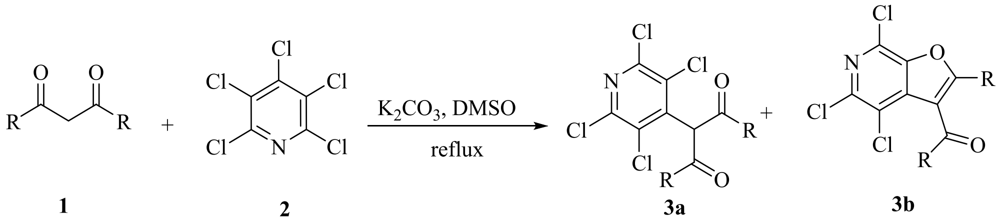

1 2 3a 3b

Figure. Reaction of 1,3- dicarbonylcompoundswith pentachloropyridine

In conclusion, we demonstrated that the reaction of 1,3- dicarbonyl compounds with pentachloropyridine proceeded firstly from carbonsite of nucleophile and subsequence from oxygen site of nucleophile in two products and in 3bcyclisation occurred with oxygen site to 3 position of pyridine ring.

References

[1] R. D. Chambers, A. Khalil, C. B. Murray, G. Sandford, A. S. Batsanov, J. A. K. Howard, Journal of Fluorine Chemistry126 (2005) 1002.
[2] R. Ranjbar-Karimi, G. Sandford, D. S. Yufit, J. A. K. Howard, Journal of Fluorine Chemistry129 (2008) 307.

C-N Bond Cleavage: A Novel Access to Sulfonamides

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Due to their efficient anticancer, antitumor, anticonvulsant, antibacterial, anti-inflammatory as well as HIV protease inhibitory, sulfonamides have found paramount importance as structural motifs in pharmaceuticals and biologically active compounds [1]. Being potent inhibitors of carbonic anhydrase [2],caspase[3] and cyclooxygenase-2 (PTGS2) are of other applications [4].Some examples of therapeutically important sulfonamides are sildenafil, amprenavir, celebrex and darunavir. To date, significant efforts have been allocated for the synthesis of sulfonamides in which all of them use from reactive amines in which lack from the requirement of additional protection/deprotectionsteps.Herein, we wish to disclose a general and novel strategy for the sulfonamidation of un-reactive amines.

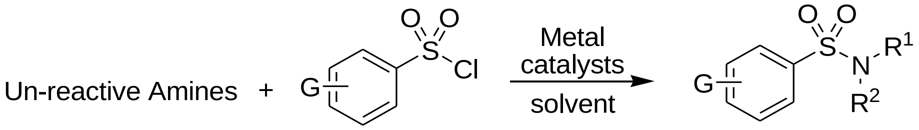

Figure 1. Scheme of the reaction.

References

[1] M. Basanagouda, K. Shivashankar, M. V. Kulkarni, V. P. Rasal, H. Patel, S. S. Mutha and A. A. Mohite, Eur. J. Med. Chem., 45 (2010) 1151.

[2] B. L. Wilkinson, L. F. Bornaghi, T. A. Houston, A. Innocenti, C. Vullo, C. T. Supuran and S.-A. Poulsen, J. Med. Chem., 50 (2007) 1651.

[3] W. Chu, J. Zhang, C. Zeng, J. Rothfuss, Z. Tu, Y. Chu, D. E. Reichert, M. J. Welch and R. H. Mach, J. Med. Chem., 48 (2005) 7637.

A Novel Access to Benzo[e]isoindole-1,3-diones via Oxidative Coupling Reactions

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Since the discovery of C-H olefination of benzene by Fujiwara at 1967 [1] numerous catalytic versions of this transformation have been developed. The vast majority of these catalytic protocols proceed under “ligandless” conditions (with Pd^{II} salts such as $Pd(OAc)_2$ as catalysts) and use oxidants such as peroxides, peroxyesters, dioxygen, polyoxometalates, Cu^{II}, or Ag^{I} to achieve catalytic turnover [2]. Glycogen synthase kinase-3β (GSK-3βa) is responsible for many important biological activities, such as Wnt and Hedgehog signaling pathways, stem-cell renewal, meiosis steps, cellular differentiation, apoptotic mechanisms, circadian rhythm, gene transcription as well as insulin action [3].Thus, the development of GSK-3βinhibitors has been regarded as a potential therapeutic approachfor these related diseases. Zou et al. found that benzo[e]isoindole-1,3-diones are of most powerful GSK-3βinhibitors [4]. However, the traditional synthesis pathways of benzo[e]isoindole-1,3-diones, are very complex, for example including sequential steps such as diazotization, low-yield benzyne formation, Diels-Alder reaction, amidation of esters, cyclization via ortholithiation and cabonization, oxidation of hemiaminal to amide and harsh dealkylation.Herein, we report a direct method to the synthesis of benzo[e]isoindole-1,3-dione derivatives via tandem oxidative coupling reactions of readily available raw materials.

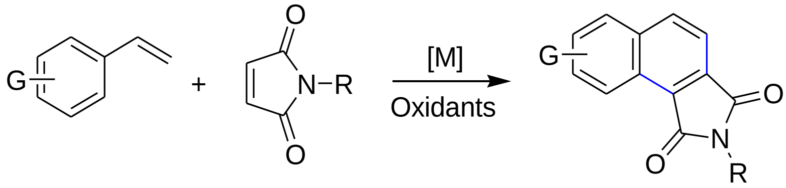

Figure 1. Scheme of the reaction.

References

[1] Y. Fujiwara, I.Moritani, S. Danno, R. Asano, S.Teranishi, J. Am. Chem. Soc., 91 (1969) 7166.
[2] J.Le Bras, J. Muzart, Chem. Rev.,111 (2011) 1170.
[3] B. W.Doble, J. R. Woodgett, J. Cell Sci. 116 (2003) 1175.

Preparatin and charactereization of thiamine-modified Al_2O_3/poly(vinyl chloride) nanocomposite films via ultrasonication assisted peocess

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Nanocomposites are materials designed for enhanced performance in any number of unique applications [1]. Alumina nanoparticles are of much interest, because of Al_2O_3 is the most cost effectiv, hardness, highstrength, excellent dielectric properties [2]. In this project, the surface modification of alumina nanoparticles (NPs) was performed in order to prevent aggregation between hydrophilic surface of NPs and improvement of NPs compatibility with the polymer matrix. The modification was carried out using Vitamin B_1 under ultrasonic irradiation. The characteristics of the modified alumina NPs were studied. Then, PVC/α-Al_2O_3-VB_1nanocomposites (NCs) containing 3, 5 and 7 wt % of modified NPs were synthesized under ultrasonic irradiation. The study of the NCs morphology with FE-SEM and TEM, showed a homogenous dispersion of NPs in the polymer matrix (Figure 1).

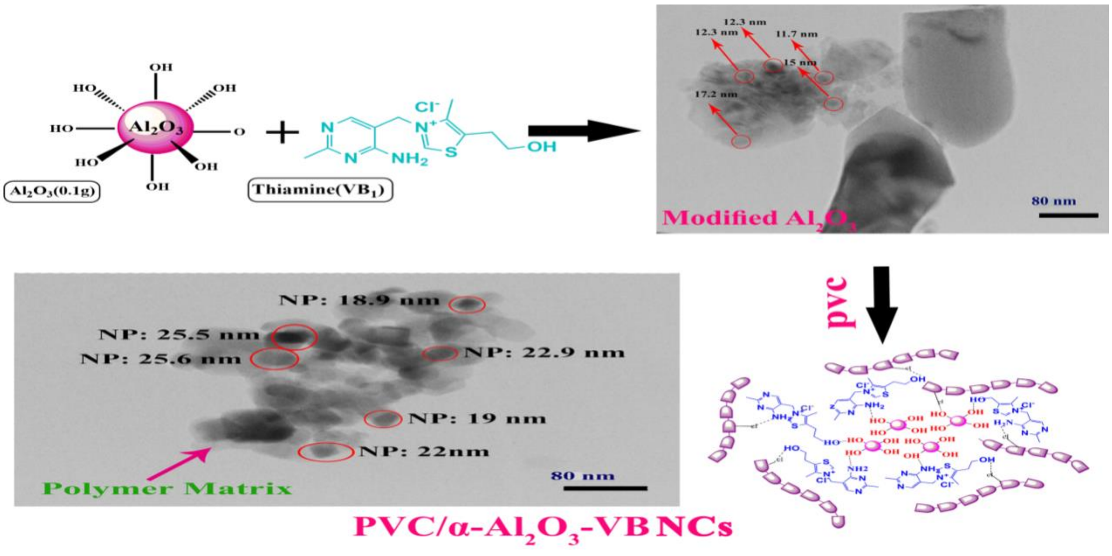

Figure 1. Reaction sequence for the preparation of PVC/α-Al_2O_3 NCs

References

[1] M. Iijima, H. Kamiya, KONA Powder and Particle Journal 27 (2009) 119-129.

[2] S. Mallakpour, E. Khadem, Journal of Molecular Structure 1075 (2014) 196-203.

Eco-friendly Methods for Polycarbonate Wastes Recycling by using Green Solvents and Nanomaterials

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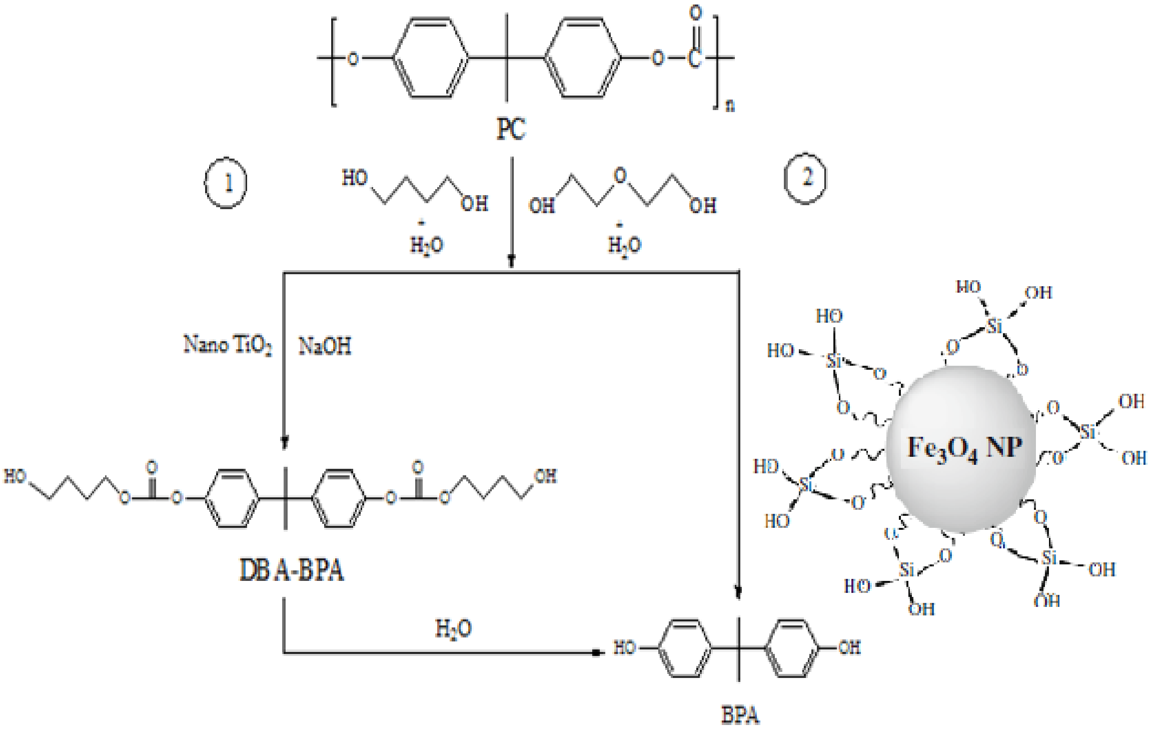
Polycarbonate (PC) is extensively used in many applications because of its very good physical and chemical properties, such as excellent transparency, high mechanical strength, good thermal stability and high heat-distortion temperature [1].The increasing amount of PC wastes from compact discs and plastic objects make their recycling development necessary [2]. Accordingly, here we report chemical recycling of wastes received from optical discs (CDs) and digital optical discs (DVDs) as polycarbonate wastes by using two methods. In the first method, chemical recycling of polycarbonate wastes in the presence of 1,4- butanediol/ water mixture as the solvent, NaOH and nano TiO_2 as catalyst and solid support, respectively and the second method, chemical recycling in presence diethylene glycol (DEG) and water as solvent and magnetic nanoparticles ($Fe_3O_4@SiO_2$) as heterogeneous catalystwere performed. In these reactions PC converts to Bis (butanol) of bisphenolate (DBA-BPA) and 4,4'-(propane-2,2-diyl) diphenol(BPA) as the major products.



References
[1] M. sala, Y. Kitahara, S. Takahashi, T. Fujii, Chemosphere 78 (2010) 42.
[2] M.M. Alavi Nikje, M. Askarzadeh,Polímeros 23 (2013) 29.

Synthesis of a novel nanocomposite TiO_2/ Fe_2O_3 /Al_2O_3 by sol-gel method and its application on PVDF membrane for removal of Cr (VI) from water

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Poly(vinylidene fluoride)(PVDF) membranes have been extensively applied to scientific research and industrial process due to its outstanding properties such as high thermal stability, good chemical resistance and membrane forming properties, in which these properties make it suitable for wastewater treatment. By possessing low level of extractable, PVDF can be considered as a pure polymer; which makes it a suitable candidate in biomedical and bio-separation applications [1].

Nanoscale particles have been widely studied in environmental separations and catalytic reactions due to their unique physical and chemical properties. Titanium oxide nanoparticles have extensively applied in industry and in different photo catalyst area for converting the contamination to the composition of the organic materials to be recovered in environment.Chrome which is present in the underground and surface water is one of the most toxic element threating humanhealth and animals [2]. Chrome has been removed in different type of ways. In this study removal Chrome fromwater was investigated by PVDF membrane involves TiO_2/ Fe_2O_3 /Al_2O_3nanocomposites. For prepared PVDF membrane we used polyvinilidenflourid (PVDF) as polymer matrix and TiO_2/ Fe_2O_3 /Al_2O_3 nanocomposite with loading content of (3% wt.) as reinforcement phase by using phase inversion technique. The influence of the parameters including pH, and chrome concentrations in a mount of adsorption were examined and the adsorption isotherms were analyzed by using Langmuir and Freundlich models. Some techniques such as XRD, Field emission scanning electron microscopy (FE-SEM) ‹have been used for studying The morphology of membranes and structural properties of TiO_2/ Fe_2O_3 /Al_2O_3 nanocomposites, and the remained concentration of chrome in water was measured by AAS device. The results show use PVDF /TiO_2/ Fe_2O_3 /Al_2O_3membrane is an effective and rapidway to remove Cr (VI)from water.

References

[1] L. L.Hench,J. K. West, Chem. Rev. 90 (2008) 33.

[2] Y. Li, F. Liu, B. Xia, Q. Du, P. Zhang, D. Wang, Z. Wang, Y. Xia, J. Hazard. Mater. 177 (2010) 876.

Synthesis of Isoxazoline Ring from the 1,3-Dipolar Cycloaddition Reaction of Nitrile oxide and 2-Indeno[1,2-b]quinoxaline-11-ylidene-1-phenyl-ethanone

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Nitrile oxide 1,afforded in situ from the reaction of dibromo formaldoxime and KHCO$_3$,reacts with the olefin compounds to give bromoisoxazolines in satisfactory yields[1-4]. Reaction of indeno[1,2-*b*]quinoxalin-11-one2 with 1-phenyl-2-(triphenyl-phosphanylidene)-ethanone3in ethanol resultedin 2-indeno[1,2-*b*]quinoxaline-11-ylidene-1-phenyl-ethanone (corresponding chalcone)4 at room temperature. 1,3-Dipolar cycloaddition of 2-indeno[1,2-*b*]quinoxalin-11-ylidene-1-phenyl-ethanone4 with nitrile oxide 1at room temperature in dichloromethane for 3 h formed a spiro compound with an isoxazole ring5(figure1).The structures were confirmed spectroscopically (IR, ^{1}H- and ^{13}C-NMR, and EI-MS) and by elemental analyses.

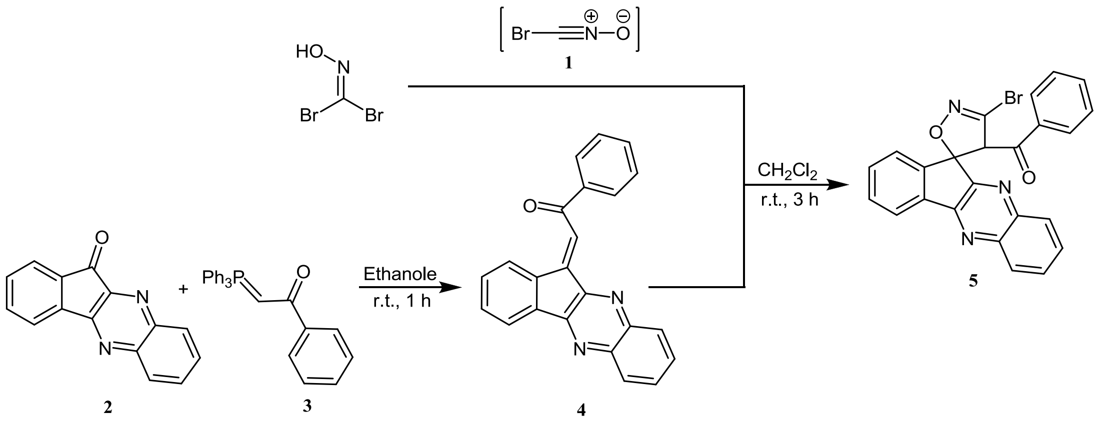

Figure3. Synthesis of isoxazole ring

References

[1] Y.Basel, A.Hassner. Synthesis(1997), 309.
[2] K.Torssell, O. Zeuthen.Acta Chem. Scand. B32 (1978)118.
[3] S. C. Sharma, K. Torssell.Acta Chem. Scand. B33 (1979)379.

The preparation of Bi_2O_3-$NiAl_2O_4$ Nanocomposite and its Catalytic Application in the Synthesis of Organic Heterocyclic Compoundsa

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Metal oxides nanocatalysts have attracted significant attention for their wide range of applications.Among these oxides, Bismuth oxide, Bi_2O_3, due to its high refractive index, dielectric permittivity, marked photoconductivity and photoluminescence, is used in a variety of areas such as sensor technologyandopticalcoatings [1]. Also, Alumina-based composites are extensively used as catalytic materials, ceramic separation membranes and catalytic membranes. Alumina properties such as high specific surface area, surface acidity and defects in their crystalline structures are theimportant factors in such wide range of applications [2].Regarding, the Bi_2O_3-$NiAl_2O_4$Nanocompositewas preparedby co-precipitationprocess. The nanocomposite was characterized by XRD, FESEM,TEM and FT-IR.

Recently, One-Pot multicomponent reactions (MCRs) have played an increasingly important role in organic and medicinal chemistry because of decreasing a number of reaction steps, lowercosts, high atom-economy, energy saving, and the avoidance of time consuming,waste consumption and expensive purification processes [3]. Hence, multicomponent reactions (MCRs) are very important for the construction of many heterocyclic compounds such as benzoxanthene and pyrimidinone derivatives. The synthesis of these compounds due to large number of biologicaland pharmacological properties has received a great deal of attention.The aims of this research were to synthesize and characterize the Bi_2O_3-$NiAl_2O_4$ nanocomposite. The catalytic properties of the nanocomposite in the synthesis of heterocyclic compounds were also investigated.

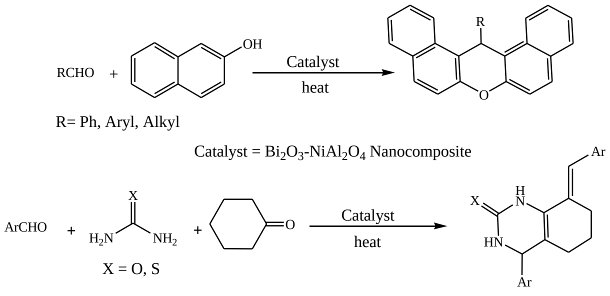

Figure 1. Scheme of the reaction

References

[1] J. Xu, Y. Ao, D. Fu, C. Yuan.Applied Surface Science 255 (2008) 2365.
[2] S.A. Hassanzadeh-Tabrizi, E. Taheri-Nassaj. Journal of Alloys and Compounds 494 (2010) 289.
[3] C. Simon, T. Constantieux, J. Rodriguez, European Journal of Organic Chemistry (2004) 4957.

Synthesis of new amidoalkylnaphthols derivatives under acidic catalyst and solvent free conditions

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1-amidoalkyl-2-naphtol derivatives are of significant importance since they have been frequently applied as hypotensive and bradycardiac agents [1]. 1-amidoalkyl-2-naphtol can be converted to 1,3-oxazine derivatives [2]. 1,3-oxazines have potentially different biological activities including antibiotic, antitumor ,analgesic, anticonvulsant, antipsychotic, antimalarial, antianginal, antihypertensive, and antirheumatic properties.

1-amidoalkyl-2-naphtol can be prepared by multicomponent condensation of arylaldehydes,2-naphtols and amide derivatives or acetonitrile in the presence of different lewis or bronsted acids as P-TSA, $ZrOCl_2$, $Yb(OTf)_3$/[Bmim]BF_4, $FeCl_3$.SiO_2, I_2, Sulfamic acid [3]. However, many of the reported methods are associated with one or more of the following drawbacks: low product yield, expensive or air-sensitive reagents, long reaction time, harsh reaction conditions, the used of toxic, corrosive and non-reusable catalysts, and the use of large amount of catalyst. Therefore, the development of more efficient procedures for the synthesis of 1-amidoalkyl-2-naphthols is still needed. A simple and eco-friendly method for the preparation of amidoalkyl naphthols derivatives via the three-component condensation reaction of aldehydes, 2-naphtol, and amidsin the presence ofacidic catalyst is described (Fig 1).

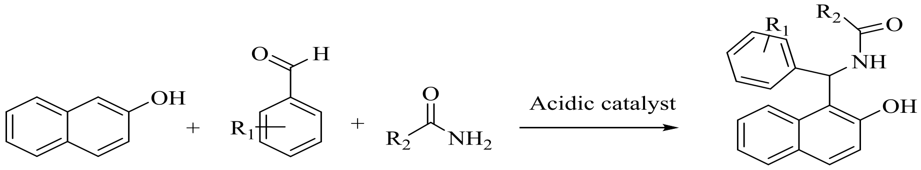

Figure 1. Synthesis of amidoalkyl naphtol by acidic catalyst

References

[1] A.Y. Shen, C.T. Tsai, and C.L. Chen. 34(1999) 877-882.

[2] M.Damodiran, N.P. Selvam, and P.T. Perumal.50 (2009) 5474- 5478.

[3] R.R .Nagawade. and D.B. Shinde. Mendeleev Communications17 (2007) 299-300.

DFT Study on the Mechanism of Chemoselectivity in [4+2] Cycloaddition Reaction Involving Electron-Poor Dienophile with DanishefskyDiene

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The Diels –Alder reaction has to be a convenient way to assemble complex six membered cycles due to its versatility as well as its high regio- and stereoselectivities [1].The scope of this class of cycloaddition is very large and allows not only the synthesis of cyclohexene derivatives but also of a variety of heterocycles by swapping carbon atoms on the diene and/or the dienophile component with heteroatoms (O, N, S for instance; the so-called hetro-Diels-Alder reaction) [2].

The reaction between indole derivatives with Danishefskydiene leads exclusively to the Diels-Alder (DA) cycloadducts resulting from the participation of the indole 2,3-carbon-carbon double bond [3].With considering the different products, we present a DFT study on the mechanism of cycloaddition reactions of indol derivatives with Danishfskydiene. Two possible mechanisms exist for this process, stepwise and concerted. The activation energies and DFT- reactivity indices was investigated for these reactions. The concerted mechanism with low activation energy is favorable path for DA and hetero-Diels-Alder(HDA) reactions. The DFT-reactivity indices can explain regioselectivity and stereoselectivity for these processes.

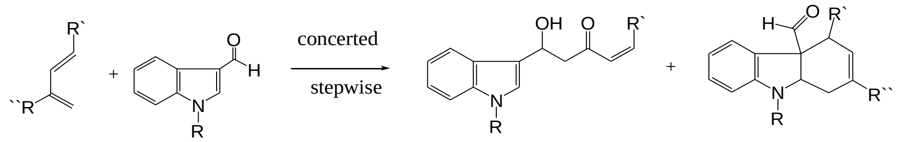

Figure 1. Scheme of the reaction

References

[1] K. C. Nicolaou, S. C. Snyder, Montagnon, T. Vassilikogiannakis, G. Angew. Chem., Int. Ed 41(2002) 1668.
[2] L. F. Tietze,G. Kettschau. Top. Curr. Chem189(1997) 1.
[3] A. Chretien, I.Chataigner, N. L. R. Piettre, J.Org. Chem 68 (2003) 7990.

Efficient Synthesis of Novel Quinolinone Derivatives

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Many quinolinones derivatives and molecules that have triazoles ring in their structure have been reported as anti-cancer agents [1]. Furthermore, some quinolinone analogs demonstrated potent anticancer activity [2]. Accordingly the quinolinoneand triazole ring scaffold is considered as an attractive heterocycle in the field of anti-cancer drug design and development.Herein, we decided to investigate novel series of 9-(4-((1-benzyl-1H-1,2,3-triazol-4-yl)methoxy)phenyl)-3,6,6-trimethyl-1-phenyl-1,4,4a,5,6,7,8a,9-octahydro-8H-pyrazolo[4,3-b]quinolin-8-one. **1**was prepared via the reaction of propargyl bromide with 4-hydroxybenzaldehyde. (Azidomethyl)benzene was separately prepared by the reaction of benzylbromide with sodium azide. One pot multicomponent reaction of 4-(prop-2-yn-1-yloxy)benzaldehyde, dimedoneand 3-methyl-1-phenyl-1H-pyrazol-5-amine in ethanol led to compound **2**which finally reacted with (azidomethyl)benzene in triethanolamine to form the desired product that was characterized by FT-IR and ^{1}HNMR spectra.

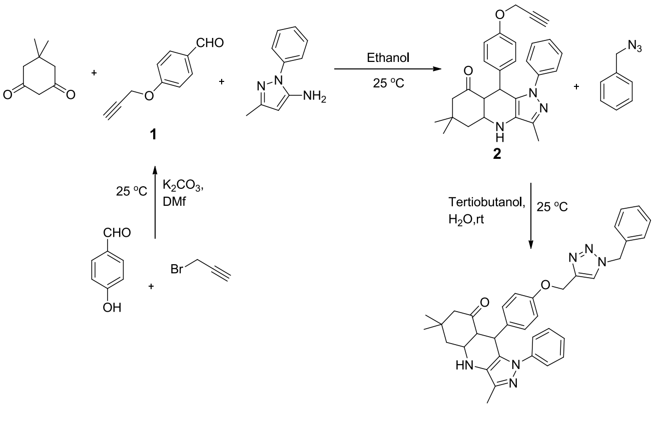

Figure 1. Synthesis of 9-(4-((1-benzyl-1H-1,2,3-triazol-4-yl)methoxy)phenyl)-3,6,6-trimethyl-1-phenyl-1,4,4a,5,6,7,8a,9-octahydro-8H-pyrazolo[4,3-b]quinolin-8-one.

References

[1] S. Philip, M. Purohit, K. L, E. S, T. Raizaday, P. S, G. Pujar. International Journal of Pharmacy and Pharmaceutical Sciences 6 (2014) 185.
[2] C. Sissi, M. Palumbo. Current Medicinal Chemistry - Anti-Cancer Agents 6 (2003**)** 439.

Biologically Synthesized Silver Nanoparticles by Aqueous Extract of *Satureja intermedia C.A. Mey* and Evaluation of Antioxidant Activity

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Developing high-yield, low cost, nontoxic and environmentally friendly methods for metallic nanoparticles is an increasing need. Using plants towards synthesis of nanoparticles are emerging and beneficial with the presence of broad variability of bio-molecules in plants which can act as capping/stabilizing and reducing agents. Among the metallic nanoparticles, Silver has been enormously utilized for its diverse applications in the fields of bio labeling, opto-biosensors, cancer cell imaging, drug delivery systems, polarizing filters, electrical batteries, staining pigments, etc. [1].

In the present attempt, we evaluated total phenolic and flavonoid contents in aqueous extract of *Saturaja intermedia C. A. Mey* (Labiateae) collected from Gardaneh Almas (2350-2400 m), between Astara and Ardabil, on June 2014. Results showed that the extract is rich in flavonoids (21.123± 0.0698 µg/mL) and phenolic compounds (25.289±0.0698 µg/mL) and the plant could be a good choice for bio reduction process. So we investigated biosynthesis of SNPs by the aqueous extract of S. intermedia and found an easy and rapid procedure. For this reason, a 100 mL aliquot of a 0.01 M solution of $AgNO_3$ was gradually added to 20 µL of theaqueous extract of S. intermedia. The mixture was kept in an ultrasonic during the addition and then was stirred in a magnetic stirrer (500 rpm) at room temperature for 48 hours. Silver nanoparticles were gradually obtained during the reaction and were washed by de-ionized water and dried for an hour in an oven at 100°C. Then the synthesized nanoparticles were characterized. UV-Vis spectrum of colloidal solution of SNPs showed a strong surface Plasmon resonance centered at 475 nm confirmed the nanocrystalline character of the particles [2]. The XRD study showed crystalline nature and face cubic center shape for nanoparticles. TEM study showed that the mean diameter and standard deviation for the silver nanoparticles were 29.29±28.18 nm. Electron donation ability of the extract and the colloidal solution of SNPs and also BHT as a standard antioxidant, were measured from the bleaching of the purple-colored methanol solution of DPPH [3]. Results showed that the aqueous extract of *S*. intermedia exhibited higher scavenging activity in concentrations 2 and 0.2 (µg/mL) compared to Ag/S. intermedia suspension and DPPH (as a standard). By reducing the concentration to 0.02 µg/mL and lower, BHT was more effective than the aqueous extract and Ag/S. intermedia suspenssion.

It can be concluded that the aerial parts of S. intermedia is a good source of flavonids and phenolic compounds, a potent antioxidant and also a valuable choice for bio-reduction and biosynthesis of silver nanoparticles.

References

[1] X. Hang, Y.W. Ngo, X.Yu, L. Yi. Current opinion in Chemical Biology 16 (2012) 429.
[2] S. Schneider, P. Halbig, H. Grau, H., U. Nickel. Photochemistry and Photobiology 60 (1994) 605.
[3] V. Bondet, W. Brand-Williams, C. Berset, C. Lebensmittel-Wissenschaft und-Technologie-Food and Science Technology 30 (1997) 609.

One-Pot Synthesis of 2-Indole-acetonitrile Derivatives via a Sequential Four Component Reaction

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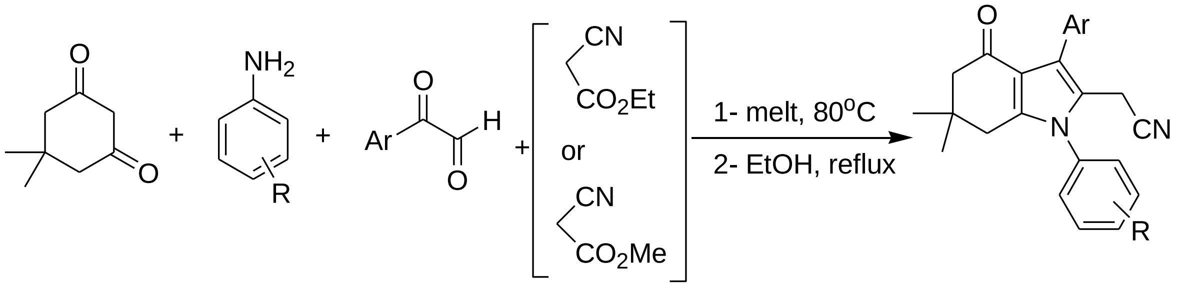
Indole derivatives displaying a broad range of biological activity in medicinal chemistry including anti hypertensive, anti proliferative, anti viral, anti tumor, analgesic, anti-inflammatory, anti microbial, anti fungal activities, etc. Although indole moiety is very small but have been the intense research interest for many years, Due to the diverse biological activities. And also, indole-based colorants are various class of organic dyes and pigments [1,2].

In this paper we report the synthesis of a new library of pharmacologically relevant 2-indole-acetonitrile (5), based on the reaction of enamines and Michel acceptor via the One-Pot , multicomponent reaction of dimedone (1), various aniline (2), aryl glyoxal(3), and ethyl cyanoacetate/methyl cyanoacetate(4), under reflux conditions respectively in melt and ethanol (fugure 1). This protocol is distinguished by its high atom-economy, yield the desired products in good to excellent yields, the use of ethanol as reaction media, and the efficiency of production without the use of any activator or metal promoters, and the pure products were acquired simply by washing the crude products with 96% ethanol. All structures were confirmed by IR, MS, ^{1}H- and ^{13}C-NMR analyses.



1 2 3 4 5

Figure 1. Synthetic Scheme for the Generation of 2-Indole-acetonitrile Derivatives.

References

[1] N.K. Kaushik, N. Kaushik, P. Attri, N. Kumar, C. H. Kim, A. K. Verma, E.H. Choi. Molecules 18 (2013) 6620-6662.

[2] T.C. Barden. Heterocyclic Scaffolds II:. Springer Berlin Heidelberg (2010) 31-46.

Preparation of a Novel Polymethylmethacrylate Nanocomposite in the Presence of PMMA-modified Graphene Oxide

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Polymethylmethacrylate can be used in many applications, but due to its rigidity in some cases does not have sufficient strength. Recently nanotechnology has been used for improving of the nanocomposites properties. Different reinforcements were used for the preparation of polymethylmethacrylatenanocomposites which graphene oxide is one of them[1].The main problem in the using of nano-materials is related to the lack of proper dispersion in the polymer matrix. Modified nanomaterials can overcome this problem partially.

In this research, the modified graphene oxide was prepared by insitu polymerization in the presence of methy methacrylate as monomer and used for this purpose [2]. Poly methyl methacrylate nano composite was prepared by Melting method [3]. FT-IR, TGA and DSC techniques were applied in order to characterization of prepared nano composites. To investigate of the mechanical properties of nano composites stretching, bending and impact tests were carried out.

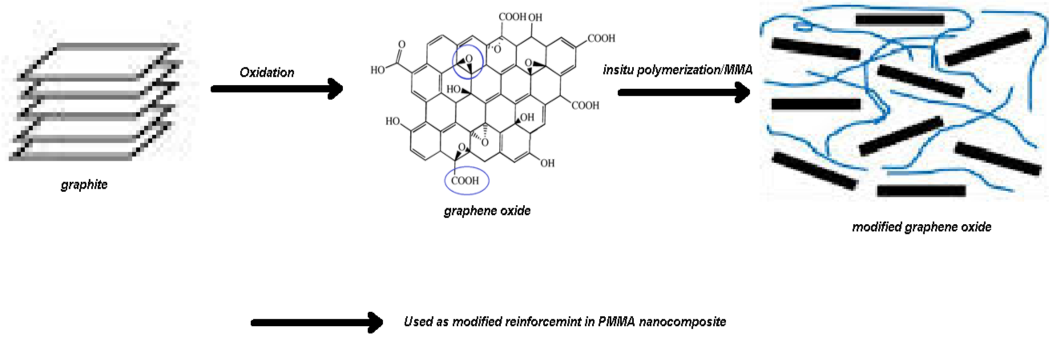

Figure1. Modification of grapheme oxide and was used in PMMA nanocomposite

References

[1] G.Caroteuto, Y.S.Her, E. Matijevic, *Ind. Eng. Chem. RES.*,35 (1996) 2929.
[2] T. Kuilla, S. Bhadra, D. Yao, N.H.Kim, S. Bose, J.H. Lee, *Prog. Polym.Sci.*,35 (2010) 1350.
[3] M.Barikani, S.Mehdipour-Ataei, H. Yeganeh. *J. Polym. Sci: Part A: Polym. Chem.*, 39 (2001) 514.

RAFT polymerization technique for the synthesis of polymers containing the dye or drug

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Nowadays, one of the concerns of human society is the cancer topic, according to numerous cancer-causing factors in the developed world.In order to overcome these problems today, drugs targeting strategy is used. Targeted drug delivery is often divided into two categories, passive and active.In active targeting, therapeutic agent along with a carrier, attached to a specific cell or tissue. Active targeting benefits include of ability to maintain drug concentration in relatively constant for a specified period of time, the possibility of delivering medicine to a particular organ or tissue, take delivery in nanometer dimensionsand etc[1,2].

We report the synthesis of a water-soluble polymer containing functional groups using RAFT polymerization technique. These polymers have a narrow molecular weight (PDI low) and is connected to an active molecules, such as dyes, drugs or antibodies. The RAFT process involves conventional free radical polymerization of a substituted monomer in the presence of a suitable chain transfer agent (RAFT agent). Sothe first step is the formation oftheN-acryloxysuccinimide(NAS)monomer,next the synthesis of pentafluorophenyl[4-(phenylthiocarbonylthio)-4-cyanovalerate] (CTA-PFP) as RAFT agent and eventuallythe synthesis of polymerthrough RAFT polymerization in Schlenk flask. These starting materials and polymerwere characterized by FT-IR and ^{1}HNMR.

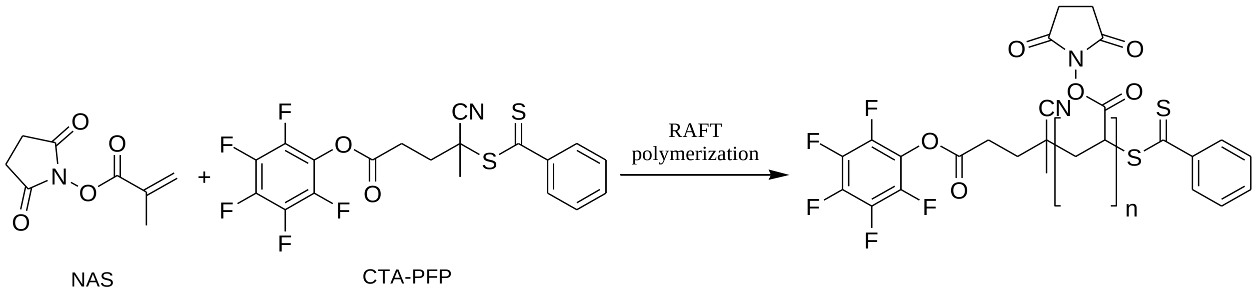

Figure 1. RAFT Polymerization of Monomer NAS in the presence of chain transfer agent.

References

[1] P.Liu, A. J.Boyle, Y.Lu, R.M.Reilly, M.A.Winnik. Biomacromolecules, 13 (2012) 2831-2842.

[2] Y.H.Bae, K.Park. Journal of Controlled Release, 153 (2011) 198.

Characterization and fabrication of poly(vinyl chloride) nanocomposite films containing zirconia nanoparticles modified with thiamine

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Excellent chemical resistance, easy modification, non-flammable and low production cost of poly(vinyl chloride) (PVC), make PVC-based materials suitable for use as the hosting matrix in the fabrication of polymer-based nanocomposites (NCs)[1]. However,poor processability, low thermal stabilityand brittleness have greatly restricted their application. To overcome this problem, PVC NCs has been fabricated by the addition of inorganic nanofillers. ZrO_2 nanoparticles (NPs) were employed as fillers to retrofit and increase the thermal stability, mechanical strengthand opticalproperties of PVC as one of the most important thermoplastics. At first, surface modification of ZrO_2NPs was performed by vitamin B_1 (VB_1) as environmental friendly coating layer, in order to prevent accumulation and increase compatibility of NPs with the organic PVC matrix [2]. PVC based NCs were prepared by the incorporation of different mass fractions of modified ZrO_2 (ZrO_2-VB_1) (3, 5 and 7 wt %) into PVC matrix by solution casting and ultrasonic dispersion methodsas a rapid, economical and green way(Scheme 1). The results indicated that PVC/ZrO_2-VB_1 NC films exhibit better thermal stability, optical, tensile and self-extinguishing properties compared withpure PVC.

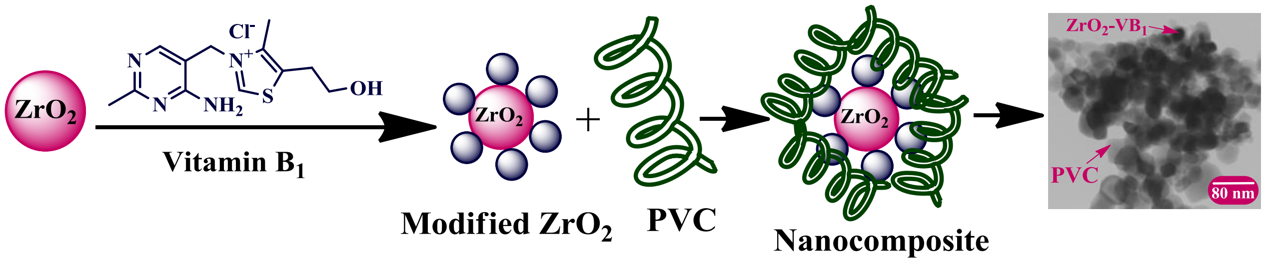

Figure 1. Reaction sequence for the preparation ofPVC/ZrO_2-VB_1 NCs

References

[1] S. Kango, S. Kalia, A. Celli, J. Nijguna, Y. Habibi, R. Kumar. Progress in polymer science, 38 (2013) 1232–1261.

[2] S. Mallakpour, M. Naghdi . Polymer Bulletin, 73 (2016) 1701-1717.

Preparation of Superabsorbent Polymers for Use as Soil Moisture Holder in Agriculture: A Green Synthetic Route

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Superabsorbent polymers (SAPs) are lightly cross-linked hydrophilic polymers that can absorb, swell and retain aqueous solutions up to hundreds of times their own weight [1].Common SAPs are generally white sugar-like hygroscopic materials, which are mainly used in disposable diapers and other applications including agricultural use and soil conditioning and as artificial soils for hydroponics, as controlled release agents for agrochemicals or pharmaceuticals, as artificial snow for skiing areas, and other numerous applications [2].In agriculture, superabsorbent polymers are used as a soil additive, as reservoir of nutrients, and as water superabsorbent in the soil.Superabsorbent polymers are used as water adsorbents to increase the capacity of the soil to absorb and retain water and this property is very important to encounter the impacts of dehydration and reduce impacts of drought stress in crops.These materials decrease the number of irrigation times by increasing the gaps of irrigation, therefore the water cost and energy will be saved [3].

In the present work, a class of superabsorbents was synthesized with different ratios of two monomers,acrylicacid and acrylamide,with a water-soluble crosslinker (*N,N'*-methylenebis (acrylamide), MBAAm)in aqueous medium.The performance of the prepared superabsorbents such aswater-holding capacity (WH) and water-retention ratio (WR) was investigated in soil samples.Other analyses such as swelling,FT-IR,TGA and SEM were alsostudied.Results showed acceptable efficiency for the prepared samples. It can be concluded that the prepared samples could be a good additive foragricultural soils as moisture holder.

References

[1] K.Kabiri, H.Omidian, S. A.Hashemi,M. J.Zohuriaan-Mehr, EUR. POLYM. J.,39 (2002)1341-1348.
[2] M. J.Zohuriaan-Mehr, K.Kabiri. Iran polym.J.17(2008) 451-477.
[3] A. Oraee, E.Ganji Moghadam. AFR. J.AGR. RES.,8(2013)1813-1816.

Synthesis of 1,3-Dimethyl-5-(9-nitro-7-phenyl-2,3,4,5-tetrahydro-1*H*-pyrrolo[1,2-*a*][1,3]diazepin-8-yl)pyrimidine-2,4,6-trione via a One-Pot , Three-Component Reaction

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Pyrrolodiazepines have CNS depressant, anti-inflammatory, anti-convulsant and anti-histamine activity.They are inhibitors of enzyme promoted prostaglandin synthesis, and protectors against the convulsive shock induced by metrazol in mice[1].Compounds based on barbituric acid show a high hypnotic and sedative activity[2].Heterocyclic ketene aminals are powerful and versatile intermediates in heterocyclic synthesis. Reactions of cyclic methylidene-aminals with a number of electrophilic reagents have been successfully used to synthesize five- and six-membered and fused heterocycles in recent years. These fused heterocyclic structures are frequently found in pharmacophores and play important roles in drug discovery. They are also used as pesticides, herbicides, antianxiety agents, and antibacterial drugs[3].

We have developed synthesis of new heterocyclic compoundsusing nitroketeneaminals multi-component reactions(Figure 1). The reaction of 1,3-dimethylbarbituric acid **1,**arylglyoxals (2) and nitroketenaminal derivatives (3)in EtOH at reflux conditions produced pyrrolodiazepin derivatives (4) in excellent yields (85-90%). The ^{1}H and ^{13}C NMR spectra of the crude products clearly indicated the formation of title compounds. The work-up procedure is simple and easy. The structures of compounds 4 were confirmed by IR, MS, ^{1}H- and ^{13}C-NMR analyses.

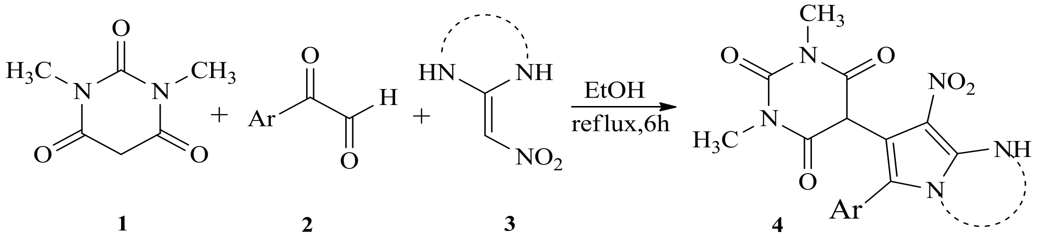

Figure 1. Synthesis of pyrrolodiazepin derivatives via a three-component reaction

References

[1] R. Katritzky, R. Jain, R.Akhmedova, Y.Jiang Xu, Arkivoc, ix(2003) 1551-7012.
[2] L. Gozalishvili, V. Beryozkina, V. Omelchenko, I.Zubatyuk, V. Shishkin, N. Kolos, Tetrahedron 64 (2008) 8759–8765.
[3] A.Alizadeh, R. Ghanbaripour, S. Weng, Helvetica Chimica Acta, 98 (2015) 663.

Synthesis of 4-(imidazolidin-2-ylidene(nitro)methyl)-2-oxo-2*H*-chromene-3-carbonitrile via a One-Pot , Three-Component Reaction

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Heterocyclic ketene aminals (HKAs) are powerful and versatile intermediates in heterocyclic synthesis. The reactions of cyclic ketene aminals with a number of electrophilic reagents have been successfully used to synthesis five- and six-membered and fused heterocycles in recent years [1]. Coumarin moieties are a large group of oxygen-containing heterocycles that are widely distributed in plants such as grasses, legumes, and fruits. Coumarins possess a wide range of biological activities including anticoagulant, inhibition of HIV-1 protease [2].

Herein, We report the synthesis of coumarin-bearing nitroketeneaminal derivatives by reaction of salicylaldehydes (1), alkyl cyanoacetate (2), diamines, and 1,1-bis(methylsulfanyl)-2-nitroethene in EtOH. The reactions of salicylaldehydes (1), alkyl cyanoacetate(2), diamines and 1,1-bis(methylsulfanyl)-2-nitroethene were performed within 3 h in EtOH to produce the targetderivatives **3** in excellent yields(Figure 1). Easy performance highly functionalized in the molecule, good yields, and easy purification are the main advantages of this method. The structures were confirmed by IR, MS, ^{1}H- and ^{13}C-NMR analyses.

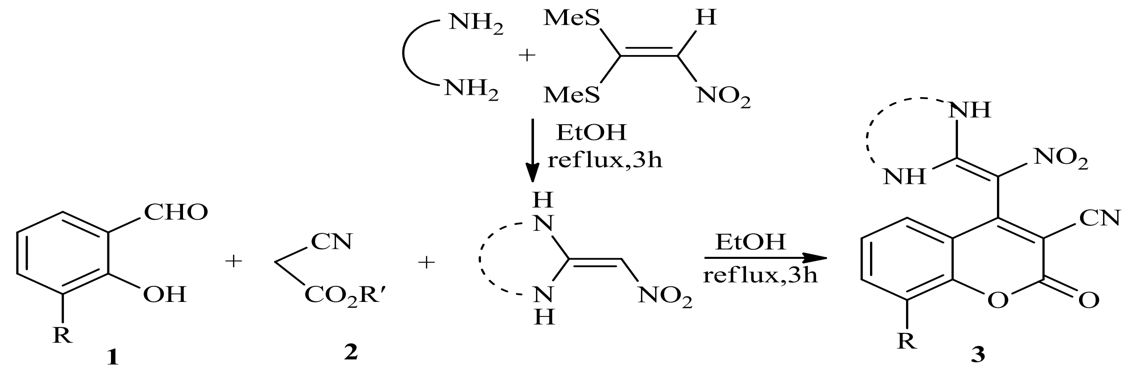

Figure 1. Synthesis **of**4-(imidazolidin-2-ylidene(nitro)methyl)-2-oxo-2*H*-chromene-3-carbonitrile**derivatives** (R=H,OMe and R'=Me,Et).

References

[1] A.Alizadeh, R.Ghanbaripour, Z. Long-Guan. Synthetic Communications,43(2013) 2575–2582.
[2] A.Alizadeh, R.Ghanbaripour, Synthetic Communications,44(2014) 1635–1640.

Synthesis, Characterization and Comparison of two Water-soluble Crosslinkers Used in the Preparation of Superabsorbent Polymers

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Superabsorbent polymer (SAPs) materials are hydrophilic networks that can absorb and retain huge amounts of water or aqueous solutions. SAPs are originally divided into two main classes: synthetic (petrochemical-based) and natural (polysaccharide and polypeptide-based) [1]. They can absorb water hundreds times of its own weight and being converted to long lasting gels, have a special place in agriculture, landscaping, erosion control and desert reduction [2].One of the most important parameters that directly effects on the superabsorbent performance, is the type of the crosslinker used in the superabsorbent synthesis. This issue involves the mechanical stability and swelling level of the synthesized superabsorbent.

In this work, two types of crosslinkers with different chain-lengths were synthesized by the reaction of ethylenediamine and propylenediamine with acryloyl chloride. The synthesized crosslinkers were then underwent superabsorbent preparation. The prepared superabsorbents were compared together and with other samples prepared with (*N*, *N'*-methylenebis (acrylamide), MBAAm) as a provided crosslinker. The performance of the samples including water-holding capacity (WH) and water-retention ratio (WR) was investigated in soil samples. Other analyses such as swelling, FT-IR, TGA and SEM were also studied. Results showed considerable changes in the performance and mechanical stability of the samples by changing the type of the crosslinker.

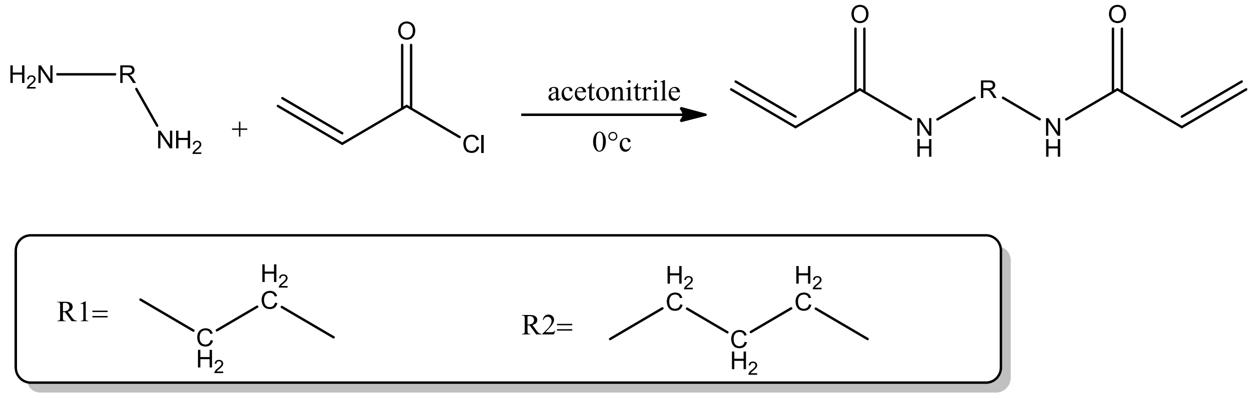

Figure 1. The synthetic route for the preparation of the crosslinkers

References

[1] M. J. Zohuriaan-Mehr, K.Kabiri. Iran Polym. J., 17(2008)451-477.
[2] R.Barihi, E.Panahpour, M.Hossein MirzaeeBeni. World Sci. J, 1 (2013) 223-228.

A friendly approach for surface treatment of SiO_2 nanoparticles by biosafe vitamin B_1 for synthesis of poly(vinyl chloride)/SiO_2 nanocomposite films with improved properties

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It is clear that, poly(vinyl chloride) (PVC) is a white and brittle solid polymer with low thermal stability which has limited its applications [1].Incorporation of various inorganic nanofillers is an effective method to overcome this problem [2].In this study, SiO_2nanoparticles (NPs) incorporated into PVC matrix to prepare nanocomposites with better mechanical, physical, and thermal properties. To prevent aggregation and to achieve a uniform dispersion of SiO_2NPs into the PVC matrix, the SiO_2 NPs were modified with vitamin B_1 (VB_1). Nanocomposites (NCs) were prepared with different percentage of modified SiO_2 NPs (3, 5 and 7 wt %)(Figure 1). The results indicated that PVC/SiO_2-VB_1 NCs exhibited better thermal stability, flexibility than pure PVC in three weight percentages.

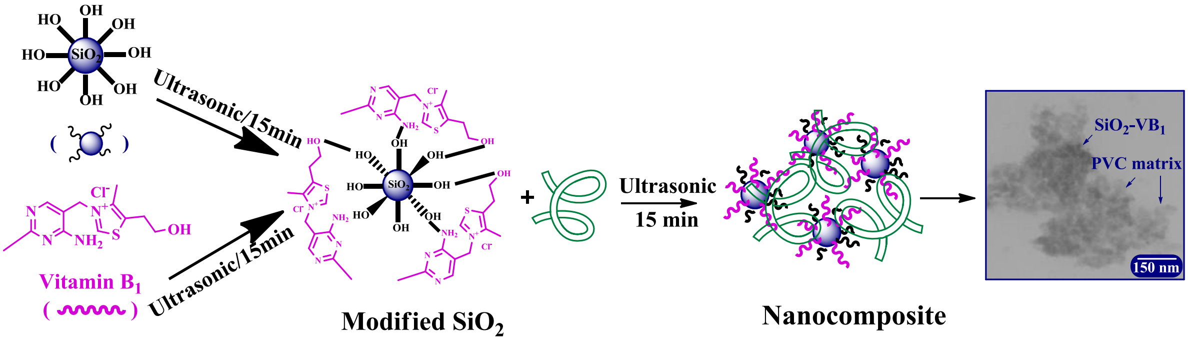

Figure 1. Reaction sequence for the preparation ofPVC/SiO_2-VB_1NCs

References

[1] S. Mallakpour, A. Jarahiyan,Journal of Thermoplastic Composite Materials,(2016) Doi: 10.1177/0892705716632857.
[2] Y.Shin, D. Lee, K. Lee, K. H. Ahn, B. Kim,Journal of Industrial and Engineering Chemistry, 14 (2008) 515–519.

Epoxy Ring Opening of Glycidylmethacrylate: Synthesis and Characterization of Bio-macromonomer

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Polymeric macromonomers are containing one or more polymerizablefunctional groups, which are typically located at the chain end(s) or side chain. They can be polymerized with low molecular weight monomers to generate brush-like [1] and complex structures such as graft copolymers, star polymers, and dendronized polymers [2]. Generally, two synthetic strategies have been used to prepare near monodispersemacromonomers: a) direct synthesis of macromonomers using a vinyl-functional initiator that does not participate in the chain-growth reaction and b) preparation of end-functionalized polymers, followed by post-polymerization modification [2]. Until recently, however, these polymers have been prepared through polymerization them by free-radical polymerization processes [3].

In this work a bio-macromonomer was synthesized by reaction of Glycidylmethacrylate (GMA) and polyvinylalcohol (PVA) in N-Methyl-2-pyrrolidone (NMP) as solvent. For this purposePVA was resolved in the solvent and then GMA was added to the solution mixture and the reaction was carried out for 24hr at room temperature under Ar atmosphere. After completion of the reaction the product was precipitated in methanol as nonsolvent and washed with ether several times.The macromonomer was characterized with Fourier transfer infrared spectroscopy (FT-IR),^{1}HNMR,^{13}C NMR, TGA and SEM analysis.

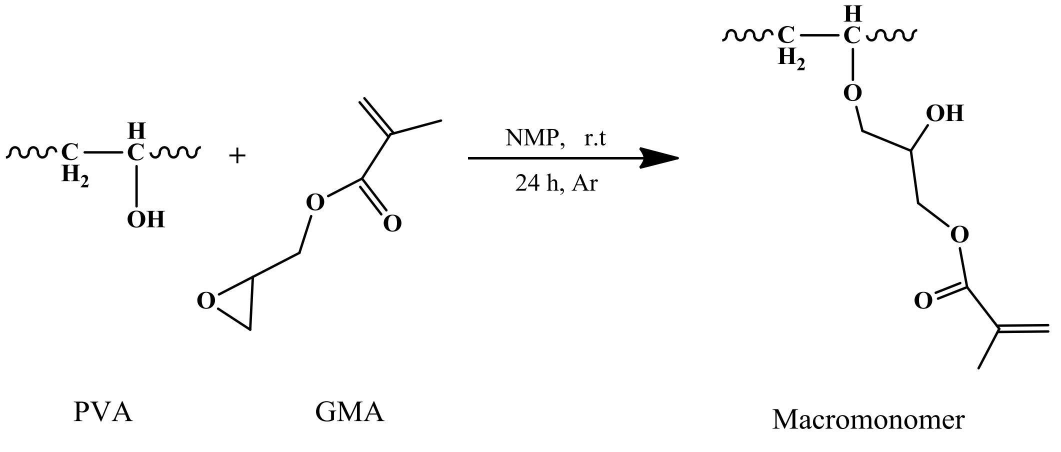

Figure 1. Scheme of the reaction

References

[1] T. Junkers, C. Barner-Kowollik. Macromol.Theory Simul.,18 (2009) 421.
[2] PengchengYang, Steven P. Armes. Macromol.Rapid Commun.,35(2014) 242.
[3] V.Heroguez, S.Breunig, Y.Gnanou, M.Fontanille. Macromolecules, Macromolecules, 29 (1996) 4459.

Synthesis and Characterization of Biodegradable Hydrogel for Drug Delivery System based on polyvinyl alcohol

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Drug delivery devices are considerable andtheme importance is because of their ability to exertspatiotemporal control over drug release locally at disease site[1]. These controlled systems based on hydrogels that are linear or three-dimention polymers networks formed by chemical or physical crosslinking to retaining large amount of water [2]. Many polymers are used for preparation of hydrogel. Among these polymersPolyvinylalcohol (PVA)is a biodegradable polymer thatcan be used in manybiomedical and pharmaceutical applications, due to its advantages such as nontoxic,non-carcinogenic, and bioadhesive characteristics with the ease of processing[3].

In thepresent study a copolymer based on polyvinylalcohol (PVA) functionalized by Glycidylmethacrylate and acrylamide was synthesized. A macromonomer was prepared with reaction of PVA and GMA in N-methylpyolydone. Then the prepared macromonomer was reacted with acrylamide monomer by free radical polymerization in dimethylacetamid (DMA) as solvent in the presence of benzoilperoxide (BPO) as initiator under Ar atmosphere.After completion of the reaction the product was precipitated and washed with acetone and deionized waterthree times.The synthesized copolymer was characterized with FT-IR,^{1}H NMR,^{13}C NMR, SEM and TGA techniques. This copolymer was investigated as drug delivery system by UV.vis analysis in different factors.

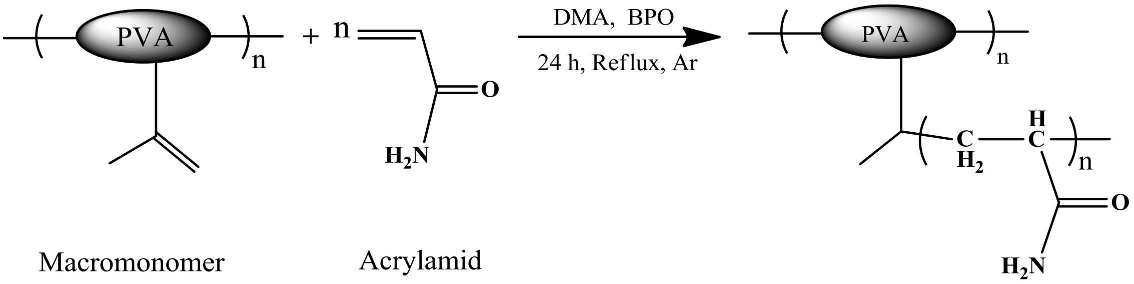

Figure 1. Scheme of the reaction

References

[1] Y.Brudno, D. J. Mooney. Journal of Controlled Release, 219 (2015) 8.
[2] N.K.Singh, D. S. Lee. Journal of Controlled Release, 193 (2014) 214.
[3] W. Cai, R.B. Gupta, ‘‘Hydrogels’’, Kirk-othmer encyclopedia of chemical technology. JohnWiley & Sons, New York.(2002).

Synthesis of β-aminocarbonyl compounds catalyzed by nitrogen and sulfur doped carbon sphere (NS-doped-CS) via multi component Mannich reactions in water

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β-Amino carbonyl compounds are attractive targets for chemical synthesis,because they are widely used as biologically active compounds and are important synthesis for a variety of pharmaceuticals.A highly diastereoselectivemulticomponentMannich reaction between cyclohexanone, aromatic aldehydes and amines in water is described.A novel heteroatom doped carbon sphere catalyzed this reaction. Reactions proceeded in good to high yields with an excellentdiastereoselectivity (Figure 1).

The best selectivity was obtained where there are weak electron donating and electron-withdrawing groups on the aldehyde. The rate formation of Mannich product is decreased when strong electron-withdrawing groups and/or electron-releasing groups are present on aldehyde; in these cases selectivity is improved if an electron-donating group is present on the amine. The catalyst is recoverable and reused for five times without significant decrease in its activity.

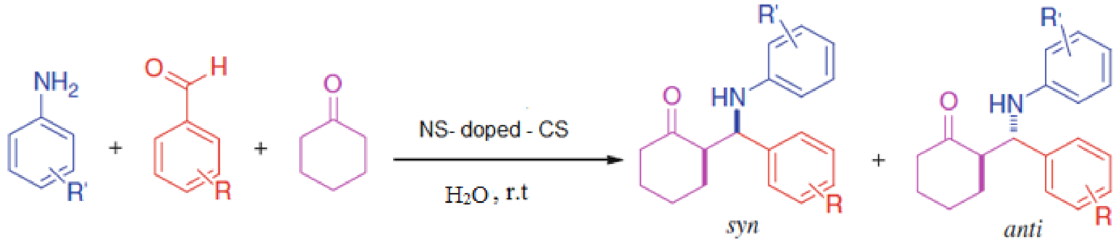

Figure1. Scheme of the reaction.

References

[1] A.A. Deshmukh, S.D. Mhlanga, N.J. Coville, Materials Science and Engineering R, 70 (2010) 1.
[2] H. Eshghi, M. Rahimizadeh, A. Javadian-Saraf, M. Hosseini, Research on Chemical Intermediates, 41 (2015)5049.
[3] H. Eshghi, M. Rahimizadeh, M. Hosseini, Monatshefte fur Chemie, 144 (2013) 197.

Chemical characterization of volatile components of *Prangosacaulis* from Iran using MAHD, HD extraction techniques and antioxidative activity ofmethanolic extract

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Microwave assisted hydrodistillation (MAHD) and hydrodistillation (HD) techniques have applied to extract essential oils from aerial parts of aromatic herb of *Prangosacaulis* from west of Iran [1]. It is a highly advanced and homogeneous family, largely used in food preparation, perfumery and medicine. We make appropriate comparisons in term of extraction yields and rates, essential oil composition, and energy consumption. The microwave method offers important advantages over traditional alternatives, shorter isolation times, environmental impact and cleaner features as no residue generation and no water or organic solvent used.

Chemical characterizations of volatile components were investigated by GC/MS. Seventeen components were characterized [2]. The major components of the oils extracted usining HD and MAHD were myrcene (7.60,5.40%) β-pinene (7.85,7.92%) and α – terpinene (5.32, 13.26%) respectively.

The methanolic extract of Prangos acaulis also was examined for free radical scavenging activity. Anti-oxidant activity was examined using 2,2-diphenyl-1-picrylhydrazy l (DPPH) assay [3]. The result indicated the free radical scavenging activity of MeOH extract (M) (IC_{50}=65.7±.0.6 µg/ml) and phenol content of sample (Gallic acid equivalent=129.2±1.1 mg/l).

Referenses

[1] S. Masoudi, Z. Aghjani, M. Yari and A. Rustaiyan, Journal of Essential Oil Research, 11(1999) 767.
[2] M.A. Ferhat, Y. Brahim, J. Smadja and F. Chemat, Journal of ChromatographyA, (2006) 121.
[3] L. Ahmadi, M. Mirza, Journal of Essential Oil Research, 11 (1999) 289.

An synthesis of tetrahydrobenzimidazo[2,1-*b*]quinazolin-1(2*H*)-one using a new ionic Brönsted acid catalyst

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Multi-component reactions (MCRs) are powerful tools in modernmedicinal chemistry, enabling straightforward access to large libraries of structurally related, drug-like compounds and thereby facilitating lead generation. Hence, combined with the use of combinatorial chemistry and high throughput parallel synthesis, such reactions have instituted an ncreasingly valuable approach to drug discovery efforts in recent years[1]. Quinazolinone derivatives have many biological activities such as analgesic, anti-inflammatory, antipyretic, antimicrobial, anticonvulsant, fungicidal, antidepressant and antitumor compounds[2,3].

In this work a newly reported ionic Brönsted acid catalystis used as an efficient and reusable catalyst in the synthesis of tetrahydrobenzimidazo[2,1-*b*]quinazolin-1(2*H*)-ones.The salient advantages of this method are mild reaction conditions, nontoxic and inexpensive catalyst, environmentally benign, high to excellent yields, shorter reaction times(figure 1).

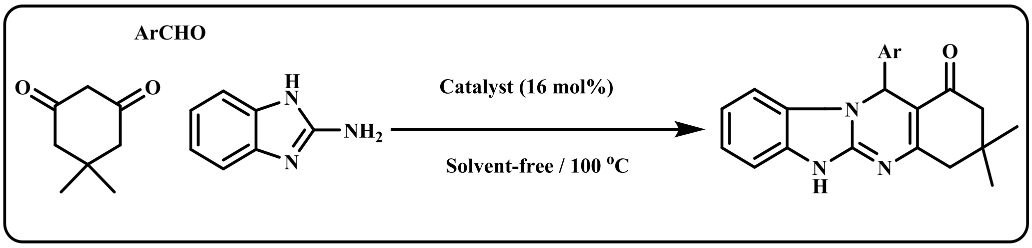

Figure 1. Synthesis of tetrahydrobenzimidazo[2,1-*b*]quinazolin-1(2*H*)-one in the presence of ionic Brönsted acid catalyst.

References

[1] M.M. Heravi, L. Ranjbar, F. Derikvand, B. Alimadadi, H.A.Oskooie, F.F. Bamoharram. Mol Divers, 12 (2008) 181-185.
[2] G. Krishnamurthy, K.V. Jagannath. J. Chem. Sci., 125 (2013) 807-811.
[3] A. Shaabani, E. Farhangi, S. Shaabani. Iran. J. Chem. Chem. Eng., 32 (2013) 3-10.

Synthesis of some pyridooxadiazine from pentaflouropyridine

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Amidoximes compounds were synthesized from reaction of corresponding nitrile compound with hydroxyl amine [1]. Pentafluoropyridine is a very versatile “building block” because, in principle, all five fluorine substituents in pentafluoropyridine could be substituted by nucleophiles. Therefore, potentially, a range of polysubstitiuted systems could be derived from this core molecule by nucleophilic aromatic substitution processes [2]. Furthermore, it is well established1 that, in general, the order of activation towards nucleophilic attack follows the sequence 4-fluorine> 2-fluorine> 3-fluorine [3].

In this project we firstly design an easy, efficient and simple approach for the synthesis of some amidoximes from nitriles under ultrasonic irradiation in short reaction times then the reaction of amidoximes with pentafluoropyridine were investigated. Reaction of some amidoximes with pentafluoropyridine in the presence of K_2CO_3 and in CH_3CN as solvent gave corresponding pyridooxadiazines compounds in good yields. The structure of new heterocyclic compounds were confirmed by ^1H NMR, ^{19}F NMR and ^{13}C NMR spectra.

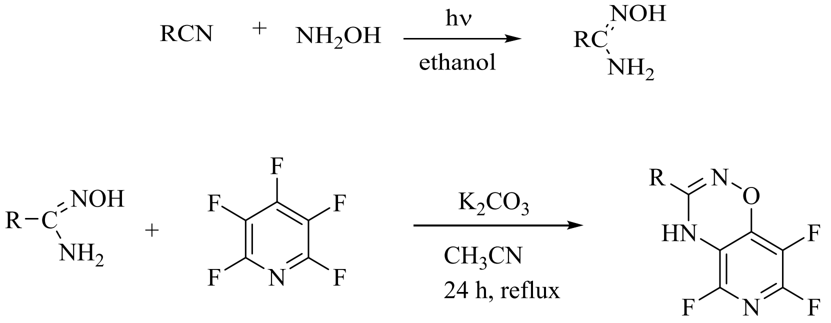

Figure 1. Scheme of the reaction

References

[1] F. Tiemann, "Effect of Hydroxylamine on Nitriles", *J. Chem. Soc.*, 17 (1884)126-129.
[2] R. E. Banks, R. N. Haszeldine, J. V. Latham, I. M. Young. *J. Chem. Soc.*,(1965) 594-597.
[3] J. M. Lehn, J. L. Atwood, J. E. D. Davies, D. D. MacNicol, F. Votgle, "Supramolecular Chemistry", OUP, Oxford., 1 (1996)11-19.

Mild and Efficient Deoxygenationof Sulfoxides to Sulfides with Silica Iodide as new Heterogeneous Reagent

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Reduction of sulfoxides to the corresponding sulfides is a main reaction that is important in both organic synthesis and biological chemistry [1]. Until now,a lot of methods have been developed for the deoxygenation of sulfoxides. In recent years, the use of reagents and catalysts supported on solid supports has received much attention. Silica gel is one of the most extensively used surface material supports for different chemical transformations in organic synthesis [2]. For example, Silica boromide and silica chloride were synthesised and used in reductionof sulfoxides to their sulfids[3][4]. We prepared a new heterogeneous reagent, SiO_2-I, as simple, mild and effective reagent for reduced sulfoxides and converted corresponding sulfides in CCl_4 at room temperature in highyeild. A wide range of diaryl, aryl-alkyl, and dialkylsulfoxidesreducedvery smoothly without any other products. EDX, FT-IR and qualitatively analysis confirmed the presence ofiodide in the heterogeneous reagent SiO_2.I.

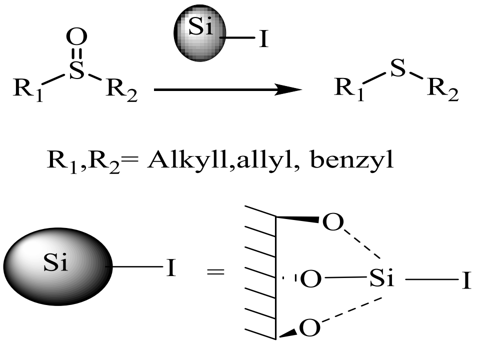

Figure 1. Scheme of the reaction

References

[1] B. W. Yoo, B. R. Yu, and C. M. Yoon, J. Sulfur Chem., 36 (2015) 358–363.
[2] P. Mehtab, M. A. Mohammed, A. L. I. Akhtar, M. Parveen, A. M. Malla, A. Ali, M. Alam, and M. F. Mustafa, Chem. Res. Chinese Univ., 30 (2014) 55–62.
[3] F. Mohanazadeh, H. Veisi, A. Sedrpoushan, M. A. Zolfigol, F. Golmohammad, S. Hemmati, and M. Hashemi, *J.* Sulfur Chem., 35 (2014) 7–13.

Comparison of Steam Distillation and Solvent Free Microwave Extraction Methods of the Analysis of Volatiles Oils of *Bifora testiculata* (L.) Spreng.

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The genus Bifora (Umbelliferae) is represented in the flora of Iran by two species, namely Bifora testiculata(L.)Spreng and *B.radians* M.B.[1]. The aerial parts of Biforatesticulata (syn: coriandrum testiculatum L.) was collected from Mehran, Province of Ilam, in July 2015. The essential oil obtained by steam distillation and solvent free microwave extraction from the stems and leaves of the plant were analyzed by GC and GC/MS.

Forty- three components representing 90.4% of the steam distillation oil and fifty- nine components representing 90.0% of solvent free microwave extraction oil of stems and leaves of B.testiculata were indentified. The main compound in two oils was (E)- 2- dodecenal (35.6% and 19.1%), respectively.Other notable constituents were in steam distillation oil dodecanal (15.6%) and decanal (7.6%) in solvent free microwave extraction oil 4aα, 7α, 7aα nepetalactone (14.0%), citronellol (10.9%), liguloxide (7.9%) and carvacrol (6.4%). The steam distillation oil of *B.* testiculata consisted mainly of aliphatic compounds (78.4%), while the solvent free microwave extraction of the plant was characterized by high amounts of monoterpens (33.4%), sesquiterpens (26.6%) and aliphatic compounds (30.0%).

References

[1] V.Mozaffarian, A Dictionary of Iranian Plants Names, Farhang Moaser publisher, Tehran, Iran(1996) 76.

Chemical Composition of the Essential Oil from Roots of *Bifora testiculata (L.) Spreng.* Obtained by Microwave Extraction Method

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Two species of genus Bifora are found in Iran, namely Bifora testiculata(L.) Spreng. (*Syn: Coriandrum testiculatum* L.) And B.radiansM.B. . B.testiculatais an annual herb with typical aroma growing along the borders of the fields, especially in chalky soils of Central Anatolia [1]. It was reported that B.radians was found to be rich in alkanals and alkenals [2]. Additionally antimicrobial andinsecticidal activity studies were carried out on this species [3].

The present work presents the chemical composition of the essential oil of roots of B.testiculatagrowing wild in Ilam, in July 2015. The yellowish oil were obtained by solvent free microwave extraction method and analyzed by GC and GC/MS.

Thirty- nine components in the root oil of B.testiculatawhich represented about 94.4% of the total oil, were identified. The root oil of the plant consisted of one monoterpene hydrocarbon (0.06%), nine oxygenated monoterpenes (24.9%), four sesquiterpene hydrocarbons (1.4%), four oxygenated sesquiterpenes (8.3%) and 21 non terpenoid compounds (59.7 %). The major components of this oil were (E)-2- dodecenal (31.6%) and thymol (15.5%).

References

[1] V.Mozaffarian, A Dictionary of Iranian Plants Names, Farhang Moaser Publisher, Tehran, Iran(1996) 76.
[2] K .H .C. Baser, B.Demircakmak, N.Ermir, F.Demirci, I.Boydag, Journal of Essential Oil Research, 10 (1998) 451.
[3] B.Ozcelik, S.Kusmenoglu, S.Turkoz, U.Abbasoglu, Pharm. Biol, 42 (2004) 526.

Wetting and Interfacial Behavior of Hydrophobic Ionic Liquid Nanodroplets on Copper Metal Surfaces: A Molecular Dynamics Simulation Investigation

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Quaternary ionic liquids (ILs) based on tetra alkyl ammonium and tetra alkyl phosphonium cations combined with bis(trifluoromethylsulfonyl)imide anion, form hydrophobic ILs, with outstanding physicochemical properties, such as high thermal stability, wide electrochemical window, non-flammability and non-volatility [1].ILs based on these classes of cations have been successfully applied as phase-transfer catalysts, solvents, electrolytes, lubricants and lubricant additives, gas capture agents, coating materials, and chemical sensors [2].Many of these applications require the knowledge of their interfacial behavior, such as wettability and adhesion.Molecular dynamics (MD) simulations method based on classical force fields is a valuable and powerful technique to study solid-liquid interface at an atomistic and molecular level, with the outcome critically comparable with experiments.In this regard, nanodroplets of triethylpentylammoniumbis(trifluoromethylsulfonyl)imide ($[N_{2225}]Tf_2N$) and triethylpentylphosphoniumbis(trifluoromethylsulfonyl)imide ($[P_{2225}]Tf_2N$) ILs were constructed without boundary condition. Four-layered Cu(100) and Cu(111) slabs were constructed in FCC lattice with experimental lattice constant of 3.615 Å.Ionic Liquids droplets were allowed to come into contact with the solid substrates.Equilibration attained after 5ns production run. Periodic boundary conditions were applied in all three directions. All MD simulations were performedusing the DL_POLY program version 2.17 [3]. Energetic contributions and binding energies calculation of ionic nanodroplets on copper surfacesled to the following orderof binding energies: $Cu(100)/[N_{2225}]Tf_2N > Cu(100)/[P_{2225}]Tf_2N > Cu(111)/[N_{2225}]Tf_2N > Cu(111)/[P_{2225}]Tf_2N$.Calculateddensity profiles exhibit pronounced oscillations near the surfaces, implying the layering of molecules. According to the density profiles, orientation of the charged species in all systems near the Cu surfaces follows the order: anion fluorine >anion oxygen > anion nitrogen >cation tail >cation head (N or P).Calculated contact angles of both ionic nanodroplets on Cu(100) and Cu(111) surfaces are lower than 90°. This indicates a favorable liquid-surface interaction. Contact angles on Cu(111) surface are lower than those on Cu(100) surface. This may be an indication of the hydrophobicity difference of these two crystallographicallydifferent copper surfaces.

References

[1] A. Stojanovic, C. Morgenbesser, D. Kogelnig, R. Krachler, B. K. Keppler and A. Kokorin, Ed.; InTech: Shangai, (2011) 657−680.

[2] B. Yu, D. G. Bansal, J. Qu, X. Sun, H. Luo, S. Dai, P. J. Blau, B. G. Bunting , G. Mordukhovich and D. J. Smolenski, *Wear*,289(2012)58–64.

[3] W. Smith, T. R. Forester and I. T. Todorov, J. Mol. Graphics, 14(1996) 136.

Enantiospecific Adsorption of Propranolol Enantiomers on Naturally Chiral Copper Surface: A Molecular Dynamics Simulation Investigation

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Most of the pharmaceutical drugs are chiral and to a large extent marketed as racemates consisting of an equimolar mixture of two enantiomers[1]. Although enantiomers have identical structures, they exhibit differences in biological activities. In order to eliminate or reduce the unwanted enantiomer from the preparation, with the feasibility of finding an optimal therapeutical treatment, much progress in chiral separation and analysis of racemic drugs in pharmaceutical as well as clinical is highly demanding.The general scheme of enantiomeric analysis and separation is based on utility of a chiral substrate. Among many other techniques, chiral metal surfacesare widely used as enantioselective chiral heterogeneous catalysts in producing enantiomerically pure compounds. The subsequent easy separation of metal from the reaction products urges the fundamental understanding of interaction between drugs and metal surfaces. Naturally chiral metal surfaces can yield much higher enantioselectivitiesthan minerals.Propranolol ((*RS*)-1-(1-methylethylamino)-3-(1-naphthyloxy)propan-2-ol) is a nonselective, beta-adrenergic receptor-blocking agent; it specifically competes with beta-adrenergic receptor-stimulating agents for available receptor sites[2]. To examine the feasibility of enantioselective adsorption of enantiomers drugs on naturally chiral metal,we carried out MD simulation adsorption of propranolol enantiomers on chiral Cu(3,1,17)^{S3} and achiral Cu(100) metal surfaces. We analyzed structural and dynamical properties, as well as adsorption energetics and the molecular orientation. Investigation of enatioselective adsorption of propranolol enantiomers on naturally chiral Cu(3,1,17)^{S} and achiral Cu(100) surfaces is quite feasible by molecular dynamic simulation. The fact that R-enantiomer binds more tightly to the Cu(3,1,17)^{S} surface than S-enantiomerby 24.7 kJmol^{-1}, gives the hope for an efficient and practical method useful in drug industries involving specific enantiomers. Thisis under the condition that drug design and advancement is highly dependent on efficient enantiomeric separation. The preferential adsorption of R-propranolol on Cu(3,1,17)^{S} over S-propranolol may roots from specific feature of the molecule having a naphtyl part and a chain part with different tendency for adsorption characteristics of each enantiomer.According to RDF graphs and average bond lengths of propranolol atoms with Cu(3,1,17)^{S} surface, R-propranolol adsorbs via naphtyl group while S-propranolol mainly adsorbs through atoms of chain part. Comparison of the bivarite maps confirms stronger adsorption of R-propranolol enantiomer. The difference in binding energies ofpropranolol enantiomers on naturally chiral Cu(3,1,17)^{S} surface is 24.70 kJmol^{-1}, which larger thanon achiral Cu(100) surface (4.19 kJmol^{-1}) by a factor of 6. Consequently the difference in binding of propranolol enantiomers towards Cu(3,1,17)^{S} surface provides the feasibility of chiral discrimination process.

References

[1] M. S. Lennard, Br. J. clin. Pharmac.,31 (1991) 623.
[2] L. A.Nguyen, H.He, C.Pham-Huy, Int. J. Biomed.Sci., 2 (2006) 85.
[3] Y. Yun, A. J. Gellman, Angew. Chem. Int. Ed., 52 (2013) 3394.

Nano-CuO catalyzed the formation of 4,5-Bis(phenylimino)-2-alkyliminoimidazolidines

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Nitrogen containing heterocyclic systems are of interest because they are key intermediates of natural products [1]. Tetrahydroimidazoles (imidazolidines) display a significant role as intermediates in the nucleotide biosynthesis [2]. Herein, we report that nano-CuO is an efficient catalytic system for guanylation of amines with carbodiimides under mild reaction conditions. A One-Pot method for direct synthesis of 4,5-Bis(phenylimino)-2-alkyliminoimidazolidines **5***via* the reaction ofaniline derivatives**1**,carbodiimides**2**,and*N*,*N*'-diphenyloxalimidoyl dichloride in the presence of CuO-NPs was developed.The structures of products**5**were assigned by IR, ^{1}H NMR, ^{13}C NMR, and mass spectral data. Various features of these transformations will be presented and discussed.

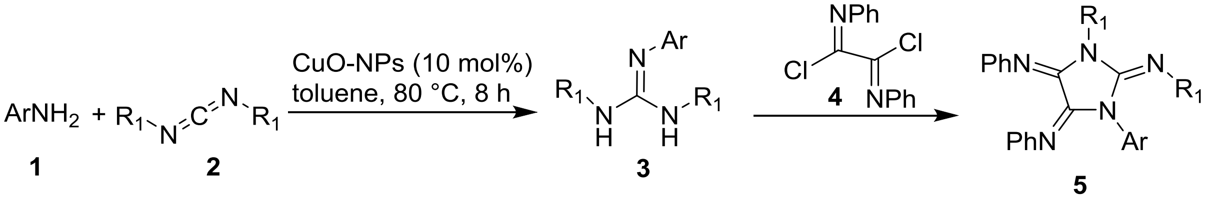

Figure 1. Scheme of the reaction

References

[1] Y. Li, Z. Wu, J. Shi, H. Bu, J. Gu, Y. Pan.Tetrahedron, 70 (2014) 3134.
[2] J. Chang-Fong, K. Benamour, B. Szymonski, F. Thomasson, J. M. Morand, M. Cussac. Chem Pharm. Bull, 48 (2000) 729.

Synthesis of Highly Polarized Carbon-Carbon Double Bonds from Cyanoacetophenone, Isothiocyanates, and Imidoyl Chlorides

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The formation of carbon-heteroatom bond is of interest due to its wide application in organic synthesis and pharmaceutical chemistry. The concept of polarized (or push-pull) olefinic systems has played an important role in organic chemistry for four decades. Substitution of one C-atom of the C=C bond with electron-donating groups and of the other with electron-withdrawing groups diminishes the C=C bond order by charge separation.[1] The polarized structure of the C=C bond is discernible by ^{13}C NMR spectroscopy due to the extreme deshielded position of the alkene C-atom on the donor side and the contrastingly shielded position of the C-atom on the acceptor side of the push-pull alkene. Various aspects of these systems will be presented and discussed.

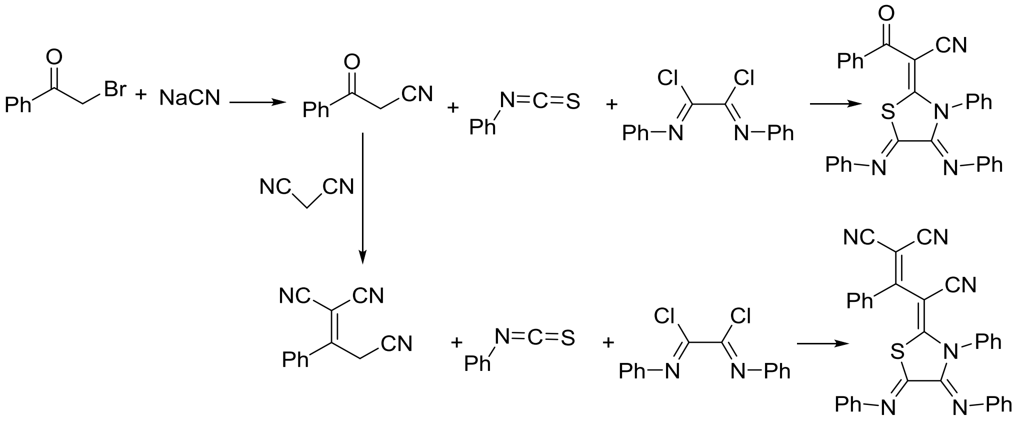

Figure 1.synthesis of push-pull olefines

References

[1] I. Yavari, M. Ghazanfarpour-Darjani, Z. Hossaini, Y. Solgi, S. Ahmadian Helv. Chim. Acta, 94 (2011) 639.
[2] A. R. Sayed Tetrahedron, 69(2013)5293.

Designing of food smart package containing preservative nanoparticles of food and pH indicator for fast determination of food deterioration

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Active packaging has been investigated for more than 40 years. The main purpose of food packaging is to protect the food from microbial and chemical contamination, oxygen, water vapor and light. The type of packaging used therefore has an important role in determining the shelf life of a food. 'Active' packaging does more than simply provide a barrier to outside influences. It can control, and even react to, events taking place inside the package [1]. Active food contact materials absorb or release substances in order to improve the quality of packaged food or to extend its shelf life. Intelligent food contact materials monitor the condition of packaged food or the surrounding environment [2].

In this study,polyethyleneterephthalate (PET)used as the packaging polymer, Eriochrome Black T as PH sensor, nanoparticles of iron oxide as the radical scavenger, copper oxide as the antibacterial, and alpha-tocopherol as the antioxidants food preservatives are stabilized on the packaging polymer. The nanoparticles are characterized by Transmission Electron Microscopy (TEM).This work confirmed that indicator, embedded on polymer, displayed a color change from Amethystine red to blue during release of amines from food which represented food spoilage in the package polymer.

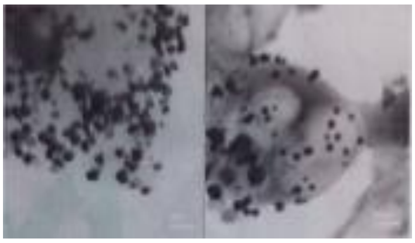

Figure 1. TEM image of nanoparticles

References

[1] J.K. Farkas, The Development of Iron-Based Oxygen Absorbing Systems Used in Food Packaging and Preservation. Ph.D. dissertation, Purdue University, West Lafayette, Indiana, USA (1998).

[2] L. Vermeiren, F. Devlieghere, M. van Beest, N. de Kruijf, J. Debevere, 10 (1999) 77.

Studies on synthesis and physiochemical properties of nanocomposites having CuO nanoparticles modified with vitamin B_1

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Polymeric nanocomposites (NCs) have been intensely investigated dueto the performance improvement achieved when a small amount of NPsare added to a polymer matrix. The remarkable changeon theproperties of polymers due to the addition of inorganic nanoparticles (NPs) is explained by the huge surface area, which increases the interaction between the NPs and the polymer matrix.In this study surface modification of CuO NPs was performed by thiamin (vitamin $B_{1)}$ as a biocompatible modifier to prevent agglomeration and enhance the dispersibility in organic solvents [1]. The process was accomplished under ultrasonic method as a fast and green way [2]. In this project, poly(vinyl chloride)/CuO-VB_1 NCs films were successfully fabricated. For this purpose different amount of modified NPs content (3, 5, 7 wt. %) incorporated to PVC (figure 1).The properties of the NCs were studied by FT-IR, XRD, UV–Vis, FE-SEM, TEM, Mechanical test and TGA techniques.

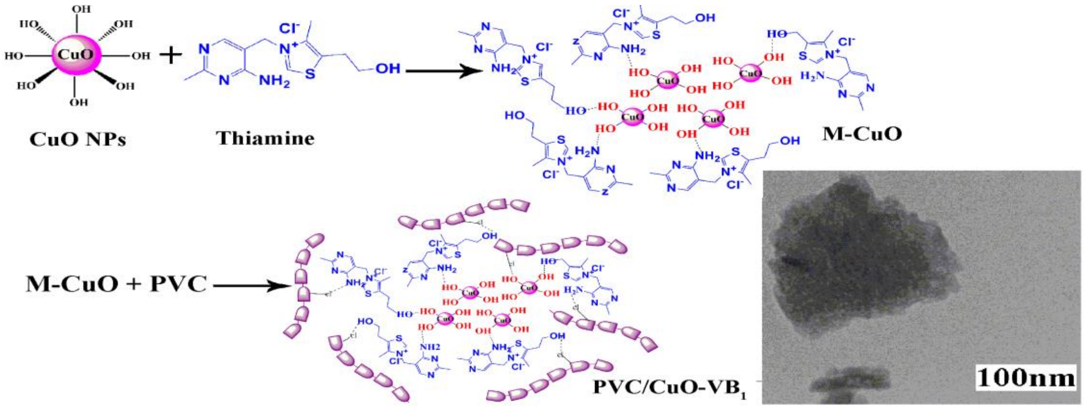

Figure 1. Preparation of PVC/CuO-VB_1 NCs

References

[1] S. Kango, S. Kalia, A. Celli, J. Njuguna, Y. Habibi, R. Kumar. Progress in Polymer Science, 38 (2013) 1232-1261.
[2] S. Gandhi, RHH Subramani, T. Ramakrishnan, A. Sivabalan, V. Dhanalakshmi, MRG Nair, R. Anbarasan. Journal of Materials Science, 45(2010) 1688-1694.

Synthesis of novel *N*,*N*'-diaryl urea derivatives possessing highly substituted imidazoles

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Since the beginning of the 21st century, ureas have staged a remarkable re-emergence inseveral fields of chemistry. The relationship between molecular structure and luminescence of a series of secondary and tertiary *N*,*N*′-diarylureas has been investigated at various temperatures [1]. These properties along with their biological properties [2], provide high performance for these compounds. Imidazoles especially polyaromatic derivatives with light emission characteristics,could also exacerbate this feature. In this work, the required tetraarylimidazoles were prepared by acid catalyzed four-component reactions of aryl aldehydes, diketone (benzil), 1,4-diaminobenzene and ammonium acetate. All synthesized imidazoles containing amino group, were the suitable precursors for reaction with phenylisocyanate to product *N*,*N*'-diaryl ureas.The urea products which were obtained in good yields and by simple work-up, have been characterized by spectroscopic data. The optical absorption and emission properties of the synthesized derivatives were then examined that exhibit a strongly enhanced fluorescence intensity.

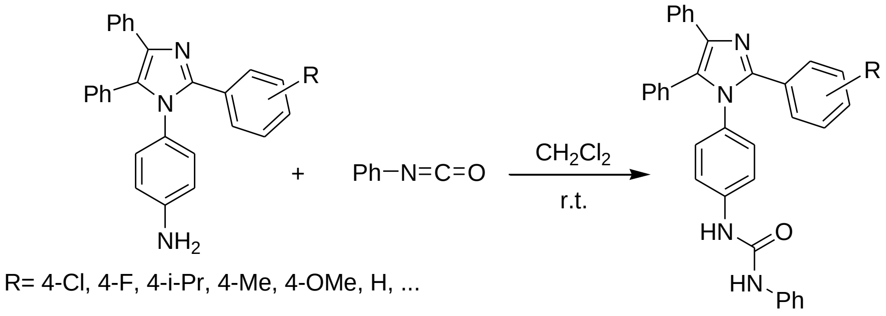

Figure 1. Scheme of the reaction

References

[1] F. D. Lewis, T. L. Kurth and W. Li.,Photochem. Photobiol. Sci.,1 (2002)30–37.
[2] L. D. Luca,Current Medicinal Chemistry, 13 (2006) 1-23.

Azide-Alkyne cyclization reactions for synthesis of new 1,2,3- triazole derivatives possessing highly substituted imidazoles

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Triazole and its derivatives are a group of organic compounds with important biological activities including anti-cancer, anti-AIDS, anti-malaria and anti-bacteria agents. They have also other wide applications in industry, agriculture and especially in the field of drug discovery [1,2]. Hence, the synthesis of these azoles has been in the center of attention formany years.The purpose of this research, is the synthesis of new derivatives of 1,2,3-triazoles containing polysubstituted imidazole rings. The polyaromatic imidazoles were prepared by four-component reactions of aryl aldehydes, diketone (benzil), 4-aminophenol and ammonium acetatein the presence of*p*-toluene sulfonic acid catalyst.All synthesized imidazoles have a hydroxy group whichwere converted into propargyl ether within treatment with propargyl chloride in the presence of a base. Propargyl etherswere used as terminal acetylenes in copper catalysed 1,3-dipolar cycloaddition reactions with benzyl azid to give the target triazole derivatives (figure 1).

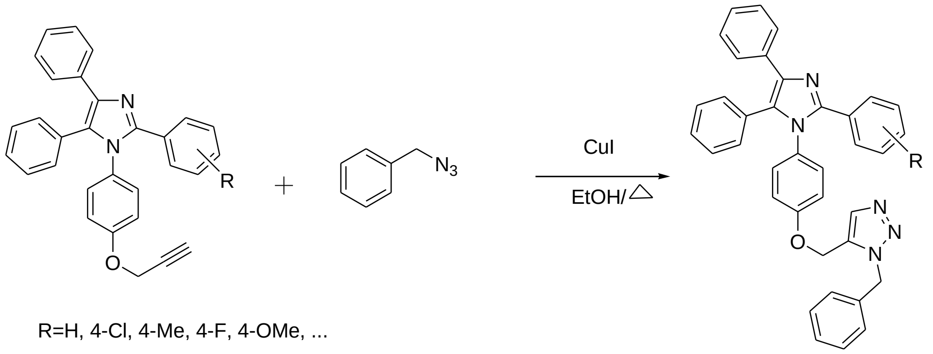

Figure 1. Synthesis of 1,2,3- triazoles containing polysubstituted imidazole rings.

References

[1] M. d. Lourdes, G. F., Pinheiro, L. C. S., Santos-Filho, O. A., Peçanha, M. D. S., Sacramento and C. Q., Machado, Medicinal Chemistry Research, 23 (2014) 1501.
[2] J. Hu, J. R. Lu, Y. Ju. Chem. Asian J., 6 (2011) 2636.

A Divergent Reactivity of a Bis(carbonyl) Ether towards Low-valent Titanium Reductive Coupling Reaction

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In the past few decades, numerous reducing metal reagents such as aluminum, cerium, iron, magnesium, manganese, niobium, samarium, silicon, titanium, vanadium, ytterbium and zirconium in their low valence state were developed extensively to operate as reductive coupling agents to afford vicinal diols or olefins [1].An unparalleled representative of this category is low-valent titanium reagents which have expanded greatly in terms of number and variety of applications for many years [2].

Hitherto we have reportedthe application of the convenient, high throughput titanium-induced reductive coupling cyclization reaction to synthesizea series of monomeric and dimeric stilbenophanes stereoisomers and their counterpart pinacolaphanes, bearing variant length alkyl chains. We persistently utilized Mcmurry coupling reaction by preparation of low valent titanium from TiCl4 and Zn in ethereal solvents as crucial step in ring- closing of the stilbenophanes and their counterpart pinacolaphanesfrom their correspondingbis(carbonyl) ethers[3].

In this context, we discovered under the typical Mcmurry coupling reaction,bis(carbonyl) ether (5) containing single etheric methylene bridge,unlike larger analogues showed a divergent behavior in respect of the products profile. Isolation and characterization of crude reaction mixture led us to compounds (1), (2) and geometric isomers (3). While it was anticipated to obtain monomeric stilbenophanes (4) besides dimers (3), instead compound 1 and 2 were unpredictably detected. These findings reflected the role of alkyl bridge length play in outcome of the reaction, eluding intramolecular coupling whatsoever and preferring less strained structures. Thus herein, in continuation of our investigation concerning the intramolecular and intermolecular coupling of bis(carbonyl) ether series (5) with various size of alkyl etheric linkage under Mcmurry reaction, we have reported the synthesis, isolation and characterization of the compound 1, 2 and 3 by NMR, Mass spectroscopy and X-ray analyses and postulated on the mechanism of the reaction leading to 1 and 2.

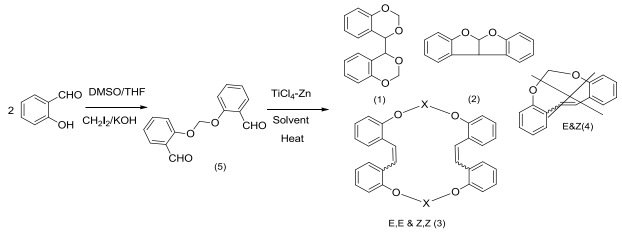

Figure 1. Schem of the reaction.

References

[1] T. Mukaiyama, N. Yoshimura, K. Igarashi, A Kagayama, Tetrahedron 57 (2001) 2499-2506.

[2] M.Ephritikhine, C.Villiers, The McMurry Coupling and Related Reactions, in Modern Carbonyl Olefination (ed T. Takeda), Wiley-VCH Verlag GmbH & Co. KGaA, Weinheim, FRG. (2003)

[3] H. R. Darabi, A. D. Farahania, M. H. Karoueia, K. Aghapoor, R. Firouzia, R. Hergesb, A. R. Mohebbi, C. Näther, .;. Supramol. Chem, 24 (2012) 653–657.

Synthesis and characterization of Pd nanoparticles supported thermo-responsive poly(*N*-isopropylacrylamide–ionic liquid) block copolymers *via* RAFT polymerization and application of Pd nanoparticles supported block copolymers in Heck coupling reaction

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Free radical polymerization is one of the most employed chain growth polymerization technique due to the versatility in terms offunctionality and reaction conditions [1]. Block copolymers are one of the most important polymeric materials in technologicalapplications and theoretical research because of their exceptional properties due to the microphaseseparation [2]. Heck reaction has proved to be a powerful method for C-C bond formation in organic synthesis since it was reported by Heck in 1968 [3].

In the present study, the synthesis and characterization of thermo-responsive PNIPAM–*b*–PIL based on modified vinylpyridine-type ionic liquid*via* RAFT techniqueis reported. At first, CTA, AIBN as initiator and *N*-isopropylacrylamide as monomer were used for the preparation of PNIPAM. Then PNIPAM is used as macro-CTA in order to produce PNIPAM-*b*-polyvinylpyridine. Afterward, PNIPAM-*b*-PIL is synthesized through the reaction of this block copolymer with1,3-propanesultone.These new polymers were characterized by FT-IR and ^{1}H-NMR spectroscopy. Block of PNIPAM-*b*-PIL supported PdNPs is prepared through the reaction with $Pd(OAc)_2$. This efficient catalyst was used for the production of a variety of substituted alkenes at 80 ^{o}Cin short reaction times and good to excellent yields. The strength and dramatic improvement in this work is related to the extremely reusability of the catalyst upon to 20 times and more, using water as a green reaction media and different catalytic behaviors below and upon its lower critical solution temperature (LCST). The catalyst was characterized by ICP, UV-Vis spectrophotometry, X-ray diffraction.

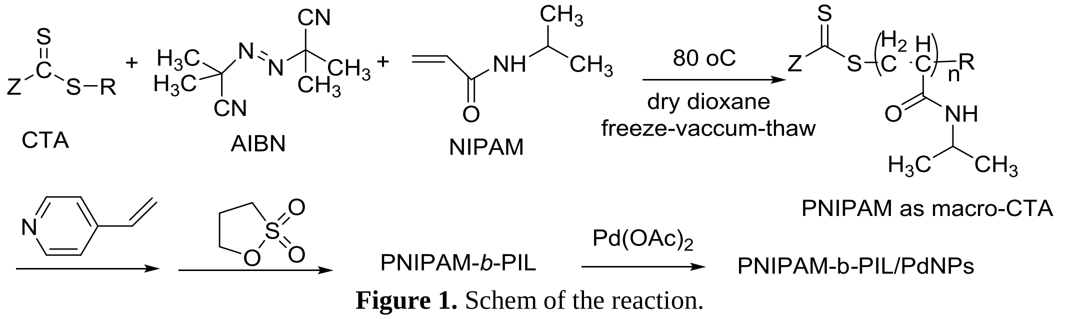

Figure 1. Schem of the reaction.

References

[1] K. Matyjaszewski, T. P. Davis, Future Outlook and Perspectives. Handbook of Radical Polymerization, John Wiley & Sons, Inc.: Hoboken, 2003, pp 895–900.
[2] J.T. Lai, R. Shea, Journal of Polymer Science Part A: Polymer Chemistry 44 (2006) 4298–316.
[3] R. F. Heck, Journal of the American Chemical Society 90 (1968) 5518.

Synthesis of quinoxalines in the presence of kaoline based magnetic nanocatalyst

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Quinoxaline and its derivatives are an important class of heterocycles displaying a broad spectrum of biological activities which have made them privileged structures in combinatorial drug discovery libraries [1]. Quinoxalines play an importantrole as a basic skeleton for the design of a number of antibioticssuch as echinomycin, actinomycin, and leromycin [2]. Quinoxalines synthesis has been done by using of catalysts $CuSO_4.5H_2O$' $Ga(OTf)_3$ [1,2]. Kaolin is very cheap and abundant raw material and has a variety of industrial uses. It is a layered silicate comprised of platelets that are interacting by means of strong hydrogen bonding between them [3].

The SEM of kaoline shows that the particle size is nanometer scale. Nano- kaoline BF_3/ Fe_3O_4as an efficient supported Lewis acid catalyst, was synthesized via reaction of nano-kaoline BF_3 with nano-Fe_3O_4 indichloromethane underultrasonic condition. Nano-kaoline BF_3/ Fe_3O_4 catalyzed reactions of 1,2-phenylen diamines and 1,2-diketones to produce quinoxalines in excellent to quantitative yields. The reactions proceed under solvent free and room temperature conditions. In conclusion, this procedure has many advantages such as mild reactions, easy work- up and good to excellent yields.

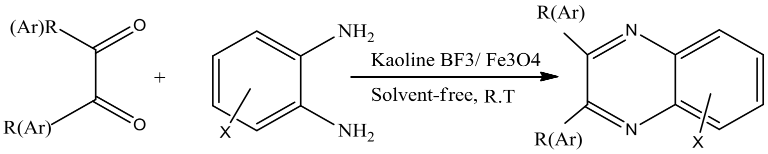

Figure 1. Synthesis of Quinoxalinein the presence of nano-kaoline BF_3/ Fe_3O_4.

References

[1] Heravi, M. M.; Taheri, S.; Bakhtiari, K.; Oskooie, H. A. Catal. Commun., 8(2007) 211.
[2] Heravi, M. M.; Baghernejad, B.; Oskooie, H. A. Tetrahedron Lett.,50 (2009) 767.
[3] Castrillo, P.; Olmos, D.; Sue, H.-J.; González-Benito, J. Compos. Struct.,133 (2015)70.

Copper Iodide nanoparticles supported on magnetic aminomethylpyridine functionalized cellulose: a new heterogeneous and recyclable nanomagnetic catalyst for the facile access to *N*-sulfonylamidines

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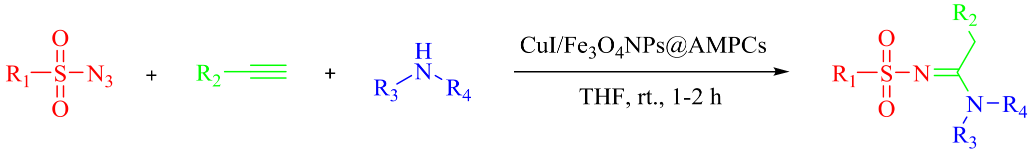
N-sulfonylamidines belong to an important class of organic compounds which include unique structural motifs in wide range of natural products and biologically active molecules.They are not only the essential part of important pharmacophores, antitumor agents and anti-proliferative, but also serve as useful synthetic intermediates and efficient coordinating ligands [1].In recent years, the emphasis and shifting of science and technology is more toward renewable resources and heterogeneous catalytic processes. Thereby natural biopolymers are attractive candidates to employ as modified supports for catalytic applications. Cellulose as one of the most important organic biopolymer, is abundantly available material in higher plants. It has many properties such as hydrophilicity, chirality, biodegradability, broad chemical modifying capacityand also large surface area [2].In this study, we report the synthesis of copper iodide nanoparticles supported on magnetically aminomethylpyridine functionalized cellulose as a heterogeneous and recyclable nanocatalyst. The application of this nanocatalyst was also investigated in the three-componentreactions between sulfonyl azides, terminal alkynes and secondary amines for synthesis of *N*-sulfonylamidines (Figure 1) which are accessible via *in situ* generated sulfonyl ketenimine intermediates.



R_1 = tolyl, phenyl, methyl

R_2 = phenyl, buthyl, penthyl

R_3, R_4 = propyl, benzyl, buthyl, isopropyl,...

4a-p

76-94%

Figure 1. Synthesis of *N*-sulfonylamidinederivatives 4a-p in the presence of CuI/Fe_3O_4NPs@AMPCs.

References

[1] (a) M. Y. Lee, M. H. Kim, J. Kim, S. H. Kim, B. T. Kim, I. H. Jeong, S. Chang, S. H. Kim and S. Y. Chang, Bioorganic Med. Chem. Lett., 20 (2010) 541; (b) Z.-L. Song, H.-L. Chen, Y.-H. Wang, M. Goto, W.-J. Gao, P.-L. Cheng, S. L. Morris-Natschke, Y.-Q. Liu, G.-X. Zhu, M.-J. Wang and K.-H. Lee, Bioorg. Med. Chem. Lett., 25 (2015) 2690; (c) T. D. Suja, K. V. L. Divya, L. V. Naik, A. R. Kumar and A. Kamal, Bioorg. Med. Chem. Lett., 26 (2016) 2072.

[2] W. Z. Yuan, J. Y. Yuan, F. B. Zhang and X. M. Xie, Biomacromolecules,8 (2007) 1101; H.-Y. Yu, G.-Y. Chen, Y.-B. Wang and J.-M. Yao, Cellulose, 22 (2015) 261.

Palladium nanoparticles supported on magnetic supramolecular ionic liquid functionalized cellulose: a novel and efficient nanocatalyst for Suzuki cross-coupling in water

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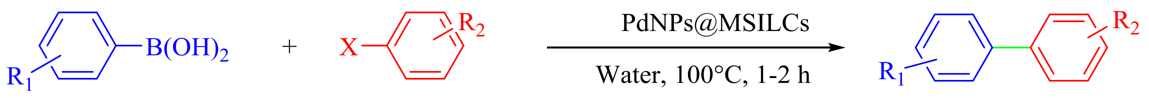
Suzuki cross-coupling represents the most popular method for production of unsymmetrical biaryls because of the friendly properties of organoboronic acids, e.g. non-toxicity, air/moisture stability and tolerance of a variety of functional groups [1]. Industrial applications have become a major concern in further development of this technique. In this context, the use of heterogeneous palladium catalysts has attracted increasing attention, because of the drawbacks of homogeneous transition metal catalysis, such as tedious catalyst separation processes, loss of expensive noble metal and residual metal impurities in the products. Therefore, a variety of heterogeneous palladium catalysts have been reported for Suzuki coupling such as commercially available Pd/C [2]. Cellulose is a naturally occurring biopolymer abundantly available in nature and serves as a bio-compatible support for the catalysts [3].In this work,we report a successful synthesis of a new class of the heterogeneous Palladium nano-particles supported on magnetic ionic liquid functionalized cellulose (PdNPs@MSILCs) and its applications in Suzuki cross- couplings in water as a green solvent (Figure 1).



R1= Ph, H, ...

R_2= $N(Me)_2$, Me, H, ...

X= I, Br

4a-V

92-99%

Figure 1. Suzuki cross-couplings of halobenzenes and boronic acids in the presence of PdNPs@MSILCs.

References

[1] (a) N. Miyaura, A. Suzuki, Chem. Rev. 95 (1995) 2457; (b) A. Suzuki, Angew. Chem. Int. Ed. 50 (2011) 6722; (c) C. C. C. Johansson Seechurn, M. O. Kitching, T. J. Colacot, V. Snieckus, Angew. Chem. Int. Ed. 51 (2012) 5062; (d) A. V. Dubey and A. V. Kumar. RSC Adv., 6(2016) 46864; (e) A. Ghorbani-Choghamarani and M. Norouzi. New J. Chem., (2016),

[2] (a) H. Li, C. C. C. Johansson Seechurn, T. J. Colacot, ACS Catal. 2 (2012) 1147. (b) M. Pagliaro, V. Pandarus, R. Ciriminna, F. Béland, P. D. Carà, Chem. Cat. Chem. 4 (2012) 432. (c) W. Chu, X. Li, Y. Hou, H. Wang, H. Li, X. Yuan, Z. Sun, Appl.Organometal. Chem. 26 (2012) 478.

[3] S. Keshipour, S. Shojaei and A. Shaabani, Cellulose, 20 (2013) 973.

TiCl$_4$/nano-cellulose: A biodegradable and eco-friendly bio-based catalyst for One-Pot synthesis of 4*H*-pyrimido[2,1-*b*]benzothiazole derivatives

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The synthesis of pyrimido[2,1-*b*]benzothiazole derivatives has been considered of greatinterest to organic chemists because oftheir potent and significant pharmacological activities.[1]In view of the importance of pyrimido[2,1-*b*]benzothiazoles, the development of effective strategies for the synthesis of these fused heterocyclic compounds will be interesting in both organic synthesis and medicinal chemistry. A common synthetic approach to pyrimido[2,1-*b*]benzothiazole derivatives involves three component condensation of 2-amino benzothiazole, aldehydes and β-ketoesters [2, 3].

Considering the new trends of science and technology towards using natural materials such as cellulose, the research efforts on green and eco-friendly methods have become popular and desirable. Cellulose is one of the most abundant natural carbon based biopolymers containing free OH groups with nucleophilic character.In this work, we have investigated about preparation of nano-cellulose by sulfuric acid hydrolysis of cotton (purest, cheap and readily available source of cellulose) and synthesis of TiCl$_4$/nano-cellulose by bonding TiCl$_4$ to OH groups of D-glucose units in nano-cellulose. TiCl$_4$/nano-cellulose was characterized by FT-IR, FESEM, XRF, EDX and XRD techniques and used as a new, biodegradable, inexpensive and eco-friendly bio-based catalyst for One-Pot synthesis of pyrimido[2,1-*b*]benzothiazoles *via* three component reaction of aldehydes, ethyl acetoacetate and 2-amino benzothiazole under thermal condition (Figure 1).

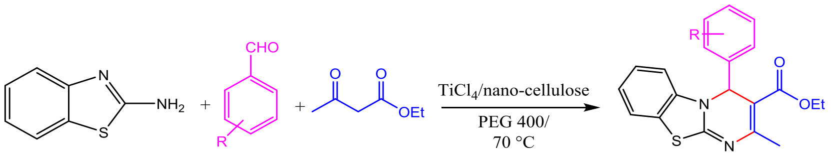

Figure 1. Synthesis of 4*H*-pyrimido[2,1-*b*]benzothiazoles in the presence of TiCl$_4$/nano-cellulose at 70 °C.

References

[1] Gabr, M. T.; El-Gohary, N. S.; El-Bendary, E. R.; El-Kerdawy, M. M. Eur. J. Med. Chem.85 (2014) 576.
[2] Nagarapu, L.; Gaikwad, H. K.; Palem, J. D ;.Venkatesh, R.; Bantu, R.; Sridhar, B. Synthetic Commun.43 (2013) 93.
[3] Sahu, P. K.; Sahu, P .K.; Gupta, S. K.; Agarwal, D. D. Ind. Eng. Chem. Res.53 (2014) 2085.

An efficient synthesis of 5-substituted 1*H*-tetrazoles in the presence of nano-$Fe_3O_4@SiO_2.SnCl_4$

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Tetrazoles are an important category of nitrogen containing heterocycles with a wide range of biological properties such as antimicrobial, antibacterial, antifungal, analgestic,anti-inflammatory, antiviral, and anti-cancer activities. Tetrazoles are widely used in many drugs such as sartan family drugs(Candesartan and Losartan) and antihistaminic drugs(Pemiroplast and Pranlukast) information recording systems, highdensityenergy materials, antifoggants in photography,ligands in coordinationchemistry , propellants and explosives .The synthesis of 5-substituted 1*H*-tetrazoles was first reported by Hantzsch and Vagt in 1901, which is based on [3,2] cycloaddition of azide with organic nitriles and its chemistry has been developed from 1980.

Generally, 5-substituted 1*H*-tetrazoles are prepared by the addition of azides to nitriles but some of the methods suffer from usual drawbacks such as long reaction time, expensive reagents, stoichiometric amounts of catalysts, strong Lewis acids, low yield and water sensitivity. Magnetic nanocatalyst$Fe_3O_4@SiO_2.SnCl_4$ is an effective heterogeneous catalyst for the [2,3]-cycloaddition of sodium azide with nitriles to afford 5-substituted 1*H*-tetrazoles in good yields.

A simple, safe and efficient method is developed for the synthesis of 5-substituted 1*H*-tetrazoles. The catalyst is reusable up to three cycles with consistent activity. The cost effectiveness and easy availability of the catalyst, simple method, excellent yield and easy work-up are the additional advantages of this protocol.

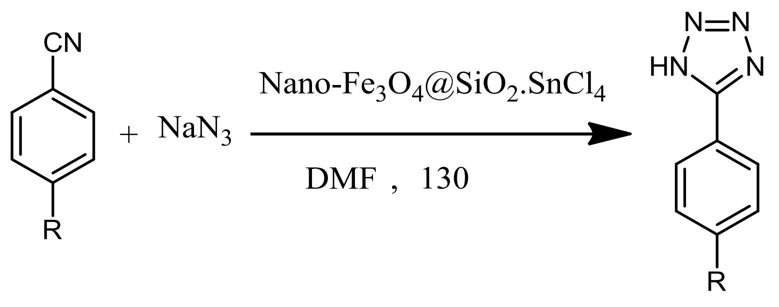

Figure 1. Scheme of the reaction

Reference

[1] K. Rama, S. Vishal, A. Alka., e. ComptesRendusChimie, (2016).
[2] L. Kantam, M., K. B. Kumar, and C. Sridhar., Advanced Synthesis & Catalysis, 347(2005) 1212-1214.

Chemical Constituents of the Essential Oil from Stems of *Salvia oligophylla Auch. ex Benth*. Which is Endemic to Iran

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The genus *Salvia* with over 900 species is probably the largestmember of the family Lamiacea and is found in both subtropical and temperate parts of the world. The two largest centers of the genus are in America and in South-West Asia. Fifty eight annual or perennial species of the genus are found in Iran of which 17 are endemic [1].

Some *Salvia* species are used in folk medicine for the treatment of asthma, eczema, psoriasis and tuberculosis. The antibacterial, antituberculous and antiphlogisticactivities of the constituents of *Salvia* species are well established [2]. The composition of volatile compounds is known for a number of species.

Water distilled oil obtained from the aerial parts of *S.sclareopsis* and *S.verbascifolia* have been the subject of our previous studies. Both oils were rich in β-caryophyllene (22.5% and 18.5%) and germacrene D (16.5% and 34.1%), respectively [3].

The stems of *S.oligophylla*, which is endemic to Iran, was collected from Ilam, in July 2015. The oil obtained by solvent free microwave extraction (SFME) method and analyzed by GC and GC/MS.

Thirty –three compounds in the stem oil of *S.oligophylla*, which represented about 86.4% of the total oil were indentified. The oil of *S.oligophylla* consisted of one oxygenated monoterpene (0.2%), twelve sesquiterpene hydrocarbons (26.3%), fifteen oxygenated sesquiterpenes (49.7%), one aliphatic compound (0.6%) and four diterpenes (9.6%). The major components of this oil were spathulenol (27.7%) and caryophyllene oxide (11.9%). Other notable constituents were β-caryophyllene (8.8%), sclareoloxide (6.9%) and bicyclogermacrene (6.3%). As can be seen from the above information the stem oil of *S.oligophylla* was characterized by high amounts of sesquiterpenes (76.0%).

References

[1] V. Mozaffarian, A Dictionary of Iranian Plant Name. Farhang Moaser Publisher. Tehran (1996)479 .
[2] Z. Abravesh, M.B.Rezaee, F. Ashrafi, Iranian. J. Med. Aromat. Plants Res, 20 (2005) 457.
[3] M.Jamzad, A. Rustaiyan, S. Masoudi, Z.jamzad, M.Yari, J. Essent.Oil Res, 21 (2006) 19.

Chemical Composition of the Essential Oil from Leaves of *Salvia oligophylla Aunch.exBenth.*from Iran

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The genus *Salvia* is the largest member of the familyLamiaceaewhichcomprises about 1000 world wide distributed species. In flora ofIran,the genus is represented by 58 species which 17 are endemic[1].Invitro pharmacologicalinvestigationsshowedits antioxidant, antibacterial, antifungal, antiviral, cytotoxic, neuroprotective, antiinflammatory, and tumorigenesis preventing as well as ecological significance such as pest-toxicand repellent and other activities [2]. Aerial parts of *Salvia* species usually contain flavonoids and triterpenoids as wellas essential oils with volatilecompounds such as monoterpenes,while diterpenoids are the main compounds in roots.

The leaves of *S.oligophylla*, which is endemic to Iran, was collected during the flowering stage from Ilam, in July 2015.The oil obtained by solvent freemicrowave extraction method and analyzed by GC and GC/MS.

Fifty constituents representing 96.2% of the total components in the oil of *S.oligophylla* were characterized byspathulenal (19.8%), β-caryophyllene (17.3%) and bicyclogermacrene (13.4%) as the main compounds.Thus,the oil of the plant consists of eight monoterpene hydrocarbons (10.9%), eight oxygenated monoterpenes (2.8%), fifteen sesquiterpene hydrocarbons (42.6%), fifteen oxygenated sesquiterpenes (34.7%),two diterpenes (4.6%) and two aliphaticcompounds(0.6%).

Previously we studied the essential oil of *S.chloroleuca*, which containedmainly bicycle-germacrene(17.0%), germacrene D (15.7%) and β-caryophyllene (11.4%) [3].

Refrences

[1] V. Mozaffarian, a Dictionary of Iranian Plant Name. Farhang Moaser Publisher, Tehran, Iran (1996)479.
[2] I. E.Orhan, F.S. Senol,N.Ozturk, G.Akaydin, B. Senser,FoodChem,132(2012)1360.
[3] M.A.Khalilzadeh, A. Esmaeili, A. Rustayan, B.Eslami,S.Masoudi, Chemistry of Natural Compounds, 46(2011)985.

Synthesis of 2-amino-4-substituted-1,4-dihydrobenzo[4,5]imidazolo[1,2-a]pyrimidine-3-carbonitriles

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Pyrimidinobenzimidazoles possess antimicrobial activity, molluscidal activities, antidiabetic, herbicidal activity, platelet anti-aggregant antiulcer activity, DNA-gyrase inhibitors and anti-inflammatory activities as well as anticancer efficacy.They can play the role of antagonists of the paralyzing action of antidiabetic activity and are important core motifs in a broad range of biologically active compounds that are frequently used in pharmaceutical and drug research, agricultural science, and dye industry [1].

In Thisstudy piperazine-1,4-diium hydrogen sulfate as a new Bronsted acidic catalyst is used for an environment-friendly three-component condensation of 2-aminobenzimidazole, an aldehyde and malononitrile, to afford the corresponding pyrimidine-based annulated di- and triheterocyclic ring systems [2].This method show eco friendly character by elimination of solvent.The other noticeable benefits of this procedure are excellent yields, short reaction times, mild reaction conditions, use of available and inexpensive materials and simple work-up procedures.

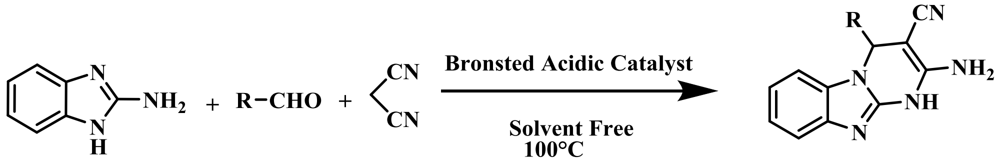

Figure 1. Synthesis of 2-amino-4-substituted-1,4-dihydrobenzo[4,5]imidazolo[1,2-a]pyrimidine-3-carbonitriles..

References

[1] M.V. Reddy, J. Oh. Y.T. Jeong. *C. R. Chimie*., 17 (2014) 484–489.
[2] A. Shaabani, A. Rahmati, A.H. Rezayan, M. Darvishi, Z. Badri, A. Sarvari. *QSAR Comb. Sci.*, 26(2007) 973 – 979.

Comparison of the Essential Oils from Leaves and Flowers of *Artemisia marschalliana Sprangel.* From Iran

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Artemisia (family Asteraceae) is a genus of small herbs or shrubs found in northern temperate regions. Thirty-four species of the genus are found in Iran of which two are endemic: A.melanolepis Boiss. And *A.kermansis* Podl [1]. The genus Artemisia has been investigated chemically and acetylenic compounds, flavonoids, cumarins and terpenoids, especially sesquiterpene lactones, have been reported [2].

Previously we reported the essential oils from the aerials parts, stem, leaf and flower of Artemisiachamaemelifolia. Menthyl acetate (26.5%, 22.0%, 20.5%, and 20.5%) and (Z)-nerolidol (20.8%, 26.3%, 14.7% and 18.1%) were the main constituents in the aerial parts, stem, leaf and flower oils, respectively [3].

The aim of our study is to identify the constituents of the essential oils of leaves and flowers of A.marschalliana, growing wild in East Azarbaijan, Iran, in July 2015. The oils were obtained by solvent free microwave extraction and analyzed by GC and GC/MS.

Thirty-one components representing 91.6% and twenty-nine constituents representing 97.3% were identified in the leaf and flower oils of A.marschalliana, respectively. The major components of both oils were spathulenol (27.7% and 24.7%), 2-propenoic acid-2-ethyl hexyl ester (11.2% and 17.3%) and bicyclogermacrene (9.2% and 10.0%), respectively and other notable components were caryophyllene oxide (8.8% and 7.7%) and germacrene D (5.1% and 9.7%), respectively.

In both oils sesquiterpenes (72.2% and 69.8%) predominated over monoterpenes (0.9% and 3.7%) and aliphatic compounds (21.5% and 14.0%), respectively.

References

[1] V.Mozaffarian, A Dictionary of Iranian Plants Names, Farhang Moaser Publishing, Tehran, Iran,(1996) 57.
[2] J.A.Marco, J.F.Sanz, F.Sancenon, A.Rustaiyan, M.Saberi. Phytochemistry, 32 (1993) 460.
[3] S. Masoudi, A.Rustaiyan, M.Vahedi, Natural Product Communication, 7 (2012) 1519.

A simple, straightforward, and environmentally benign synthesis of quinazolinone derivatives by DABCO-based ionic liquid

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DABCO-Based ionic liquid was utilized for the preparation of quinazolinone derivatives in the expeditious procedures. These methods involve three-component reaction between aldehydes, *β*-diketones, and 3-amino-1,2,4-triazole or 2-aminobenzimidazole in present of 1,4-disulfo-1,4-diazabicyclo[2.2.2]octane-1,4- diium dihydrogen sulfate ([DABCO]$(SO_3H)_2(HSO_4)_2$) as reusable and economical catalyst at 100 °C. This method also show eco-friendly character by elimination of solvent. The other noticeable benefits of this procedure are excellent yields, short reaction times, mild reaction conditions, use of available and inexpensive materials and simple work-up procedures [1, 2].

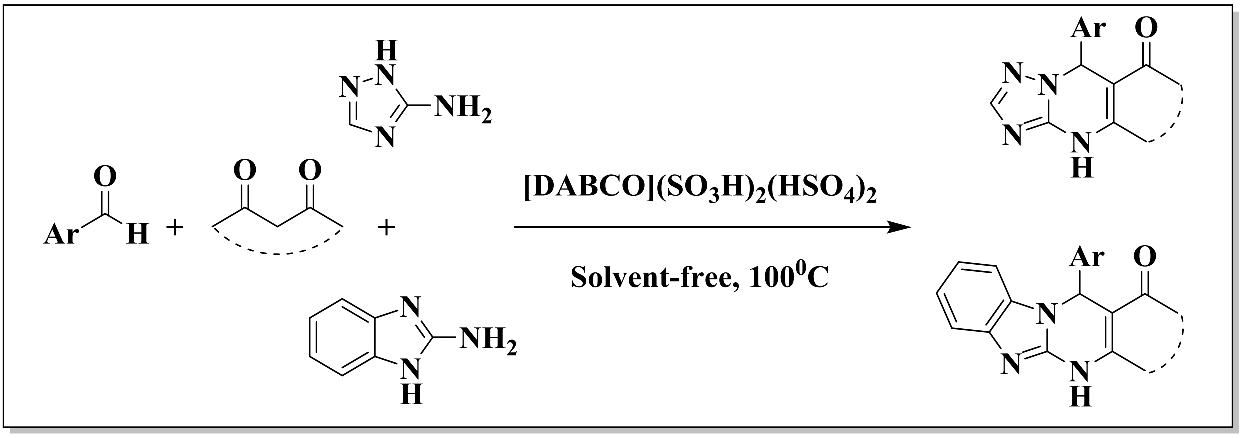

Figure 1. Synthesis of benzimidazoquinazolinone derivativesusingof the [DABCO]$(HSO_3)_2(HSO_4)_2$.

References

[1] E. M. Gordon, R. W. Barret, W. I. Dower, S. P. Fodor, M. A. Gallop, J. Med. Chem., 37 (1994) 1385.
[2] M. A. Gallop, R. W. Barret, W. J. Dower, S. P. Fodor, E. M. Gordon, J. Med. Chem., 37 (1994) 1233.

Synthesis of benzofuran derivatives via ionic liquids

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Benzofuran exist in various natural and synthesized products. Here, some of benzofuran derivatives is prepared *via*ionic liquid. α-halo ketones and different 2-hydroxy aldehydes were mixed in ionic liquid as solvent at temperature. High yield of product, easy work-up and ability of ionic liquid recycling are of the most advantages of this study[1].

We synthesis benzofuran derivatives from o-hydroxyacetophenone and salicylaldehydeand ethyl bromoacetate in K_2CO_3 and ionic liquid [hmim] Clattemperature.

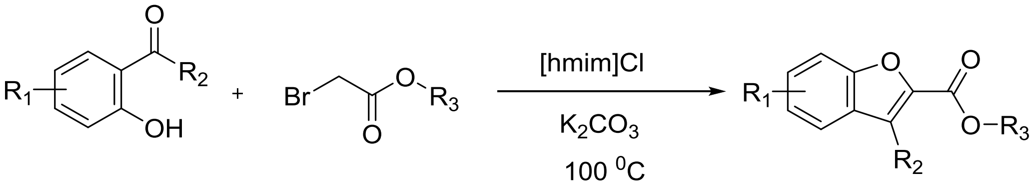

Figure 1. Schem of the reaction.

Also, we synthesis benzofuran derivatives from reaction of salicylaldehydes with diverse phenacyl bromide under the action of potassium carbonate in ionic liquid [hmim]Cl as solvent at temperature of 100 ^{O}C to yield substituted benzofuran derivatives.

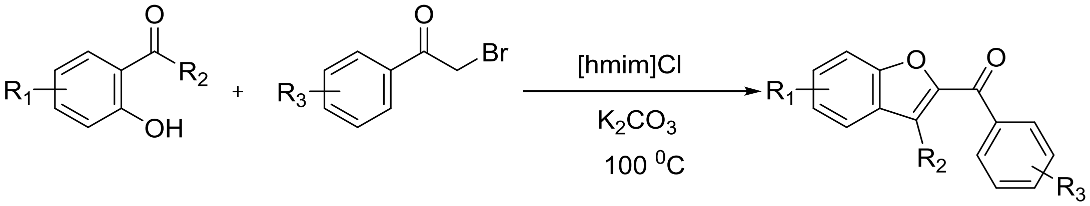

Figure 2. Schem of the reaction.

References

[1] J. Liu,Ch.Mi,X. Tang,Y. Cao,Z. Li,Res ChemIntermed, 40 (2014) 2083.

Comparison of the Essential Oils from Leaves and Stems of *Ferula oopoda (Boiss & Buhse) Boiss*. Growing Wild in Iran

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The gerus Ferula, includes about 170 species occurring from central Asia westward throughout the Mediterranean region to northern Africa.The flora of Iran comprises 30 species of Ferula of which 15 are endemic [1].The Ferula genus has been found to be a rich source of gum-resin.The resin enjoys a reputation as a folklore medicine. It is considered to be a sedative, carminative, antispasmodic digestive expectorant, laxative, analgestic, anthelminitc, antiseptic and a diuretic in its properties [2].Only a few studies have reported the chemical composition of Ferula essential oils. A water distilled oil obtained from the aerial parts of F.ovina, has been the subject of our previous studies. F.ovina oil contained α-pinene (50%) and limonene (11.5%) were the major components [3].

The aim of our study is to identify the constituents of the essential oils of leaves and stems of F.oopoda, collected from Ilam, Iran in July 2015. The oils were obtained by solvent free microwave extraction method and analyzed by GC and GC/MS.Thirty-three components representing 93.9% and thirty-one constituents representing 86.4% were identified in the leaf and stem oils of F.oopoda, respectively. Spathulenol (17.7%), β-eudesmol (11.4%) and β-caryophyllene (10.2%) were the major components in the leaf oil of the plant whereas bornyl acetate (26.0%) was the main component in the stem oil. Other notable components were caryophylene oxide (7.7%) in leaf oil and β-eudesmol (9.8%) and limonene (8.6%) in stem oil of the plant.The leaf oil of F.oopoda was characterized by large amounts of sesquiterpenes (74.2%) while in the stem oil monoterpenes (63.4%) predominated over sesquiterpenes.

References

[1] V. Mozaffarian, A Dictionary of Iranian Plant Names, Farhang Moaser Publisher, Tehran, Iran (1996) 229.
[2] D.Eigner, D.Scholz, Pharmazie, 19 (1990) 141.
[3] B.Rahmani, N.Zabarjad, N.Masnabadi, S.Masoudi, ARustaiyan, J. Essent. Oil Res., 20 (2008) 232.

Chemical Composition of the Essential Oil from Stems of *Artemisia marschalliana Sprengel.* Obtained by Microwave Extraction.

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The genus Artemisia is the largest and most distributed genera within the family Asteracea. Thirty-four species of the genus are found in Iran, of which two are endemic: A.melanolepis Boiss. And A.kermansis Podl [1]. Many members of the genus Artemisiaare aromatic plants. Many Artemisia species are distributed in Europe, Asia, and North America. Artemisia species are well known for their volatile oil that is used in the food and pharmaceutical industries and in folk medicine to treat gastrointestinal diseases [2].

The chemical composition of essential oils from various Artemisia spp. have been analyzed in previous studies. Previously we reported the essential oil from the aerial parts of A.turcomanica. 1,8-Cineol (5.5%), spathulenol (15.2%), camphor (14.8%), santolina alcohol (14.6%) and trans-β- terpineol (11.6%) were the main constituents [3].

The aim of our study is to identify the constituents of the essential oils of leaves and flowers of A.marschalliana, growing wild in East Azarbaijan, Iran, in July 2015. The oils were obtained by solvent free microwave extraction and analyzed by GC and GC/MS.The stems of Artemisia marschalliana was collected from East Azarbaijan, Iran, in July 2015. The oil was obtained by solvent free microwave extraction and analyzed by GC and GC/MS.Fourteen constituents, representing 95.3% of the total components in the oil of A.marschalliana were identified. The oil was characterized by large amounts of aliphatic hydrocarbons (68.8%) with dodecane (41.4%), tridecane (12.4%) and undecane (11.5%) being the major constituents. The sesquiterpenes amounted to (18.0%) with spathulenol (13.9%) being the important one. In the oil of the plant we couldn’t identify any monoterpene.

References

[1] V.Mozaffarian, A Dictionary of Iranian Plants Names, Farhang Moaser Publishing, Tehran, Iran (1996) 57.
[2] J.A.Marco, J.F.Sanz, F.Sancenon, A.Rustaiyan, M.Saberi. Phytochemistry, 32 (1993) 460.
[3] S. Masoudi, A.Rustaiyan, M.Vahedi, Natural Product Communication, 7 (2012) 1519.

Volatile Constituents of the Flower of *Ferula oopoda (Boiss & Buhse) Boiss.* Obtained by Solvent Free Microwave Extraction

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The genus Ferula, which belongs to the Umbelliferae family, is widespread in the mediterranian area and Central Asia.The flora of Iran comprises 30 species of Ferula of which 15 are endemic [1].The resins of the plants have been used in China as a remedy for malaria and dysentery and also as an insecticide.Toxicity in cattle due to Ferula is well known as ferulosis, which is a hemorrhagic disease caused by F.communis and many other Ferula species, mostly due to their 4-hydroxylated and phenylated coumarins [2].The chemical composition of the oil of F.latisecta have been the subject of our previous studies. (Z)-Ocimenone (32.4%), (E)-ocimenone (20.3%) and cis-pinocarvone (11.4%) were the main constituents of this oil [3].

The present work presents the chemical composition of the essential oil of flower of F.oopoda growing wild in Ilam in July 2015.The yellowish oil were obtained by solvent free microwave extraction and analyzed by GC and GC/MS.Forty-one components in the flower oil of F.oopoda, which representing 92.6% of the total oil, were identified.The flower oil of F.oopoda consisted of thirteen monoterpene hydrocarbons (67.8%), seventeen oxygenated monoterpenes (18.2%), seven sesquiterpene hydrocarbons (3.4%), two oxygenated sesquiterpenes (2.3%) and one aliphatic compound (0.9%). The major components of this oil were limonene (17.7%) and α-phellandrene (10.0%). Other notable constituents were δ-3-carene (8.3%), myrcene (6.4%) and bornyl acetate (6.1%). As can be seen from the above information, in the flower oil of the plant monoterpenes (86.0%), predominated over sesquiterpenes (5.7%).

Rererences

[1] V. Mozaffarian, A Dictionary of Iranian Plant Names, Farhang Moaser Publisher, Tehran, Iran (1996) 229.
[2] S.Tagliapietka, M.Aragno, G.Ugazio, G.M.Nano, Res. Commun. Chem. Pathol. Pharmac., 66 (1989) 333.
[3] Z.Habibi, P.Salehi, M.Yousefi, Y.Hejazi, S.Masoudi, A.Rustaiyan, Chemistry of Natural Compounds, 42(2006) 689.

Chemical Constituents of the Essential Oil of *Salvia Persepolitana Boiss.* Obtained by Steam Distillation

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Salvia is a fascinating plant genus and one of the wide spread members of the Labiatae family, which comprises about 900 herbs and shrubs, growing in the temperate and warmer zone of the world. Fifty eight are described in the flora of Iran, among which 17 are endemic [1]. Some of these species feature prominently in the pharmacopoeias of many countries through out the world [2]. The volatile oils of Salvia are chemically complex mixture, often containing in excess of 100 individual components. They have low boiling points and can be recovered from the plant tissues by steam or hydrodistillation, In addition to flovoring foods, volatile oils can also act as anti-oxidants and preservatives against food spoilage, while a broad range of applications in aromatherapy and health care has been observed. Previously we studied the essential oil of S.brachysiphon which contained β-caryophyllene (28.1%), α-pinene (20.6%), limonene (11.5%) and β- pinene (10.6%) was found to be the major constituents [3].

The leaves and steams of S.persepolitana, which is endemic to Iran, growing wild in Ilam, in July 2015. The oil obtained by steam distillation and analysed by GC and GC/MS.Thirty five components representing 84.4% of steam distillation oil from leaves and steams of S. persepolitana were identified.The main compounds of the oil were 6, 10, 14-trimethyl 2-pentadecanone (20.7%) and spathulenol (13.5%). Other notable constituents were caryophyllene oxide (8.1%) and phytol (5.4%). The oil of the plant was characterized by high amounts of sesquiterpenes (35.8%) and aliphatic compounds (27.7%). The monoterpenes fraction was relatively small, representing (7.5%) of the total oil.

References

[1] V.Mozaffarian.A Dictionary of Iranian Plant Name, Farhang Moaser Publisher, Tehran, Iran (1996) 479.
[2] H. Hitikoto, S. Morozumi, T. Wauke, S. Sakai, H. Kurata, Appl. Environ. Microbiol, 39 (1980) 818.
[3] M. Jamzad, A. Rustaiyan, S. Masoudi, Z. Jamzad, M.Yari, J.Essent. Oil Res., 21 (2006) 19.

Chemical Composition of the Essential Oil of *Salvia Persepolitana Boiss*. Obtained by Solvent Free Microwave Extraction

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Salvia the largest genus of the family Lamiacea, includes about 900 species widespread all over the world. Sixty species are found in Iran, seventeen of which are endemic [1]. Some of these species are used as medicinal, aromatic and ornamental plants. Salviaofficinalis L. is one of the most widespread species and since ancient time, has been used in the treatment of various disorders, such as tuberculosis, psoriasis and seborrheic eczema.

Previous chemical investigations on different species of Salvia have shown the presence of flavonoids, diterpeniods and even the rare sesterterpenes [2].Theleaves and stems of Salvia persepolitana, which is endemic to Iran, was collected from Mehran, Province of Ilam, in July 2015. The essential oil obtained by solvent free microwave extraction (SFME) from the leaves and stems of the plant were analyzed by GC and GC/MS.Fortyfour components representing 90.0%of solvent free microwave extraction oil of Salviapersepolitana were identified.The main compounds were spathulenol (26.6%), bicyclogermacrene (14.4%) andβ-caryophyllene (14.8%).Other notable constituents were bornylacetate (7.2%) and δ-elemene (6.3%).The oil of the plant was characterized by large amounts of sesquiterpenes (73.7%) and small amount of monoterpenes (26.4%).Spathulenol (14.6%) was also the main component of the oil of S. urumiensis [3].

References

[1] V.Mozaffarian.A Dictionary of Iranian Plant Name, FarhangMoaser Publisher, Tehran, Iran (1996) 479.
[2] A.Rustaiyan, S.Masoudi, M.Tabatabaei-Anaraki, Natural Product Communication, 2 (2007) 1031.
[3] M.A.Khaliazadeh, A. Esmaeili, A.Rustaiyan, B.Eslami and S.Masoudi, Chemistry of Natural Compounds, 46 (2011) 985.

On the Reaction of Benzothiazole with Alkyl Propiolates

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The development of efficient synthesis of heterocyclic compounds is of interest in organic chemistry because most of the biologically active compounds contain a heterocyclic scaffold as a fundamental unit in their structure [1].The reaction between benzothiazole(1) and alkyl propiolates 2 in ETOH/H_2O (4:1) solvent system, proceeded smoothly at room temperature to afford product 3 and4 in about 9:1 ratios. The effect of solvent on the product ratio will be presented and discussed. The structures of product3 and 4 were deduced by NMR and IR spectroscopy.

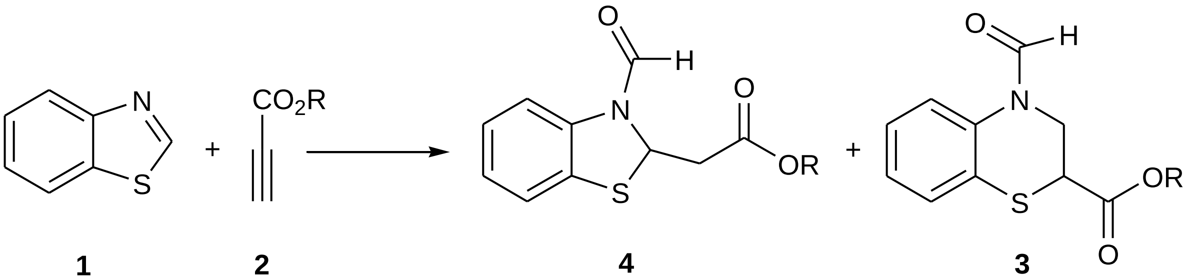

Figure 1. Scheme of the reaction

References

[1] Katritzky, A. R.; Rees, C. W.; Bird, C. W.; Cheeseman, G. W. H. (Eds.); Comprehensive Heterocyclic Chemistry; Pergamon Press: New York, (1987) 1.

An efficient synthesis of 2-amino-tetrahydro-4*H*-pyrans using a basic catalyst

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4*H*-Pyrans and 4*H*-pyran-annulated hetrocyclic scaffolds represent a "privileged" structural motif well distributed in naturally occurring compounds with a broad spectrum of significant biological activities that include anticancer, cytotoxic, anti-HIV, antihyperglycemic and etc [1-3]. The conventional synthetic method for the preparation of this type of compounds is based on the condensation of ethyl acetoacetate with aromatic aldehydes and malononitrile. For this purpose, a variety of catalysts have been used to facilitate the reaction that has some disadvantages such as toxicity, expensiveness and difficulty in the preparation of the catalyst. In this work we report the applicability of a basic organo-catalyst for the simple, efficientsynthesis of 4*H*-pyran derivatives. The present methodology suggests several advantages such as ease of the preparation, reusability of the catalyst, high yields, simple and green procedures, low cost, short reaction times, easy work-up and preformation of the reaction in water as a green solvent(figure 1).

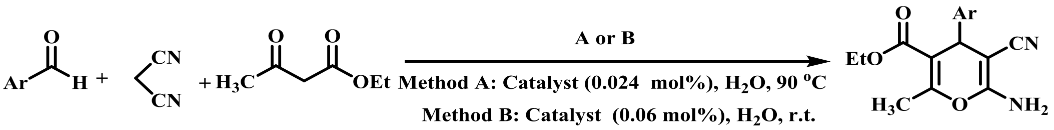

Figure 1. Synthesis of 4*H*-pyran derivatives in the presence of basic catalyst.

References

[1] Wu, J. Y. C.; Fong, W. F.; Zhang, J. X.; Leung, C. H.; Kwong, H. L.;Yang, M. S.; Li, D.; Cheung, H. Y. Eur. J.Pharmacol, 473 (2003) 9.

[2] Raj, T.; Bhatia, R. K.; Kapur, A.; Sharma, M.; Saxena, A. K.; Ishar,M. P. S., Eur. J. Med. Chem., 45, (2010),790.

[3] Rueping, M.; Sugiono, E.; Merino, E., Chem.Eur. J., 14(2008), 6329-6332.

Efficient synthesis of pyrano[2,3-*d*]pyrimidine-2,4(1*H*,3*H*)-diones in the presence of organo catalyst

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Barbituric acid and its derivatives show a variety of pharmaceutical properties. Pyrano[2,3-d]pyrimidine-2,4(1*H*,3*H*)-diones as important derivatives of barbituric acid has also received significant attention from many pharmaceutical and organic chemists essentially because of the broad spectrum of their biological and pharmaceutical properties such as antitumor, analgesic, antibacterial, and fungicidal activities [1-3].

In this work, we have introduced an efficient, simple and green method for the synthesis of pyrano[2,3-d]pyrimidine-2,4(1*H*,3*H*)-diones derivatives using a saccharin as an efficient organo catalyst. Easy work-up procedure, mild and green reaction conditions, high reaction times and excellent yields of the products are significant advantages of this method(figure 1).

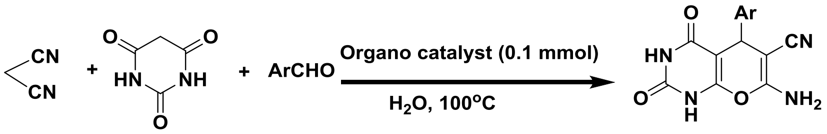

Figure 1. Synthesis of pyrano[2,3-d]pyrimidine-2,4(1*H*,3*H*)-diones.Derivatives in the presence of saccharin as an efficient organo catalyst

References

[1] Suguira, K.; Schmid, F.A.; Schmid, M.M.; Brown, G.F. Effect of compounds on a spectrum of rat tumors. Cancer Chemother. Rep. Part 2, 3(1973) 231-238.

[2] Regnier, G.L.; Canevar, R.J.; Le Douarec, J.C.; Halstop, S.; Daussy, J.Triphenylpropylpiperazine derivatives as new potent analgetic substances. J. Med. Chem., 15(1972) 295-301.

[3] Pershin, G.N.; Sherbakova, L.I.; Zykova, T.N.; Sakolova, V.N. Antibacterial activity of pyrimidine and pyrrolo-(3,2-d)-pyrimidine derivatives. Farmakol. Taksikol,35 (1972) 466-471.

Introduction of a new organo-catalyst for the synthesis of 2-amino-tetrahydro-4H-pyrans derivatives

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Pyran derivatives are ordinary structural subunits in a variety of important natural products, including carbohydrates, alkaloids, polyether antibiotics, pheromones and iridoids. Tetrahydrobenzo pyrans are important class of heterocyclic scaffolds in the field of drugs and pharmaceuticals.

These compounds are widely used as anti-coagulant, diuretic, spasmolytic, anticancer and anti-anaphylactic agents. Numerous methods have been reported for the synthesis of 4H-benzo pyrans. Each of these methods has its own advantages with some limitations such as extreme experimental conditions, long reaction times, low yields and effluent pollution [1,4].

Herein, we wish to report the efficient method for the synthesis of 2-amino-tetrahydro-4H-pyrans using hydantoin as an efficient organo-catalyst.

The most important advantages of this method are: simplicity, mild reaction conditions, easy work-up, short reaction times, high yields of the products and reusability of the catalyst (figure1).

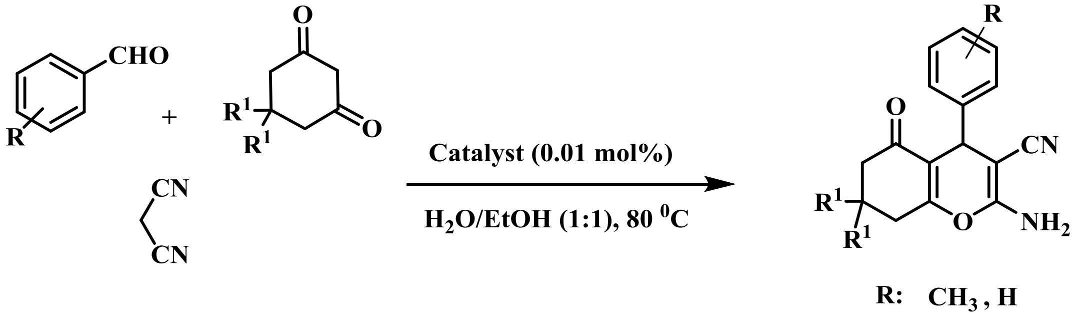

Figure 1. Synthesis of 2-amino-tetrahydro-4*H*-pyran derivatives in the presence of hydantoin as an efficient organo catalyst.

References

[1] L. L. Andreani, E. Lapi, Boll. Chim. Farm., 99(1960) 583.
[2] X. S. Wang, D. Q. Shi, S. T. Tu, C. S. Yao, Synth. Commun., 33(2003) 119.
[3] J. Tu, Y. Gao, C. Guo, D. Shi, Z. Lu, Synth. Commun. 32(2002) 2137.

Synthesis of N-substituted phthalimides

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Phthalimide subunit existed widely in both natural and synthetic compounds with broad activities against AIDS, cancer and inflammation [1,2].Moreover, many phthalimidederivatives has been reported to show antimicrobial activity. Recently, however as far as we knew, few of themwas applied in controlling phytopathogenic fungi [3,4].

In this work we wish report a new and efficient One-Pot synthesis of N-alky- phthalimides via reaction of dialkylacetylenedicarboxylate in the presence of triphenylphosphine and aryglyoxals. Treatment of triphenylphosphine with dimethylacetylenedicarboxylate in the presence of phthalimide produces β-aminophosphoranes.Then the reaction followed by attack on aryl glyoxal and after that the elimination of 3- dimethyl 5-oxo-4-phenyl-2,5-dihydro-1H-pyrrole-2,3-dicarboxylate occurred and attack of anion of phthalimide to another arylglyoxanlproduced the product(figure 1). This new product was characterized by FT-IR and ^{1}HNMR spectra.

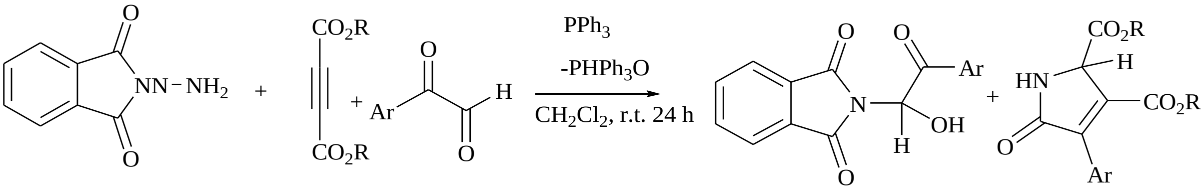

Figure1. The synthesis of N-substituted phthalimides**.**

Refrences

[1] V.L.M. Sena, R.M. Srivastava, R.O. Silva, V.L.M. Lima. Part V, Farmaco, 58(2003)1283.

[2] S. Nagarajan, S. Majumder, U. Sharma, S. Rajendran, N. Kumar, S. Chatterjee, B. Singh, Bioorg. Med. Chem. Lett., 23 (2013) 287.

[3] G. Singh, A. Saroa, S. Girdhar, S. Rani, S. Sahoo, D. ChoquesilloLazarte, Inorg. Chim.Acta 427 (2015) 232.

Synthesis of biologically active compounds: 7-(4-(1-benzoyl-4-cyano-9-oxo-9H-fluoren-3-yl)piperazin-1-yl)-1-cyclopropyl-6-fluoro-4-oxo-1,4-dihydroquinoline-3-carboxylic acid

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The functional azafluorenones, being the core structural unit in non-naturally and naturally occurring products, serve as "privileged structures" in many biologically active molecules and pharmaceutical substances [1]. they have also been found in natural alkaloids, such as onychine(I), polyfothine(II), isoursuline(III), which exhibit powerful antimicrobial, DNA damaging, and anticandidal activity as well as anti-malarial effects [2].

Multi-component domino reactions (MDRs) have been successfully applied to the total synthesis of natural and naturallike products [3] becoming one of the key tools that allow the creation of several bonds in a One-Pot manner and offer remarkable advantages like convergence, operational simplicity and facile automation [4]. we found another new HOAc promoted MDR of arylglyoxal monohydrates with Ciprofloxacinand 1,1-dicyanomethylene-3-indanone yielding polyfunctionalized 2-azafluorenones.This new product was characterized by FT-IR and ^{1}HNMR.

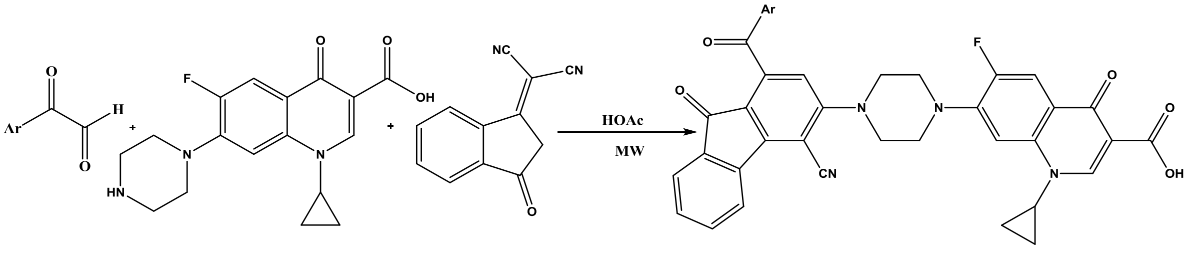

Figure 1 The synthesis of polysubstituted 2-azafluorenones.

Refrence

[1] D. Mueller, R. A. Davis, S. Duffy, V. M. Avery, D. Camp and R. J. Quinn, J. Nat. Prod., 72 (2009) 1538.
[2] G. A. Kraus and A. Kempema, J. Nat. Prod., 73 (2010)1967.
[3] B. B. Toure and D. G. Hall, Chem. Rev., 109(2009)4439.

One-Pot synthesis of substituted hydantoinsusing triphenylphosphine, α-bromoketones and parabanic acid derivative

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Wittig reactions are often used for the synthesis of acyclic and cyclic alkenes [1-3].We report One-Pot , and efficient condensation reactions oftriphenylphosphine, α-bromoketones and N,N'-diphenylparabanicacid in the presence of triethylaminein xylene reflux that led to new substituted hydantoins.The reactions afford to the corresponding products in good to high yields. Satisfactory yields of products, as well as a simple procedure, isolation and purification of the products make it a useful protocol for this synthesis. The structures of the synthesized compounds were characterized by ^{1}H, ^{13}CNMR and IR spectroscopy as well as mass spectrometry.

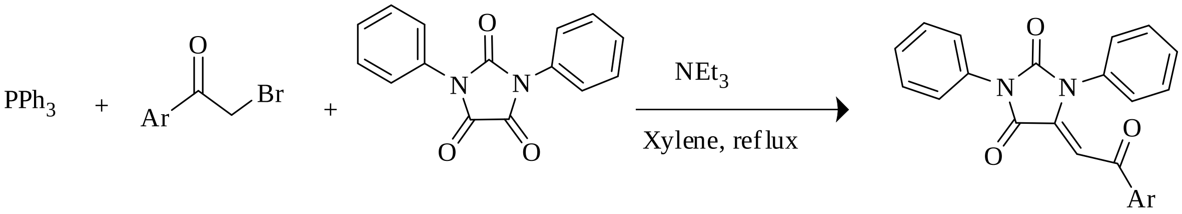

Figure 1. Scheme of the reaction

References

[1] S. HakanÜngören, I. Kani, A. Günay, Tetrahedron Letters, 53 (2012) 4758.
[2] F. Palacios, C. Alonso, D. Aparicio, G. Rubiales, J.M. de Los Santos, Tetrahedron, 63 (2007) 523.
[3] V.M. Abdou, Phosphorus Sulfur Silicon, 177 (2002) 325.

Three-component reactions of triphenylphosphine, α-haloketones and *N,N'*-diphenylthioparabanic acid in the presence of NEt_3

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Five-membered rings containing two heteroatoms are privileged structures with proven utility in medicinal chemistry [1-3].In this research, we synthesized the substituted thiohydantoin derivatives via three-component reactions of triphenylphosphine, α-haloketones andN,N'-di phenyl thioparabanic acid in the presence of NEt_3 in toluene. The wide ranges of substituted α-haloketoneshave been used in the reactions that led to the corresponding products in high to excellent yields. We have described a simple and rapid procedure for the synthesis of variously substituted thiohydantoins from thioparabanic acids by chemoselective Wittig reactions. The structures of thiohydantoin derivatives were deduced from ^{1}H,^{13}CNMR and IR spectroscopy as well as mass spectrometry.

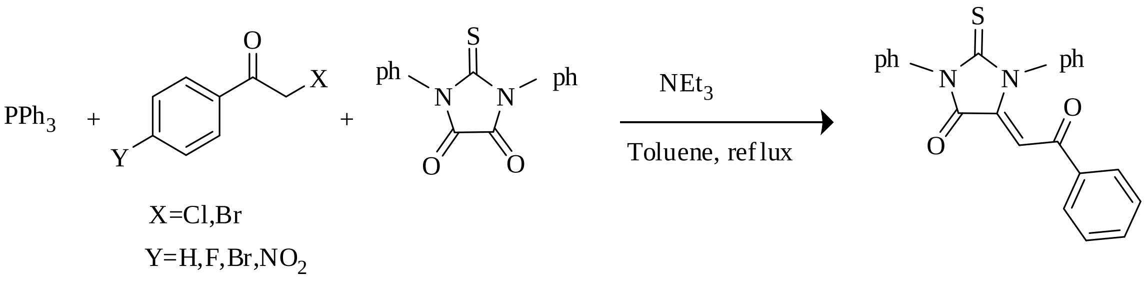

Figure 1. Scheme of the reaction

References

[1] S. Hakan Üngören, I. Kani, A. Günay, Tetrahedron Letters, 53 (2012) 4758.
[2] T. Kurz, K. Widyan, Tetrahedron Lett., 45 (2004) 7049.
[3] M. Meusel, M.Gütschow, Org. Prep. Proced. Int., 36 (2004) 391.

Cu (II)-Van-MCM-41 as a recyclable catalyst system for synthesis and oxidation of sulfides

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Symmetrical and unsymmetrical diaryl sulfides are a class of important synthetic reagents and intermediates in organic, bio-organic, heterocyclic chemistry and medicinal [1, 2].They are found in numerous drugs displaying a broad spectrum of therapeutic activities such as anti-diabetes, anti-Alzheimer's, anti-inflammatory, anti-cancer, anti-Parkinson's, and anti-HIV [3].In this work we used of vanillin for immobilization onto MCM-41 silica support to preparation of safe and appropriate Schiff base ligand. The aim of the present study was to report a simple and highly efficient protocol for synthesize of symmetrical diaryl sulfides.

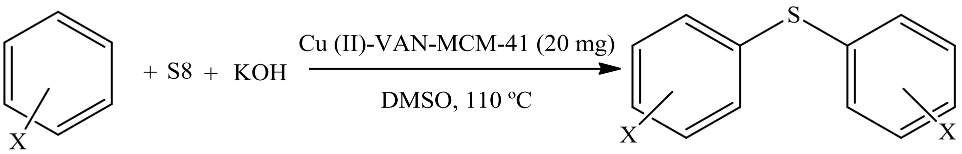

Figure 1. Synthesis of symmetric sulfides

Consequently, an efficient and environmentally friendly procedure has been used for the synthesis of symmetric sulfidesin the presence of catalytic amounts of Cu (II)-Van-MCM-41. Furthermore, the catalyst could be isolated with simple filtration and reused for several times.

References

[1] B. Movassagh, M. Soleiman-Beigi, Monatsh Chem., 140 (2009) 409.
[2] B. Movassagh, A. Yousefi, Monatsh Chem., 146 (2015) 135.
[3] A. Rostami, A. Rostami, N. Iranpoor, M. A. Zolfigol, Tetrahedron Lett., 57 (2016) 192.

Synthesis and characterization of VO-Vanillin complex immobilized on MCM-41 and its facial catalytic application in the sulfoxidation reaction in green media

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Sulfoxides are useful for stereo control in asymmetric synthesis and they are important targets of pharmaceutical interest [1]. They have been used as reagents in functional group transformations such as the oxidation of thiols[2,3].The objective of this work was introducing VO-Vanillin-MCM-41 as an economical, environmentally benign, heterogeneous, and highly selective catalyst. Using of this catalyst in the preparation of sulfoxides leads to selectivity and excellent conversion.MCM-41 and preparedcatalyst was characterized by small angle XRD, SEM, EDS, FT-IR, TGA analysis and N_2 adsorption-desorption analysis.Furthermore, the catalyst could be isolated with simple filtration and reused for several times witout significant loos in its activity.

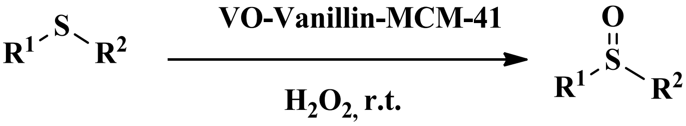

Figure 1. Oxidation of sulfide to sulfoxie in the presence of VO-Vanillin-MCM-41

References

[1] A. Ghorbani-choghamarani, S, Sardari, Chin J Catal., 31 (2010) 1347.
[2] O. G. Lowe, *J Org Chem*., 40 (1975) 2096.
[3] M. M Abu-Omar, S. I. Khan, Inorg Chem., 37 (1998) 4979.

A Novel Access to Benzo[e]isoindole-1,3-diones via Oxidative Coupling Reactions

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Since the discovery of C-H olefination of benzene by Fujiwara at 1967 [1] numerous catalytic versions of this transformation have been developed. The vast majority of these catalytic protocols proceed under "ligandless" conditions (with Pd^{II} salts such as $Pd(OAc)_2$ as catalysts) and use oxidants such as peroxides, peroxyesters, dioxygen, polyoxometalates, Cu^{II}, or Ag^{I} to achieve catalytic turnover [2]. Glycogen synthase kinase-3β (GSK-3βa) is responsible for many important biological activities, such as Wnt and Hedgehog signaling pathways, stem-cell renewal, meiosis steps, cellular differentiation, apoptotic mechanisms, circadian rhythm, gene transcription as well as insulin action [3].Thus, the development of GSK-3βinhibitors has been regarded as a potential therapeutic approachfor these related diseases. Zou et al. found that benzo[e]isoindole-1,3-diones are of most powerful GSK-3βinhibitors [4]. However, the traditional synthesis pathways of benzo[e]isoindole-1,3-diones, are very complex, for example including sequential steps such as diazotization, low-yield benzyne formation, Diels-Alder reaction, amidation of esters, cyclization via ortholithiation and cabonization, oxidation of hemiaminal to amide and harsh dealkylation.Herein, we report a direct method to the synthesis of benzo[e]isoindole-1,3-dione derivatives via tandem oxidative coupling reactions of readily available raw materials.

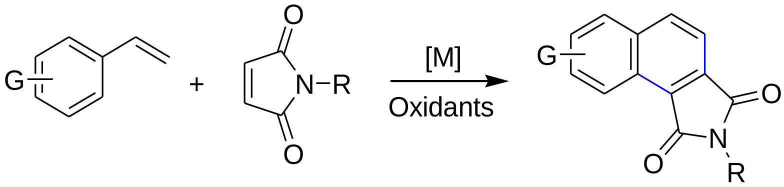

Figure 1. Scheme of the reaction

References

[1] Y. Fujiwara, I.Moritani, S. Danno, R. Asano, S.Teranishi, J. Am. Chem. Soc., 91 (1969) 7166.
[2] J.Le Bras, J. Muzart, Chem. Rev.,111 (2011) 1170.
[3] B. W.Doble, J. R. Woodgett, J. Cell Sci., 116 (2003) 1175.

Organically functionalized mesoporous silica nanoparticles as an effective nano-carrier for curcumin delivery

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In this study, the synthesis of novel PEGylatedimidazolium ionic liquid and Citric PEGylated functionalized MSN nanoparticles and also the evaluation of their potential in the loading and release of curcumin have been investigated. Due to the high surface area and their capability for the desired organically functionalization, their application provide convenient opportunity to introduce high efficient nano-carriers. The size, the loading amount and release efficiency were investigated in in-vitro conditions. Techniques such as BET, XRD,DLLS, UV-Vis, TGA, FT-IR and TEM were applied for characterization.

Herein, a PEGylated functionalized imidazolium ionic liquid and Citric PEGylated functionalized MSN nanoparticles has been fabricated. Then it has been evaluated as an effective nanocarrier for improving the transport and delivery of CUR to cancerous cell lines. Indeed the structure of PEGylatedimidazolium ionic liquid and Citric PEGylated functionalized MSN nanoparticles was fully characterized and confirmed by a variety of techniques. Then CUR was loaded on the surface of the modified NPs. MTT assay technique was applied to examine the efficiency of PEGylatedimidazolium ionic liquid and Citric PEGylated functionalized MSN nanoparticles as anticancer. Our data suggest that CUR loaded PEGylatedimidazolium ionic liquid and Citric PEGylated functionalized MSN nanoparticles has more cytotoxic effect on MCF-7 as the cancerous model cell versus pure CUR.

References

[1] (a) A. Shafiee, European journal of medicinal chemistry 68 (2013) 291-300; (b) M,Mahdavi. Synlett 25 (2014)0385-0388.
[2] S.E.Sadat-Ebrahimi. Journal of Chemical Research, 39.9 (2015).
[3] M.Mahdavi. European journal of medicinal chemistry, 95 (2015)492-499.

The synthesise of chromones derivatives under solvent free condition

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Chromones are major categories of heterocyclic compounds containing oxygen that due to their reactivity and biological activity have found more synthetic importance.In this research, the reaction between salicylaldehyde derivativesand DMAD was done on solid bed of zinc oxide in room temperature and under solvent free conditionby grinding method. Chromoneshydroxyl derivativeswere synthesized and characterized with suitable efficiency in 1-1.30 hours. The IR and ^{1}H-NMR spectrawere compared with previous reported compounds and the results showed that these compounds have been synthesized.

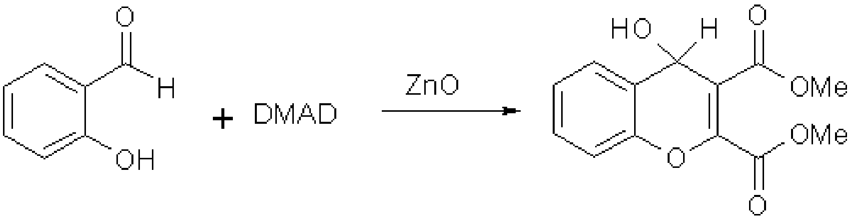

Figure 1. Scheme of the reaction

References

[1] Daniel O. Bennardi, Diego M. Ruiz, Gustavo P. Romanelli, Graciela T. Baronetti, Horacio J. Thomas and Juan C. Autino. Letters in Organic Chemistry, 5 (2008)607-615.

Noncovalent functionalization of graphene oxide with Schiff bases compounds as antibacterial materials

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Graphene is a singleatomthick two-dimensional graphiticcarbon material. In the field of biomedicine,functionalized graphenes have been used for drug delivery, gene transfection,biosensing, as well as tumorimaging and photothermal therapy [1].Recently,research attention has been drawn towards the antibacterialactivity of graphene and graphenebasedNanocomposites [2]. Although whether and how graphene oxide(GO) presents antibacterial activity are still under debatebut suggested that the GO antimicrobial action contributes to both membrane disruption and oxidative stress [3].

Graphene oxide is produced by Hummer method. The Schiff base compounds were placed on the graphene oxide surface by non-covalent approach. It seems that π-π stacking interactions between the rings of chromene and graphene, is the most important factor for staying compounds on the surface of graphene oxide. The structure of the synthesized compounds was confirmed by FT-IR, UV-VIS, EDX and FE-SEM analysis. The purpose of synthesis these hybrid nanomaterials, is evaluation of their antimicrobial activity on the Escherichia coliand Staphylococcus aureus microorganisms.

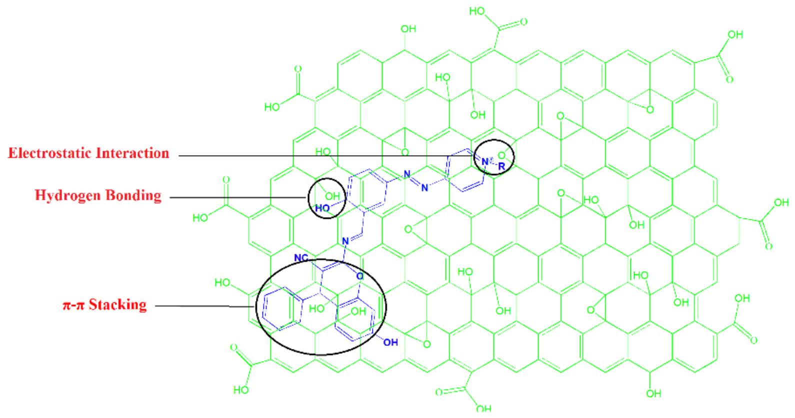

Figure 1. Scheme of the reaction

References

[1] Zh. Liu, J. T. Robinsonb, S. M. Tabakmanb, K. Yanga, H. Dai. Materials Today, 14 (2011) 316.
[2] B. S. Wu, H. N. Abdelhamid, H. F. Wu. RSC Adv., 4 (2014) 3722.
[3] O. Akhavan, E. Ghaderi.AcsNano, 4 (2010) 5731.

Synthesis and evaluation of in vitro antibacterial and antioxidant activity of 4-((3-formyl-4-hydroxyphenyl) diazenyl)-alkylpyridinium derivatives

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Monoazo compounds, which have the common structure unit of the azo chromophore, -N=N-, linking two aromatic systems.Delocalizedintegratedπ-orbitals systems in aryl azo compounds causes theappearance ofbright colorsfromyellowto red. According to thenon-toxicity, thiscompounds use inpainting, biologyand medicalstudies. The pharmaceutical importance of compounds including an arylazo group has been extensively reported in the literature [1]. Also, azo dyes are reported to have a broad range of antibacterial, antifungal, antitumor and anti-oxidant activities [2, 3].

The simple reaction of 2-hydroxy-5-(pyridin-4-yldiazenyl) benzaldehyde (A) with n-alkyl bromides generated five novel azo pyridinium salts in good to excellent yields. The UV-Vis absorption spectra of synthesized compounds indicated enol–keto tautomeric, solvatochromism and cis-trans isomerization. The solvatochromism behavior of compounds due to intramolecular hydrogen bond in enol–keto tautomeric, dipole moment changes and depends on the substitution, solvent, pH and temperature. Antibacterial activity was studied by disc diffusion and MIC methods. Diphenylpicrylhydrazyl (DPPH) assay was used to determine the antio-xidant property.

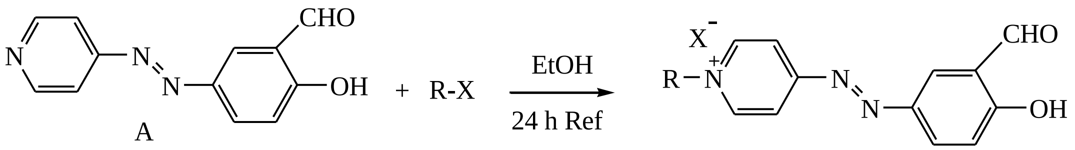

Figure 1. Scheme of the reaction

References

[1] H.G. Garg,R.A. Sharma.J Med Chem., 12 (1996) 1122.
[2] A. Kakanejadifard, F. Azarbani, A. Zabardasti,S. Kakanejadifard, M. Ghasemian, F. Esna-ashari, S. Omidi, S. Shirali, M. Rafieefar. Dyes and Pigments, 97 (2013) 215.
[3] M. Ghasemian, A. Kakanejadifard, F. Azarbani, A. Zabardasti, S. Kakanejadifard. Spectrochimica Acta Part A: Molecular and Biomolecular Spectroscopy, 124 (2014) 153.

The preparation of dimethyl-4-hydroxy-8-methoxy-4-hydro chromone -2, 3-dicarboxylate in presence of ZnO under solvent free condition

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The increasing use of chromones compounds for the synthesis of other required compounds and derivatives have been caused that the appropriate procedures base on green chemistry were developed.In this work, the reaction between 3- methoxysalicylaldehyde and DMAD was done on solid bed of zinc oxide in room temperature and under solvent free condition by grinding method. Dimethyl-4-hydroxy-8-methoxy-4-hydrochromone-2,3-dicarboxylate was synthesized and characterized with suitable efficiency (60%) in 1 hour. The IR and 1H-NMR spectra were compared with previous reported compounds and the results showed that these compounds have been synthesized.

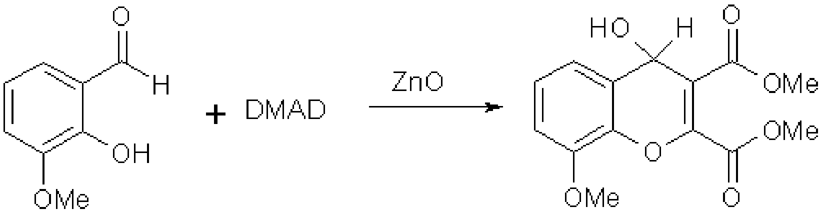

Figure 1. Scheme of the reaction

References

[1] D. Sharma, J.K. Makrandi, 2 (2009)157-159.

Synthesis of triacetoxybenzoic acid and triacetoxybenzoyl chloridefrom gallic acid and study on comparison of their antibacterial activity

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Gallic acid (GA) or 3,4,5-trihydroxybenzoic acid is a polyhydroxy phenolic compound and found in various plants such as tea, green tea and fruits [1].Variousderivatives of gallic acid have shown good bioactivity including antibacterial, antifungal, antiviral, anticancer, antioxidant, antitumor activities [1,2].In this study, we first synthesized triacetoxybenzoic acid(ACGA) and 3,4,5-triacetoxybenzoyl chloride(ACGACl) from GA and then evaluated the antibacterial activity of the synthetic compounds against nine microorganisms using disc diffusion method and compared with the GA activity.

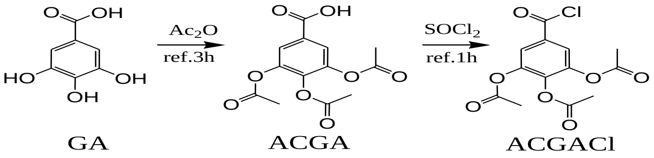

Figure 1. Scheme of the reaction

The three compounds prevented the growth of all the microorganisms. However the activity of GA was more potent than its derivatives. The results as diameter of inhibition zone in term of millimeter (mm) are shown in the table 1. The decreasing of ACGA and ACGACl activity may be due to changing of hydroxyl groups to acetoxy and chloride.

Microorganism	GA mm	ACGA mm	ACGACl mm	Vancomicin Positive control (mm)
Pseudomonas aeruginosa **Gram-negative**(-)	12	8	7	8
Escherichia coli(-)	14	8	8	18.33
Staphylococcus coagulase(-)	12	8	7	16.33
Citrobacter frurdii(-)	12	8	8	Non active (na)
Enterobacter aerogenes(-)	14	8	8	na
Acinetobacter baumannii(-)	19	8	8	21
Serratia marcescens(-)	12	8	7	na
Klebsiella pneumoniae(-)	12	8	8	8.5
Streptococcus pneumoniae **Gram-positive**(+)	16	12	10	14

References

[1] R.Kaur, K. Kaur, L. Gupta, N. Dhir, G. Preet. SInternational Journal of Pharmaceutical Sciences Review and Research, 28 (2014) 16.
[2] J. P. Rauha, S. Remes, M. Heinonen,A.Hopia, M. Kähkönen, T. Kujala, K. Pihlaja, H. Vuorela, P. Vuorela. International journal of food microbiology, 56 (2000) 3.
[3] Y. Wanga, J. Ronga, B. Zhanga, L. Hua, X. Wanga, C. Zenga. Bioorganic & Medicinal Chemistry.

Synthesis of some new azo compounds via coupling reaction of 2-aminotiophenes with phenolic compounds

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Azo compounds refer to the chemical compounds bearing the functional group R-N=N-R′ in which R and R′ can be either aryl or alkyl group [1] and they are useful in the fields of dyes, pigment and advanced materials. But they have several other applications too as, for example, dyes for drug, food and cosmetic applications, biomedical field [2] chiral receptors, liquid crystals and new glassy materials [3].

In this work, we initially prepared the two 2-aminotiophene derivatives from the starting materials cyclopentanone (or cyclohexanone), malononitrile and sulphur *via*Gewald three-component reaction. Then, the obtained 2-aminothiophenes were reacted with some phenolic compounds under the normal azo coupling reaction conditions tosatisfactorily give the desired products in good yields. Finally, structure of the productswas confirmed by spectroscopic methods.

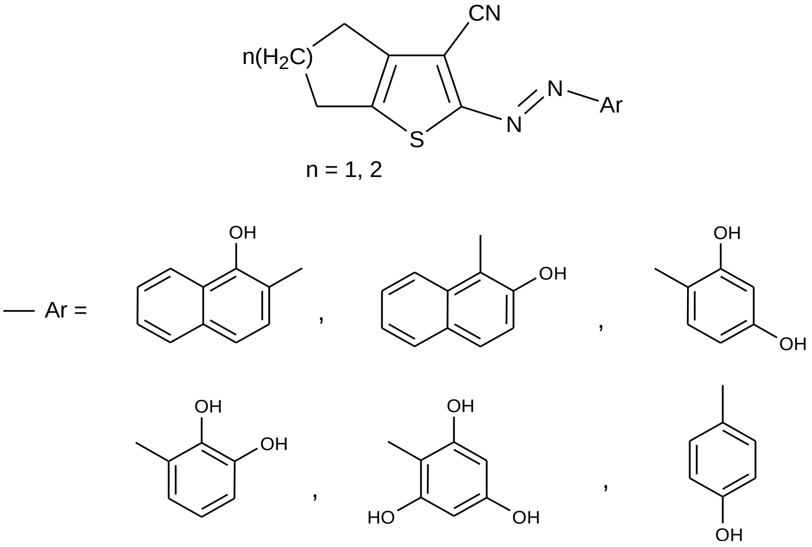

Figure 1. Scheme of the reaction

References

[1] L. Sekhri. Asian Journal of Chemistry, 17 (2005) 1474.
[2] T. S. Jagodzinski. Chemical Reviews, 103(2003) 197.
[3] Y. He, X. Gu, M. Guo, X. Wang. Optical Materials, 31(2008) 18.

Highly Efficient Protocol for One-Pot Ring Opening of Cyclic Ethers (Ether Bond Cleavage) via Cyanuric Chloride (CC) and Carboxylic Acids

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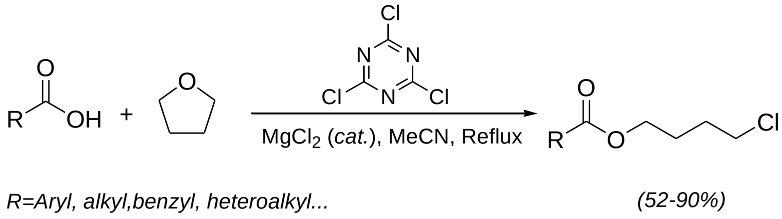
The cleavage of a C-O bond of ethers is a versatile and nearly ubiquitous transformation in organic synthesis for the production of many pharmaceuticals and other fine chemicals. In this connection, a variety of reagents and methods in which are capable of cleaving ethers have been developed[1].Among them, the most conventional method involving acylative cleavage of ethers with acyl chlorides is one of the attractive methods for the preparation of esters. Thus, it is of great interest in the development of the convenient and practical catalytic methods for the transformation of ethers into esters. There are some reports on the acylative cleavage of ethers with acyl chlorides using Lewis acids. However, these methods involved some disadvantages, such as the use of harsh, toxic, expensive, unstable reagents or catalysts, drastic conditions, and low yields of products.

Cyanuric chloride (2, 4, 6-trichloro [1, 3, 5]-triazine) (CC or TCT) is a stable, non-volatile, inexpensive and a safe reagent which has long been used in various organic transformations [2].In recent years, we developed the application of CCin various organic transformations as a useful reagent for the synthesis of sulfonamides from amine-derived sulfonate salt, One-Pot synthesis of N-acyl sulfonamides,synthesis of ynones, andalso One-Pot regioselective N-acylation of nucleobases [3].Encouraged by the intense research activities in the field of ethers' C-O bond cleavage and also in pursuit of our ongoing interest in utilizing cyanuric chloride in organic transformation; hereby, we disclose cyanuric chloride as an efficient reagent for ring opening of cyclic ethers (ether bond cleavage) via carboxylic acids(Scheme 1). To this end, diverse activated carboxylic acids by CC were used to react with cyclic ethers using catalytic amount of $MgCl_2$ in anhydrous MeCN at reflux condition. The influence of parameters on this protocol including the type of solvent, base and temperature were assessed. Good to excellent yields of chloroalkylesters were obtained exploitingthis current approach.



Scheme 1. One-Pot ring opening of cyclic ethers using cyanuric chloride and carboxylic acids

References

[1] R. C. Larock, Ether cleavage In Comprehensive Organic Transformations; Wiley-VCH: New York, NY, (1999).

[2] M.N. Soltani Rad, A. Khalafi-Nezhad, Z.Asrari, S.Behrouz, Z.Amini, M.Behrouz, Synthesis, (2009) 3983.

[3] M. N. Soltani Rad, S. Behrouz, Z. Asrari, A. Khalafi-Nezhad, Monatshefte für Chemie - Chemical Monthly,145(2014) 1933.

Consecutive Condensation, C-N and N-N Bond Formation: A Copper-Catalyzed One-Pot Three-Component Synthesis Of 2*H*-Indozole

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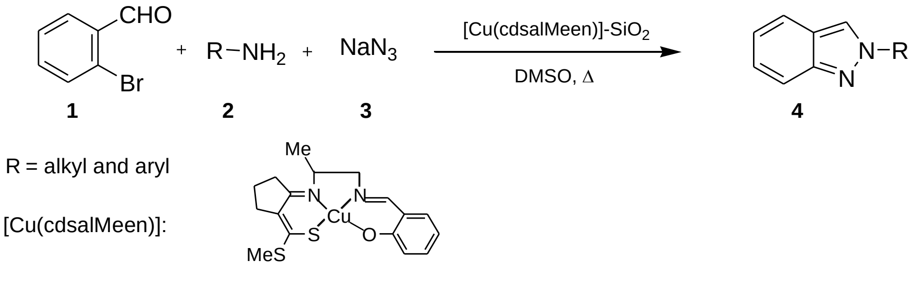
Indazole derivatives have received an increasingly significant attention in modern drug discovery since the indazole unit is a key structural motif in various drug substances exhibiting a wide spectrum of biological activities like anti-platelet, anti-inflammatory, anti-cancer, anti-tumour, anti-contraceptive, anti-depressant, anti-microbial and anti-HIV. In addition, indazoles act as efficient bioisosters of benzimidazoles and indoles [1].

Due to the unique biological activities of indazole derivatives, a number of synthetic methods were developed to access indazole scaffold. However, most of the existing approaches have led to the thermodynamically favoured 1*H*-idazoles or a mixture of 1*H*- and 2*H*-indazoles [2]. Accordingly, the difficulty in the synthesis of 2*H*-indazoles led to much less study on the applications of 2*H*-indazoles. Thus, the development of efficient and applicable methods for selective synthesis of 2*H*-indazoles is of great significance to synthetic chemists.

In 2011, Rao and coworkers reported the efficient copper-catalyzed intramolecular cyclization of 2-azidoimines through N-N bond formation to afford the corresponding 2*H*-indazoles [3]. However, this method requires multi-steps process for preparation of the prerequisite 2-azidoimines as the key starting material. In the light of remarkable advantages of multi-component reactions in organic synthesis, the three component synthesis of 2*H*-indazoles from 2-bromobenzaldehydes, amines, and NaN_3 would be a highly advantages and attractive strategy. In this regard, we now report a highly efficient and straightforward synthesis of 2*H*-indazoles via one-pot three-component reaction of readily available 2-bromobenzaldehyde, structurally diverse amines, and NaN_3 in the presence of {methyl-2-{[1-methyl-2-(2-phenolate)methylidyne nitrilo] ethyl}-aminato(-1)-1-cyclopentenedithio carboxy-late Copper(II), [Cu(cdsalMeen)] as the novel and highly efficient heterogeneous catalyst (Scheme 1).



Scheme 1. One-pot three-component synthesis of 2*H*-indazoles

References

[1] M. J. Haddadin, W. E. Conrad, M. J. Kurth, Mini-Reviews in Medicinal Chemistry 12 (2012) 1293.
[2] N. Cankařová, J. Hlaváč, V. Krchňák, Organic Preparations and Procedures International 42 (2010) 433.
[3] J. Hu, Y. Cheng, Y. Yang, Y. Rao, Chemical Communications 47 (2011) 10133.

Optical, mechanical and thermal behavior of Poly(vinyl chloride) composite films embedded with modified TiO_2 usingvitamin B_1 as modifier agent

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Poly(vinylchloride) (PVC) is the most widely used polymer after polyethylene and polypropylene. One of the major problems that limit the practical use of the PVC is its lower thermal stability and brittleproperties [1]. Utilizing metal nanoparticles (NPs) into polymeric matrices has been studied extensively to improve features and capacities [2]. According to the agglomeration of NPs, different organic or inorganic materials can be used as modifiers to surface modification of NPs [3]. In this study, vitamin B_1 (VB_1) asbiosafe and naturally synthesized molecule, was used to surface modification of NPs for the first time. In addition, TiO_2NPs due to their nontoxicity, chemical and biologicalineffective and low cost, was used as modifier for PVC matrixand the effect of various amounts of modified NPs on prepared nanocomposites (NCs) was studied (figure 1).

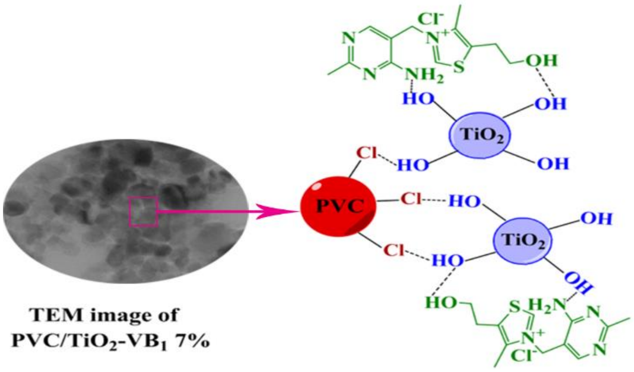

Figure 1. Schematic image and TEM micrograph of the prepared PVC/modified TiO_2 NC film.The significant advantages of this procedure are: a) surface of TiO_2NPs was modified with biosafe materials b) ultrasonic technique was used as a simple and green methodc) thermal stability and mechanical properties of the NCs were enhanced after incorporation of modified NPs.

References

[1] H. Mudassir, M. Lee, Progress in Natural Science, 24 (2014) 579-587.
[2] M. Zarrinkhameh, A. Zendehnam, S. M. Hosseini, Journal of Industrial and Engineering Chemistry. 30 (2015) 295-301.
[3] S. Mallakpour, M. Naghdi, Polymer Bulletin.73 (2016) 1701-1717.

Multi-component synthesis of xanthenediones by the lanthanum triflate catalyst

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Xanthene derivatives possess agricultural, antibacterial, antiviral, anticoagulant, anticancer, diuretic, spasmolytic and anti-inflammatory properties which are also widely applied in photodynamic therapy [1]. Xanthenediones are important building blocks in a number of natural products and have been used as versatile synthons because of the inherent reactivity of the inbuilt pyranring [2,3].

Here, we wish to report our preliminary results on the synthesis of xanthenedione derivatives catalyzed by the lanthanum triflate catalyst from the reaction of dimedone and different aromatic aldehydes at 60 °C under solvent free conditions (Figure 1).

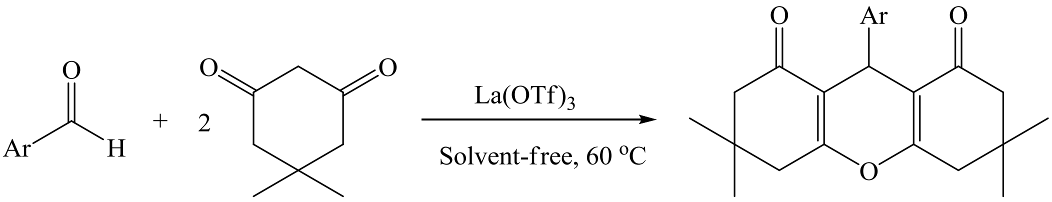

Figure 1. Synthesis of different xanthenediones by the La(OTF)$_3$ catalyst

References

[1] T.S. Jin, L.B. Liu, Y. Zhao, T.-S. Li, Synth. Commun.,(2005) 2379.
[2] S. Hatakeyma, N. Ochi, H. Numata, S. Takano, J. Chem. Soc.,Chem. Commun.,(1988) 1202.
[3] G.M. Cingolant, M. Pigini, J. Med. Chem.,(1988) 531.

Eco-friendly method for recovery of polyol from flexible polyurethane foam

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Polyurethane foams are disposed of not only at the end of their use but also as scrap during slabstock manufacturing, leading to an environmental and economic problem [1]. A detailed study of the main reaction parameters affecting the reaction and properties of the recovered polyol has been carried out. They include zinc oxide concentration as a catalyst, reaction temperature and mass ratio of treated foam to the glycolysis agent. Reactions were studied using various DEG and castor oil ratios and the recovered polyols were characterized and data compared with an authentic sample[2].

The goal of chemical recycling of flexible foams is to regain the polyols suitable for manufacturing new PUR foam. Glycolysis of PUR gives a mixture of original polyol, low-molecular-weight urethanes with hydroxy-end groups and other, secondary products such as aromatic amines, etc. The glycolysis of commercially manufactured flexible foams has been studied in order to obtain directly the polyol product that can be used in the production of new foams[3].

References

[1] C. Molero, A. de Lucas, J.F. Rodrıguez.Polymer Degradation and Stability, 94 (2009) 533–539.
[2] M. M.AlaviNikje and K. M.Tavassoli. Current Chemistry Letters, 1 (2012) 175–180.
[3] H. Benes, J. Rosner, P. Holler, H. Synkova, J. Kotek and Z. Horak. Polym. Adv. Technol., 18 (2007)149–156.

Synthesis of BiscoumarinDerivatives Catalysed by Cyclohexane-1,4-diyl bis(hydrogen sulfate) under Solvent-free Conditions

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Coumarins play an important role in both natural and synthetic organic chemistry because of their potential applications in fragrance, pharmaceutical and agrochemical industries [1]. Biscoumarins are generally synthesized by combination of two equivalents of 4-hydroxycoumarin and different aldehydes. In the recent few years several methods have been reported for this synthesis which includes the use of different catalysts [2].

Sulfonated materials were usually synthesized through the oxidation of carbon materials by sulfur acid or oleum to produce sulfonic acid groups on the surface.It was before reported in the literature that sulfonic acid derivative is good catalyst for the synthesis of biological compounds[3].Cyclohexane-1,4-diyl bis(hydrogen sulfate) [CBDH]was prepared by reaction between cyclohexane-1,4-diol and chlorosulfonic acid (figure 1).

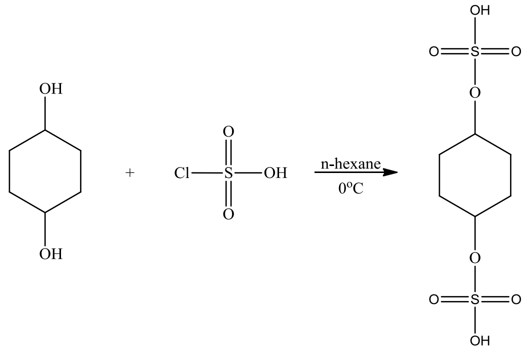

Figure 1. Preparation of cyclohexane-1,4-diyl bis(hydrogen sulfate)

Herein we report a mild, efficient, and environmentally benign procedure for the synthesis of bis-coumarins from reaction of aromaticaldehydes and 4-hydroxycoumarin in the presence of [CBDH] under solvent-free conditions as an efficient catalyst (figure 2).

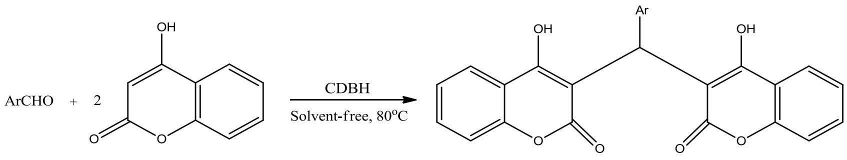

Figure 2. Synthesis of bis-coumarins in the presence of [CBDH]

References

[1] J.W. Hinman, H. Hoeksema, E.L. Caron, W.G. Jackson, Journal of the American Chemical Society, 78 (1956) 1072.
[2] Z. Siddiqui, F. Farooq, Catalysis Science and Technology, 1 (2011) 810.

Agar–sulfuric acid catalyzed synthesis of tetrahydro-4*H*-chromene-3-carbonitrile derivatives

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Tetrahydrobenzo[*b*]pyran, pyrano[2,3-d]pyrimidine, and pyrano[*c*]chromene derivatives have attracted much attention due to their wide range of biological properties [1].4H-pyrans and their derivatives have also attracted great attention due to their useful biological and pharmacological properties [2]. Furthermore, substituted 4H-pyrans also constitute a structural unit of a series of natural products [3].

On the other hand organic reactions under solvent-free conditions have also attracted much interest from chemists particularly from the viewpoint of green chemistry. The possibility of performing multicomponent reactions under solvent-free conditions using an environmentally friendly catalyst could enhance the efficiency from an economic as well as ecological point of view[4].In continuation of our efforts to develop new, green chemistry methods as well as our interest on applications of heterogeneous-catalyzed organic reactions,we decided to explore the possibility of synthesizing tetrahydro-4H-chromene-3-carbonitrilederivatives via a One-Pot , three-component condensation of dimedone, aromatic aldehydes and malononitrile under solvent-free conditions using agar–sulfuric acid [ASA] as a recyclable catalyst (figure 1).

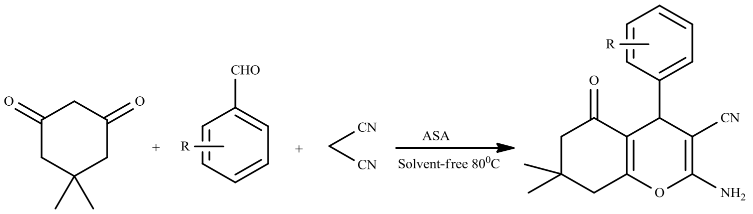

Figure 1: Synthesis of 4H-chromene derivatives using ASAunder solvent-free conditions

References

[1] L.L. Andreani, E. Lapi, Bollettino Chimico Farmaceutico., 99 (1960) 583.
[2] L. Bonsignore, G. Loy, D. Secci, European Journal of Medicinal Chemistry, 28 (1993) 517.
[3] S. Hatakeyama, N. Ochi, H. Numata, S. Takano, Journal of the Chemical Society, ChemicalCommunication, (1988) 1202.

Chemoselectivity of some S and N centered nucleophiles toward pentachloropyridine

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Perhalogenated aromatic and heteroaromatic compounds are important starting materials for synthesis of other heterocyclic and macrocyclic compounds [1,2].Polychloroheterocycles played an important role in the synthesis of the corresponding polyfluorocomponds. For example, pentachloropyridine used as intermediates for synthesis of other useful material such as pentafluoropyridine. Pentachloropyridine reacted with larger nucleophiles at 2-position of pyridine ring and with small nucleophiles at 4-position of pyridine ring. However, the outcome of nucleophilic substitution on pentachloropyridine is not as clear-cut as it seems at first sight. Therefore, substitution reactions are often solvent dependent [3].

In this work we investigated the reaction of pentachloropyridinewithbis(dithiocarbamate salt) and 3,4-dihydropyrimidine-2(1H)-thione derivatives. Dithiocarbamate salt of amines can be prepared according to the procedure given in literature [4,5]. Reaction of Dithiocarbamate saltand 3,4-dihydropyrimidine-2(1H)-thione derivatives with pentachloropyridinegave products rising from the substitution of the most activated chlorine atom at the 4-position of pyridine ring (figure 1, 2). Products confirmed by ^{1}H-NMR and ^{13}C-NMR spectroscopy data.

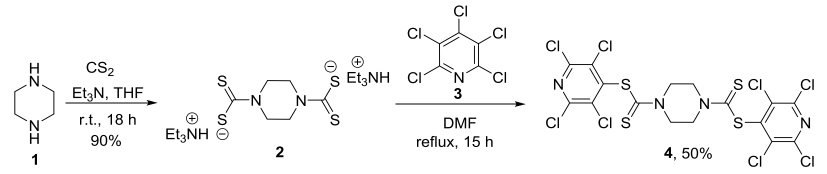

Figure 1. Reaction of salt **3** with pentachloropyridine

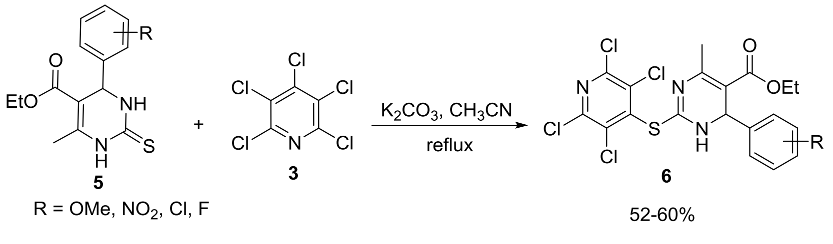

Figure 2. Reaction of 3,4-dihydropyrimidine-2(1H)-thione with pentachloropyridine

References

[1] R. D. Chambers, A. Khalil, C. B. Murray, G. Sandford, A. S. Batsanov, J. A. K. Howard, Journal of Fluorine Chemistry, 126 (2005) 1002.
[2] R. Ranjbar-Karimi, G. Sandford, D. S. Yufit, J. A. K. Howard, Journal of Fluorine Chemistry, 129 (2008) 307.
[3] H. Suschitzky, Polychloroaromatic Compounds, Plenum Press London and New York, (1974).

Synthesis of novel tetra-tert-butylcalix[4]arene derivatives linked to two series of substituted 1,2,4-triazole and 1,3,4-oxadiazole

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Two series of 1,2,4-triazole-5-thiones and 1,3,4-oxadiazole-5-thiones substituted tetra-tert-butylcalix[4]arenederivatized at lower rim were synthesized by the reaction of 1,2,4-triazole-5-thione and 1,3,4-oxadiazole-5-thione with 5,11,17,23-tetra-*tert*-butyl-25,27-bis(3-bromopropoxy)-26,28-dihydroxy calix[4]arene**(2)**. The synthesized compounds were characterized by FT-IR, ^{1}H NMR, ^{13}C NMR, spectral data elemental analysis and ESI-MS.

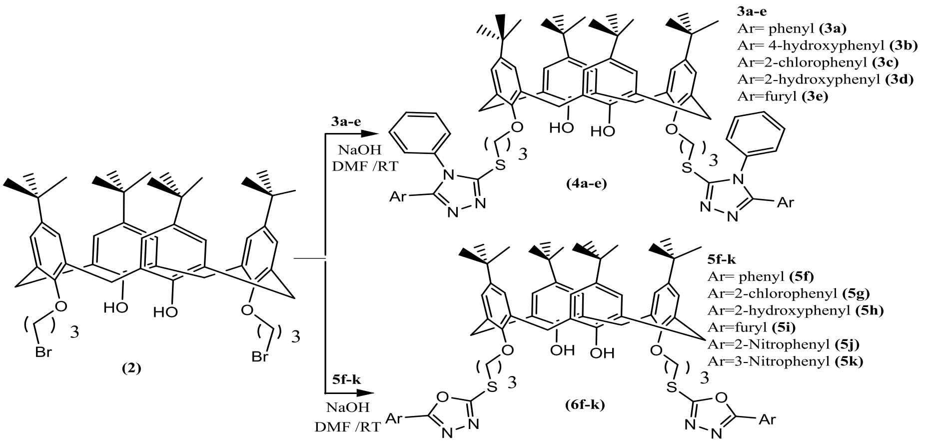

Figure 1. Scheme of the reaction

References

[1] C. D. Gutsche, M. Iqbal. Org. Synth.,68 (1990) 234.
[2] Z. T. Li, G. Z. Ji, C. X. Zhao, S. D. Yuan, H. Ding, C. Huang, A. L. Du., M. Wei. J. Org. Chem., 64(1999)3572.
[3] 36. R. Iqbal, K. H. Zamani., N. H. Rama. Turk. J. Chem., 20(1996)295.

Synthesis of Pyrrolobenzothiazole Derivatives from Benzothiazole and Acetylenic Esters

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Molecules that contain benzothiazole moieties are attractive targets fororganic synthesis because they often exhibit diverse and important biological properties [1]. Therefore, thesyntheses of benzothiazole derivatives have received an increasing attention to synthetic organic chemists and medicinal chemistry [2]. Pyrrolo[2,3]benzothiazole cyclization reactions of 2-methylbenzothiazole with dialkylacethylcarboxylates/alkylpropiolates and succinimide at room temperature under metal- and radiation- free conditions are described. Various aspects of these transformations will be presented and discussed.

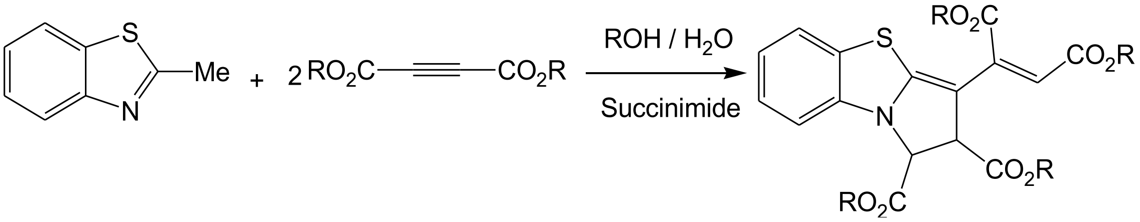

Figure 1. Scheme of the reaction

Refrences

[1] D.Cressier,; Prouillac, C.;Hernandez, P.; Amourette, C.; Diserbo, M.; Lion, C.; Rima, G. Bioorg. Med. Chem., 17 (2009) 5275.
[2] Yao, S.; Ahn, H. Y.; Wang, X.; Fu, J.; van Stryland, E. W.; Hagan, D. J.; Belfield,K. D. J. Org. Chem.,75 (2010)3965.

Optimization and purity Determination of Curcuminextracted from *Curcuma(longa) L.* by HPLC

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Medicinal plants have been used for mankind as source of medicines since a long time ago. More than 35,000 plant species have been reported to be used in various human cultures around the world for medical purposes [1].

Curcumin, 1,7-bis(4-hydroxy 3-methoxy phenyl)-1,6-heptadione-3,5-dione is a dietary phytochemical obtained from the dried rhizomes of the turmeric plant *(Curcuma longa)*. Traditionally curcumin has been used as a colouring, as a flavouring substance and as a food preservative.Because of its wide spectrum of biological activity, an extensive number of studies have been focused on curcumin. Recently, curcumin has also been shown to display anti-oxidant, anti-cancer, anti-viral, anti-infectious and anti-amyloidogenic properties.

Moreever, there are some methods for extraction of curcuminoids such as supercritical carbon dioxide extraction, microwave assisted extraction, ultra-sonic assisted extraction [2], maceration and Soxhlet extraction techniques. Here we have discussed about three methods of curcuminoidsextraction from Curcuma longa by using ethanol as a solvent. These methods are maceration, Soxhlet extraction andultra-sonic assisted extraction techniques. Firstthe yields of different extraction were studied and thenthe amount of curcumin was obtained from different extraction techniques discussed with HPLC. The results of HPLC have been shown that maceration technique is the best method for extraction of curcumin.

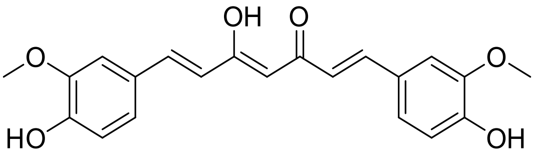

Figure 1. Scheme of the reaction

References

[1] W, Yee.Ching, Y.B. Yusoff, and W.Nurdiyana B. Wan. Journal of Food Chemistry and Nutrition, 2.1 (2014) 01.

[2] P.S. Wakte, B.S. Sachin, A.A. Patil, D.M. Mohato, T.H. Band, D.B. Shinde. Separation and Purification Technology, 79.1 (2011) 50.

Phytochemical study and evaluation the effects of different alcoholic extracts of *turmeric* on colon cancer cells HT29

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Turmeric is commonly known for its medicinal values in the majority of traditional medicinesystems.Curcumin is a main coloring substance in Curcuma longa and two related compounds, demethoxycurcumin and bisdemethoxycurcumin, are altogether known as curcuminoid.Curcumin, the most active curcuminoid found in Turmeric, has been shown to possess a multitude of beneficial effects in the treatment of cancers, cardiovascular disease, and inflammation [1].

The goal of this studying is evaluation of anticancer and anti-oxidant properties of Turmeric (Curcuma longa) on colon cancer cells HT29 and phytochemical analysis.The phytochemicals of turmeric have been identified by phytochemical methods [2]. The phytochemical tests have been done in this study are alkaloid, glycoside, flavonoid, tannin, saponin and fixed oils.In order to evaluate cytotoxic and anti-oxidant characteristics, ethanolic extracts from Turmeric has been obtained, using maceration, Soxhlet extraction, ultra-sonic assisted extraction techniques. The effects of these extracts on HT29 have been evaluated using MTT and NBT tests.

The results of photochemical showed that alkaloid, glycoside, flavonoid and fixed oils compounds, but no saponins and tannins are detected. The results of MTT showed the least cell survival value of treated cancerous cell was concerned to Soxhlet apparatus. Furthermore, the results of this research showed that the Turmeric extract by ultra-sonic displays peroxidant characteristics and drives the cancerous cell toward apoptosis. The existence of numerous compounds ethanolic extracts from Turmeric have been identified anti-oxidant and peroxidative properties of different extracts of Turmeric.

References

[1] S.J.Kulkarni, K.N. Maske, M.P.Budre,R.P.Mahajan. Int. J. Pharmacol. Pharm. Tech, 1 (2012) 2277.
[2] N. Deb, P.Majumdar, A. K.Ghosh. J Pharm Sci Tech, 2 (2013) 81.

Synthesis of Fe_3O_4@C-SO_3H nanoparticles as magnetically acid catalyst for the preparation of dihydropirimidinone

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Recently, the carbon based solid acid catalysts with high acidity and thermal stability have received wide attention [1]. Although the sulfonated carbon catalyst is active its speration from the reaction mixture is still achallenge during the practical application. The catalyst is generally recovered by the filtration or centrifugation methods which are dependent on special apparatus and time consuming. More recently, a magnetic sulfonatedmesoporous silica catalyst was reported for thehydrolysis of biomass, indicating that the magnetismseparation could be a feasible way to separate thecatalytic material from the reaction residues [2, 3].

Herein we report a method for the synthsis ofnew Magnetic Nano-catalyst with core-shell structure (Fe_3O_4@C-SO_3H).Fe_3O_4@C-SO_3H has been synthesized through the hydrothermal carbonization of glucose with magnetic cores and sulfonation of carbonaceous intermediate with PTSA (Scheme). Subsequently, the structure and morphologyof the preparednanocatalyst were studied with some differentspectroscopic, microscopic andthermogravimetric techniques such as FT-IR, XRD, FESEM and CHNS-Analysis.The magnetic Fe_3O_4 core makes the catalysts easily separated from reaction mixtures by using the externally applied magnetic field.

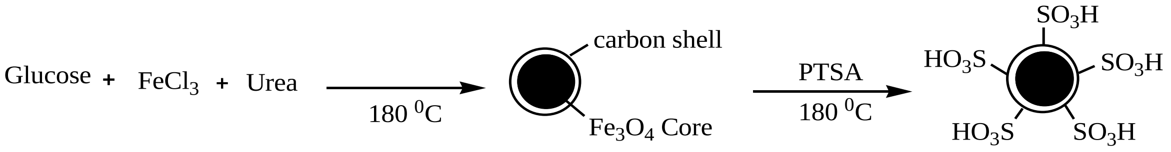

Figure 1. Scheme of the reaction

The application of this new nanocatalyst allows the synthesis of a Dihydopirimidinone through the reaction of aldehydes with urea and β-ketoesters undersolvent-free conditions. This synthetic pathway is a green protocol offering significant advantages, suchas easy preparation of the catalyst, mild reaction conditions and minimization of chemicalwaste.

References

[1] X.Liang. Chem. Eng. J., 264(2015)251-257.
[2] C.Zhang, H.Wang, F.Liu, L.Wang, H. He, Cellulose, 20(2013)127-134.
[3] B.Zhang, J.Ren, X. Liu, Y.Guo, G. Lu, Y.Wang. Catal. Commun., 11(2010) 629-632.

Formation of Nanostructured Thin Films at Liquid-Liquid Interface and Their Applications in the Organic Dye Degradation

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Textile industries produce effluents contain a large amount of colored dye contents which are toxic, non-biodegradable and has been considered as an important source of water pollutions in the world[1]. Mixing even only small proportion of these dyes with water cause environmental pollution and some other severe problems. Refractory azo dyes with one or more azo group (–N=N–) are one of the main class of colorants, constitute about a half of global production and used in tattooing, cosmetics, foods products, paper and texture industries and are commonly detected in texture wastewater (about 15% of them end up in wastewaters after dyeing operation processes).Due to their high surface to bulk ratio, nanoparticles possess high catalytic activity, have emerged in the treatments of several toxic chemicals in the environmentsuch as removing chemical wastes from water due to their potentials as promising candidates for sensors and catalysts. Oil/water interface strategy is introduced to provide effective platforms for rapid fabrication of large-area self-assembled nano films composed of different nanosized structures such as nanoparticles at room temperature [2, 3].

In this study, the reactions between some azo dyes and $NaBH_4$ catalyzed by nanoparticles thin films have been investigated. Here, we report insitu degradation of methyl orange, methyl red and bismarck brown by using thin films that monitored by UV–Vis spectroscopy. We used different thin films such as Pt, PtPd and $PtFeFe_2O_3$nanoparticle films and activity of these films was compared in the degradation of different dyes. Rate constants for the catalyzed reactions have been determined. PtPd nanoparticles thin film has shown the highest rate constant for the degradation of methyl orange.

References

[1] A. Bhankhar, M. Giri, K. Yadav, N. Jaggi, Indian Journal of Physics, 88 (2014) 1191.
[2] S.J. Hoseini, M. Rashidi, M. Bahrami, Journal of Materials Chemistry, 21 (2011) 16170.
[3] S.J. Hoseini, M. Bahrami, M. Dehghani, RSC Advances, 4 (2014) 13796.

Palladium-Based Nanoalloys as Catalyst for Suzuki-Miyaura Reaction

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In organic synthesis, palladium is one of the most useful catalysts for various C-C bond formations such as Suzuki-Miyaura reaction. Despite the important role of Pd catalysts, the use of Pd have some disadvantages, including the catalyst reusability and high cost attributed to the scarcity of the metal, thus postponing their industrial applications[1]. Some researchers developed alloying strategy to overcome these problems and prepare heterogeneous Pd catalysts[2]. Immiscible liquid interface route is an effective and low cost strategy for rapid fabrication of large-area self-assembled nano films of various nanosized structures which has the extraordinary physical and chemical properties. To achieve this goal, various two immiscible liquids were used for a contact angle of 90° of the particles with the water/oil interface which is essential for the interfacial entrapment of nanostructures [3].

In this study, palladium bimetallic nanoalloy thin films were prepared by a simple reduction method at toluene/water interface and employed as catalyst in the Suzuki−Miyaura reaction. The morphology and structure of the prepared thin films were characterized by X-ray diffraction (XRD), transmission electron microscopy (TEM) and energy dispersive analysis of X-ray (EDAX). TEM analysis exhibits a sponge structure for PdFe/Fe_2O_3 bimetallic nanoalloy thin film, snowman like structure for PdPt and spherical structures for PdNi and PdCu thin films. The cross-coupling reactions were performed under aerobic condition. These efficient and reusable catalysts pave away to green chemistry, with great potential for industrial applications.

References

[1] D. Astruc, Inorganic Chemistry, 46 (2007) 1884.
[2] S.J. Hoseini, M. Dehghani, H. Nasrabadi, Catalysis Science and Technology, 4 (2014) 1078.
[3] S.J. Hoseini, M. Bahrami, M. Roushani, RSC Advances, 4 (2014) 46992.

Fe_3O_4@Ni: A High Performance Recyclable Catalyst for Preparation of Oximes

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Oximes are highly crystalline materials and oximation isvery efficient method for characterization and purification ofcarbonyl compounds. These compounds not only represent auseful series of derivatives of carbonyl compounds but alsomay be used as intermediates for the preparation of amides bythe Beckmann rearrangement, nitrones, hydroximinoylchlorides, nitrile oxide and chiral α-sulfinyl oximes [1].The usual method for thepreparation of oximes involves treatment of aldehydes orketones with hydroxylamine [2]. In addition, a largenumber of other methods have been reported for performingof this transformation [3]. However, some methods in thisarea are not very satisfactory due to drawbacks such as lowyields, inability for the preparation of aromatic ketoximes, long reaction times, tedious work up and effluent pollution.In this work, we have used the nanomagnetic core-shell Fe_3O_4@Ni as a heterogeneous catalyst for thepreparation of oximes in water (Figure 1).

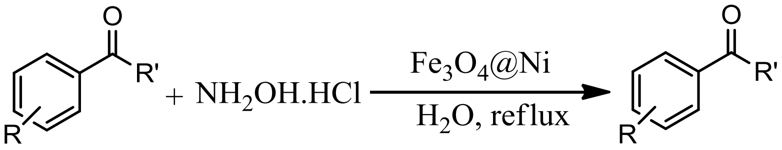

Figure 1. Scheme of the reaction

References

[1] A.R. Hajipour, F. Rafiee, A.E. Ruoho, J. Iran. Chem. Soc.7(2010) 114.
[2] I.J.Finar, G.H. Lord, J. Chem. Soc. 1957, 3314.
[3] H.Zang, M.Wang, B. W.Cheng, J.Song, Ultrason. Sonochem.16 (2009) 301.

Nano Core-Shell Iron Oxide@Copper Hydroxide: A High Performance Recyclable Catalyst for $NaBH_4$ Reduction of Nitroarenes to Arylamines

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The reduction of nitroarenes is an important process as the products, aromatic amines, are versatile intermediates and precursors in the preparation of dyes, pharmaceuticals, pigments, agrochemicals and polymers [1,2]. A variety of procedures and reducing agents are available for this purpose [3]. The main limitations of these works were prolonged reaction time, low yields, harsh conditions, use of harmful organic solvents, tedious work-up procedures and the use of expensive catalysts.In this work, we have used the nanomagnetic core-shell $Fe_3O_4@Cu(OH)_x$ as a heterogeneous catalyst for reduction of nitroarenes to arylamines in water (Figure 1). Remarkable reusability and easy separation of the nanocatalyst, high yields and mild reaction conditions as well as the benefits of using water as a green solvent are the advantages which make this protocol a perfect candidate for the reduction of nitroarens.

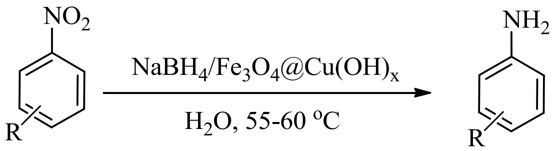

Figure 1. Scheme of the reaction.

References

[1] A. Saha, B. Ranu, J. Org. Chem. 73 (2008) 6867.
[2] Q. Shi, R. Lu, L. Lu, X. Fu and D. Zhao, Adv. Synth. Catal.349 (2007) 1877.
[3] X. Liu, Z. Ma, J. Xing, H. Liu,J. Magn. Magn.Mater.270 (2004) 1.

Synthesis of Novel Pyridopyrazoles by Reaction of Aminomethylene Malondialdehydes and 5-Amino-3-methylpyrazole Derivatives

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

Recently, we have been able to show that the principles embodied in transformations of simple indolenines *via* Vilsmeier formylations can be incorporated into more complex bisindolenine systems [5].

As a part of our continued interest to the amino heterocycles [6] we have now demonstrated the *p*-TSA catalyzed and green synthesis of novel pyridopyrazoles 2a-e by condensations of variously aminomethylene malondialdehydes 1 with electron-rich amino heterocycles in water (Scheme 1).

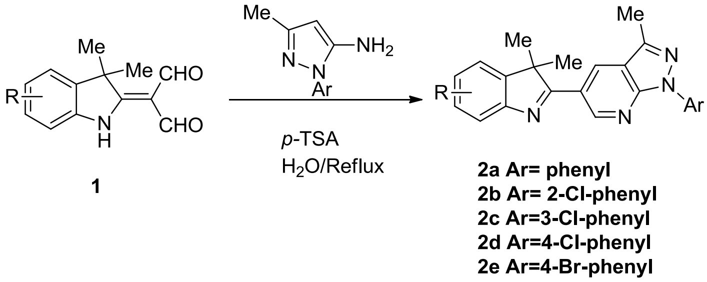

Figure 1. Scheme of the reaction.

References

[1] Baradarani, M. M.; Afghan, A.; Zebarjadi, F.; Hasanzadeh, K.; Joule, J. A. J. Heterocycl. Chem 2006, 43, 1591.
[2] Helliwell, M.; Afgan, A.; Baradarani, M. M.; Joule, J. A. Acta Crystallogr. Sect. E 2006, 62, o737.
[3] Rashidi, A.; Afghan, A.; Baradarani, M. M.; Joule, J. A. J. Heterocycl. Chem 2009, 46, 428.

One-Pot Three-Component Heterocyclizations of 5,6-Dihydro-1*H*-pyrrolo[3,2,1-*ij*]quinolone-1,2(4*H*)-dione, 6-Aminouracil Derivatives and Dimedones in Water

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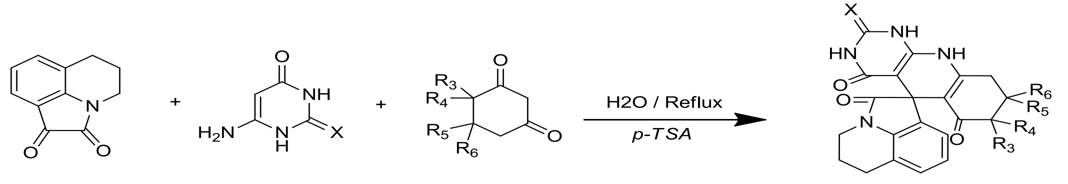
Multicomponent reactions (MCRs) became increasingly useful tools for the synthesis of biologically active compounds. These reactions enable multi-step syntheses to be conducted in a One-Pot fashion to obtain a variety of invaluable products. Moreover, MCRs can dramatically reduce the generation of chemical waste and reduce the cost of the starting materials [1]. Uracil and its annelated analogs occupy a unique place in the field of medicinal chemistry as useful anticancer and antiviral drugs [2]. The versatility of uracil derivatives for the synthesis of nitrogen-containing heterocycles of biological importance has been well documented in the literature [3]. As a part of our continued interest to the synthesis of novel spirocyclic compounds [4-6] we decided to examine One-Pot , *p*-TSA catalyzed reaction of 5,6-dihydro-1*H*-pyrrolo[3,2,1-*ij*]quinolone-1,2(4*H*)-dione 1, 6-amino uracil 2a and 1,3-dicarbonyl compound 3a in refluxing H_2O.Evidence for the compound 4a came from a study of the H-nmr spectra of the product. Encouraged by this success, we extended this reaction to various dimedones 3b-c and 6-aminthiouracil 2b under similar conditions, furnishing the compounds 4b–e in good yields.



1

2
2a X=O
2b X=S

3
3a R^3, R^4, R^5, R^6=H
3b R^3, R^4=Me, R^5, R^6=H
3c R^3, R^4=H, R^5, R^6=Me

4
4a R^3, R^4, R^5, R^6=H, X=O
4b R^3, R^4=Me, R^5, R^6=H, X=O
4c R^3, R^4=H, R^5, R^6=Me, X=O
4d R^3, R^4, R^5, R^6=H, X=S
4e R^3, R^4=H, R^5, R^6=Me, X=S

Figure 1. Schem of the reaction.

References

[1] Muravyova, E. A.; Tkachenko, V. V.; Desenko, S. M.; et al. Arkivoc 2013, (iii), 338.
[2] Macilwain, C. Nature (London) 1993, 365, 378.
[3] Bradshaw, T. K.; Hutchinson, D.W. Chem Soc Rev 1997, 6, 43.

Core-Shell of Pd@NiZn/Reduced-Graphene Oxide Thin Film at Toluene-Water Interface as an Efficient Catalyst in Suzuki- Miyaura Reaction

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Metallic particles have attracted tremendous interest because of their large surface areas and large numbers of edge and corner atoms, which dramatically improve their catalytic performances [1].Core-shell nanoparticles have given rise to great research interest because of their different novel properties. These nanoparticles have rised at the frontier between materials chemistry and other fields, such as electronics, biomedical, pharmaceutical, optics, and catalysis [2]. Core-shell nanoparticles often exhibit improved catalytic properties compared to their alloyed counterparts or to mixtures of monometallic nanoparticles. In addition to the improved material properties, core-shell materials are also significant from an economic aspect. A precious material can be coated over an inexpensive material to reduce the use of the precious material compared with making the same sized pure material [3].

In this study, a facile and efficient method was used to prepare the Pd@NiZn/reduced-graghene oxide and Pd@NiZn core-shell nano films. The morphologies and structures of the prepared thin films were characterized by X-ray diffraction (XRD), transmission electron microscopy (TEM) and energy dispersive analysis of X-ray (EDAX). Our study shows that both of these core-shell nanostructures display superior activity and durability in catalyzing Suzuki–Miyaura coupling reaction. Compared to the classical reactions, this method consistently has the advantages of a green solvent, short reaction times, low catalyst loading, high yields and reusability of the catalyst.

References

[1] X. Chen, G. Wu, J. Chen, X. Chen, Z. Xie, X. Wang, Journal of the American Chemical Society 133 (2011) 3693.
[2] S.J. Hoseini, M. Bahrami, M. Dehghani, RSC Advances 4 (2014) 13796.
[3] S.J. Hoseini, M. Rashidi, M. Bahrami, Journal of Materials Chemistry 21 (2011) 16170.

Synthesis and characterization of novel S-(5-aryl-1,3,4-oxadiazol-2-yl) 2-chloroethane- thioate linkage tetra-*tert*-butyl calix[4] arene derivatives

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A series of S-(5-aryl-1,3,4-oxadiazol-2-yl)2-chloroethanethioate**(2a-e)** substituted tetra-tert-butyl calix[4]arene derivatized at lower rim were synthesized by the reaction of S-(5-aryl-1,3,4-oxadiazol-2-yl)2-chloroethanethioate with tetra-*tert*-butylcalix[4]arene **(1)**. The synthesized compounds were characterized by FT-IR, ^{1}H NMR, ^{13}C NMR, elemental analysis.

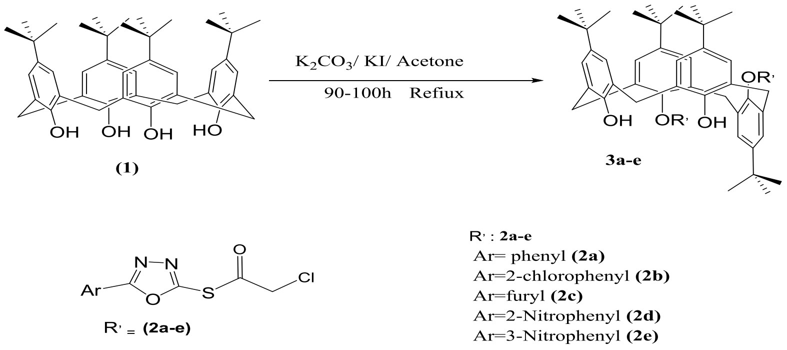

Figure 1. Scheme of the reaction.

References

[1] C. D. Gutsche., M. Iqbal. Org. Synth. 68, 234 (1990).
[2] R. Iqbal, K. H. Zamani., N. H. Rama.Turk. J. Chem. 20, 295 (1996).
[3] (a) I. K. J. Al-Joubory, T. F. K. Albayati, K. A. J. Albayati., T. S. M. Al-Joubory, Diyala. J. Pure. Sci.9, 47 (2013). (b) C. H. Lee, H. I. Cho., K. Lee. J. Bull. Korean Chem. Soc. 22, 1153 (2001).

Industrial proparation of Rivastigmine tartarate and synthesis of its Azolic derivatives

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Alzheimer disease (AD) is a complex neurological affection that is clinically characterized by loss of memory. Rivastigmine, an acetyl cholinesterase (AChE) inhibitor approved in 2000 for the treatment of AD, bears a carbamate moiety in its structure, which is able to react covalently with the active site of the enzyme [1,2].

Our process for the straight forward synthesis of enantiomerically pure Rivastigmine Tartarate, (S)-N-ethyl-N-methyl-3-[-(dimethylamino)ethyl]-phenyl carbamate hydrogen-(2R,3R)-tartarate withUSP38 has been efficiently carried out under mild reaction condition with NaOMe as a basic catalyst, that is easy to scale up in industry and suitable for the manufacture of Rivastigmine in active pharmaceutical ingredient (API) demand.

This process is convenient operation and purification and completes the synthesis of RivastigmineTartarate in 93% overall yield. The purity of product was characterized by HPLC analysis.

On the basis of previous studies on a series of benzopyrano[4,3-b]pyrrolecarbamates asacetyl cholinesterase (AChE) inhibitors, we designed and synthesis a series of conformationally analogues of Rivastigmine by including the N-ethyl-N-methyl carbamoyl moiety in different azolic systems.

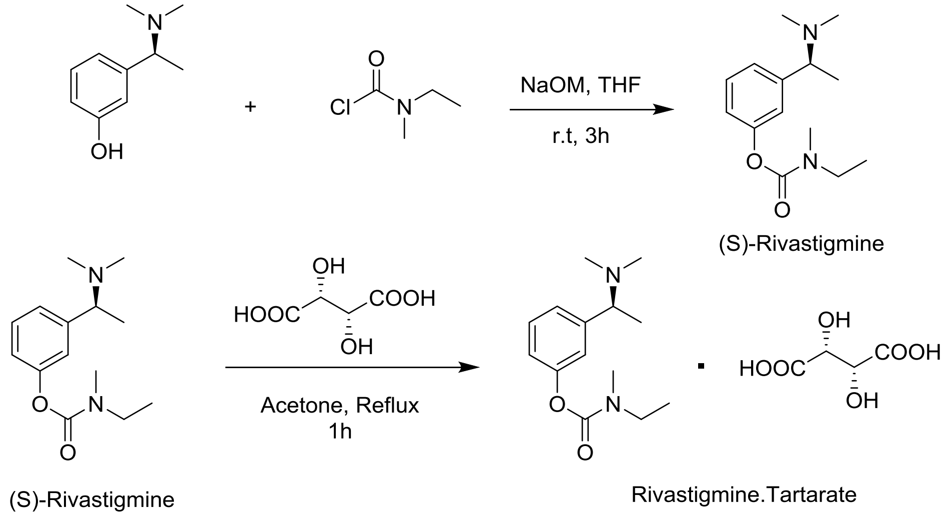

Figure 1. Scheme of the reaction.

References

[1] P.C. Yan, G.L. Zhu, J.H. XiE, Journal of Organic Process Research & Development 17 (2013) 307.
[2] M.L. Bolognesi, M. Bartolini, A. Cavalli, Journal of Medicinal Chemistry 47 (2004) 5945.

Poly (Vinylimidazolium\divinylbenzene)-copper Complex: A Highly Active and Robust Heterogeneous Catalytic System for Click Reaction

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Mesoporous polymers have receivedconsiderable attention inthe broad- range of applications such as catalysis[1]separation [2] and ect.Because of their large surface area, high thermal and mechanical stability.Herein a functionalized mesoporous polymer, poly (Vinylimidazolium –divinylbenzene)-copper complex, was successfully synthesized by free radical polymerization of vinyl imidazolium and DVB. The resulting heterogeneous catalyst is shown to be an efficient catalyst for the synthesis 1, 4-disubstituted of 1, 2, 3-triazoles(the Huisgen reaction)[3] at room temperature in high yields (Figure 1). Nitrogen adsorption measurements and electron microscopy were used to examine the porous structures. The catalyst could be recovered and was reused several times without significant loss of activity.

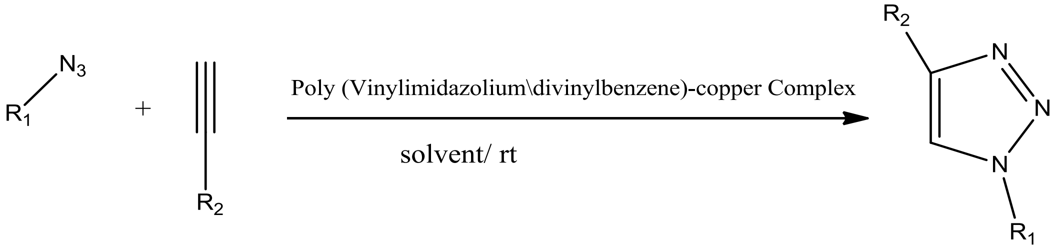

Figure 1.Click Reaction Catalyzed by Poly (Vinylimidazolium\divinylbenzene)-copper Complex

[1] Adv. Synth. Catal.2008, 350, 2065.
[2] J. Polym. Sci.,Polym. Lett.Ed. 1985, 23, 103.
[3] Huisgen, R. Pure Appl. Chem. 1989, 61, 613.

Synthesis of new sulfur-containing heterocycles through the One-Pot multicomponent reactions

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Due to the presence of sulfur atom in many of the biologically and pharmaceutically active molecules, introduction of sulfur atom into the organic compounds has received much interest in the organic synthesis [1]. The best way to approach this aim is the formation of carbon-sulfur bond.On the other hand, multicomponent reactions (MCRs) are important to provide efficient routes for the synthesis of heterocyclic compounds.Although significant advances have been madein the case of MCRs, there is still a high demand for newprocesses for the synthesis of heterocyclicmolecules [2]. In this presentation we wish to report One-Pot multicomponent procedures for the synthesis of various sulfur-containing heterocyclic compounds from the reaction of primary amines and carbon disulfide (or phenyl isothiocyanate) in the presence of electrophiles such as dimethyl acetylene dicarboxilate, 2-chloroacetaldehyde, chloroacetylchloride, acryloyl chloride, and α,β-unsaturated aldehydes.

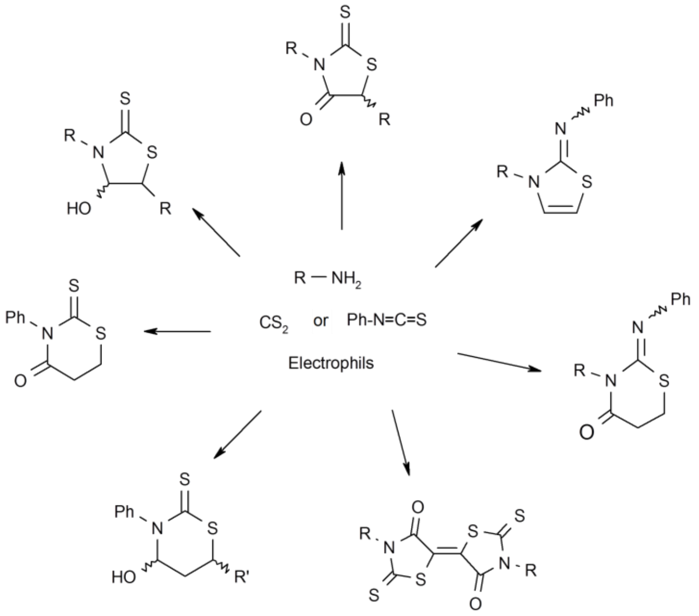

Figure 1.scheme of the reaction

References

[1] For a list of the top selling sulfur-containing drugs in 2012 with structures, see: http://cbc.arizona.edu/njardarson/group/top-pharmaceuticals-poster

[2] J. D. Sunderhaus, S. F. Martin, Chemistry 15 (2009) 1300.

Synthesis of Naphthofuran Derivatives in the Ionic Liquids

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The last two decades have seen an explosion of interest in ionic liquids, much of the interest in ionic liquids has centered on their possible use as green solvent. IL's are salts consisting completely of organic cations and inorganic or organic anions [1].

A facile and efficient approach for the synthesis naphthofuran derivatives isusing ionic liquid as solvent. reaction of β-Naphthoxyketones in IL's are obtained in good to excellent yields of naphthofuran.

In this work, first we synthesis β-Naphthoxyketone from β-naphtol and α-boromoketon in K_2CO_3/acetone [2], then use acidic ionic liquid [bmim]HSO_4, and [hmim]$FeCl_4^-$ for synthesis of naphthofuran derivatives.

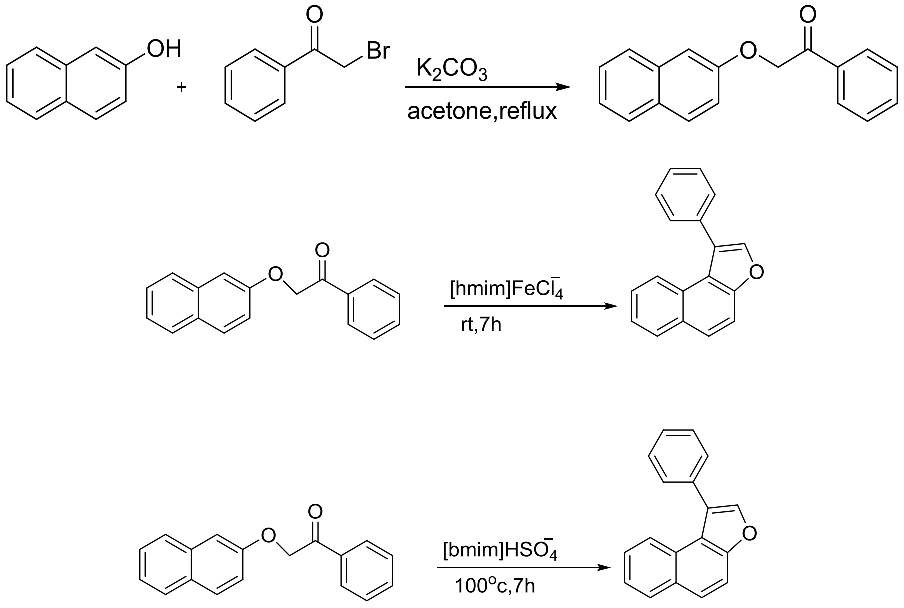

Figure 1. Scheme of the reaction.

References

[1] P. Wasserscheid, T. Welton, (eds) (2007) Ionic Liquids in Synthesis, 2nd edn, Wiley-VCH Verlag GmbH, Weinheim.

[2] H. Meizi, Y. Ning, S. Chunlal, Y. Xiaojin, Y. Ming, Medicinal chemistry research 20 (2011) 200-209.

A novel One-Pot , four component synthesis of 2-amino-1, 4-dihydropyridin derivatives

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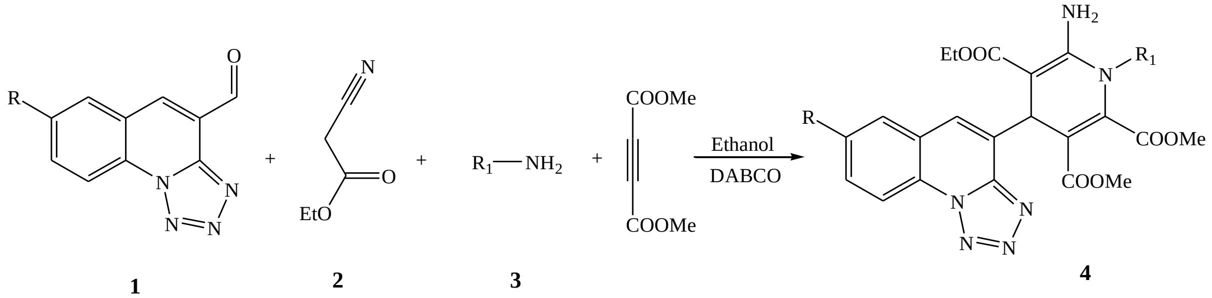
Quinoline ring systems represent a major class of heterocycles in which benzene ring is fused with pyridine ring. The derivatives of quinoline exhibit diverse biological and physiological activities such as antimalarial, anti-inflammatory, antitumor, DNA binding capacity, and antibacterial properties. Recently, quinoline has been employed in the study of bio-organic and bio-organometallic processes. The quinoline skeleton is often used as a key intermediate for the design of many pharmacologically important synthetic compounds [1]. The fusion of quinoline to the tetrazole ring is known to increase the biological activity [2].

In this work, we wish to report an efficient One-Pot four component synthesis of 2-amino-1,4-dihydro pyridine derivatives 4 from the reaction of tetrazolo[1,5-a]quinoline-4-carbaldehydese**1**, ethyl-2-cyanozcetat 2, primary amines 3, and di methyl acetylenedi carboxylate in the presence of DABCO in ethanol. The reaction was completed in 4 hr to give products in moderate yields.



R: H, CH_3

R_1: propyl, benzyl, phenethyl, paramethoxyphenethyl

Figure 1. Scheme of the reaction.

References

[1] S.S. Sonar, S. A. Sadaphal, R.U. Pokalwar, B.B. Shingate, M.S. Shingare Journal of Heterocyclic Chemistry 47 (2010) 441.

[2] A. Mukherjee, M.S. Akhtar, V.L. Sharma, M. Seth, A.P. Bhaduri, A. Agnihotri, P.K. Mehrotra, V.P. Kamboj Journal of Medicinal Chemistry 32 (1989) 2297.

Serendipitous synthesis of 4-thioxochromen-2-one derivatives through the One-Pot three-component reaction of primary amines, carbon disulfide, and 4-chlorocoumarin-3-carbaldehyde

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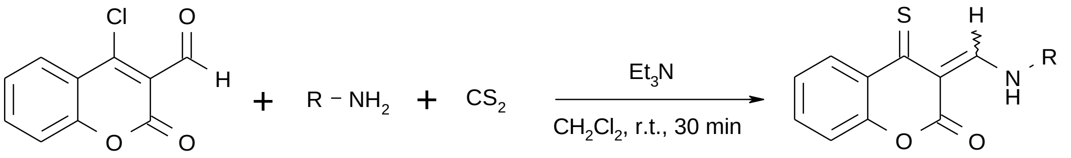
Coumarins are an important class of natural and synthetic compounds that show various biological activities [1], which often depending on the substituent on the benzopyran moiety. For example, some coumarine derivatives having pyridine substituted at 3- or 4-position of the coumarine ring possess CNS depressant activity [2]. Also a number of coumarin derivatives used as an intermediate to produce various biologically active compounds [3]. In addition, these compounds are useful as organic electroluminescent materials [4].

In this paper we wish to report One-Pot three component reaction between 4-chlorocoumarin-3-carbaldehyde andprimary amines in the presence of carbon disulfide and thriethylamine leads to 4-thioxochromen-2-one derivativesin good to excellent yields.



R:propyl, isopropyl, ethyl-1-ol, propyl-2-ol, benzyl, phenethyl, *p*-methoxyphenethyl, (*S*)-1-phenyl ethyl

Figure 1. Scheme of the reaction.

References

[1] M. Małecka, E. Budzisz,crystal engineering communication16 (2014) 6654.
[2] RB.Moffett,Journal of Medicinal Chemistry7 (1964) 446.
[3] T. Dubutfet, O. Muller, S.S.Simonef, J.J.Descomhes, M. Laubie, T.J. Verheuren, G. Lavidle,Bioorganic& Medicinal Chemistry Letters 6 (1996) 349.

Pd-S-Benzylisothiourea on Fe_3O_4 magnetic nanoparticles: efficient and reusable nanocatalyst for organic reactions

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Palladium is one of the most crucial metals in catalysis and it has been commonly applied as one of the most powerful tools for the organic reactions such as Carbon−Carbon bond formation or organic synthesis. In particular, palladium-catalyzed cross-coupling reactions of aryl halides such as Suzuki and Heck coupling reactions have become a powerful stay in modern synthetic organic chemistry for the preparation of natural products, agrochemicals, pharmaceuticals, biologically active compounds, herbicides, UV screens, preparation of hydrocarbons, polymers, liquid crystal materials and advanced materials [1]. Homogeneous Pd-catalysts have been extensively studied in synthetic organic chemistry because of their higher catalytic activity and selectivity. Removal of palladium from organic products at the end of the reaction is highly desirable because of its high cost and toxicity. Therefore, to combine the advantages of both heterogeneous and homogeneous catalysts, immobilization of homogeneous catalysts on the nanoparticles is the best choice, which efficiently bridges the gap between heterogeneous and homogeneous catalysts. However, the all supporting nanocatalyst have some disadvantages such as difficult or time consuming and expensive separation of fine particles from a reaction mixture. This drawback can be overcome by magnetic nanoparticles, which can be rapidly and easily isolated from the reaction mixture using an external magnet [2].

Herein, we reported a new complex of palladium that immobilized on Fe_3O_4 MNPs and further used as an excellent nano organometal catalyst for the Suzuki reaction and One-Pot synthesis of polyhydroquinoline derivatives, because polyhydroquinoline derivatives have been reported to possess a wide range of pharmaceutical activities and biological properties [3, 4].

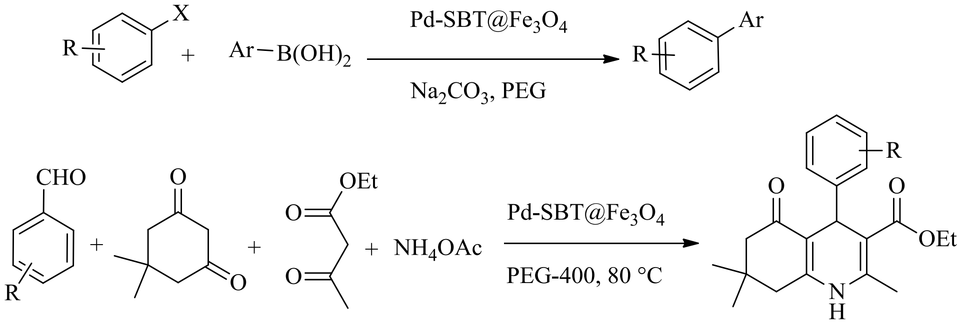

Figure 1. Scheme of the reaction.

References

[1] A. Ghorbani-Choghamarani, B. Tahmasbi, P. Moradi, RSC Advances6 (2016) 43205.
[2] A. Ghorbani-Choghamarani, B. Tahmasbi, P. Moradi Applied Organometallic Chemistry 30 (2016) 422.
[3] M. Hajjami, B. Tahmasbi, RSC Advances5 (2015) 59194.

New complex supported on magnetic nanoparticles: as efficient and reusable nanocatalyst for synthesis of sulfide derivatives

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In recent years, supported catalysts on the nanoparticles have attracted much attention in organic reactions. The main drawback of these catalysts is their separation; because nanoparticles have diameters of less than 100 nm, which cannot be separated by conventional methods such as filtration techniques [1]. This draw back can be overcome using magnetic nanoparticles (MNPs), which can be easy recovered from the reaction mixture by external magnet. Furthermore, magnetic separation of the MNPs is more effective and easier than filtration or centrifugation [2]. MNPs are readily available and high-surface-area resulting in high catalysts loading capacity and outstanding stability. The functionalized of MNPs are a kind of novel functional materials, which have been widely used in biotechnology and catalysis studies [3]. Existence of many hydroxyl groups on the MNPs surface leads to reaction with alkoxysilane reagents and formation of Si–O bonds which support terminal functional groups available for immobilization of other substances [4]. Herein, we reported a new complex of Ni that immobilized on Fe_3O_4 MNPs and further used as an excellent nano organometallic catalyst for the synthesis of sulfide derivatives, because sulfide derivatives have been reported to possess a wide range of pharmaceutical activities and biological properties and also sulfides are starting material in organic synthesis [5].

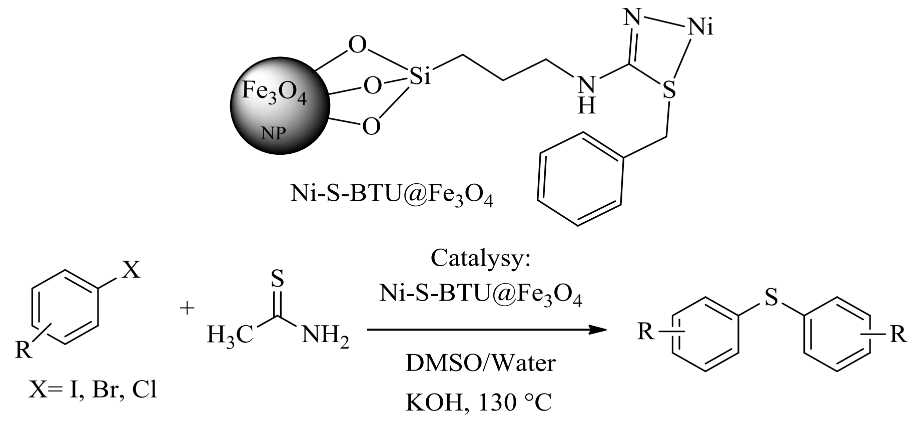

Figure 1. Scheme of the reaction.

References

[1] F. Havasi, A. Ghorbani-Choghamarani, F. Nikpour, New Journal of Chemistry 39 (2015) 6504.
[2] A. Ghorbani-Choghamarani, B. Tahmasbi, P. Moradi Applied Organometallic Chemistry 30 (2016) 422.
[3] C.W. Lim, I.S. Lee, Nano Today 5 (2010)412.

Carbon coated Cu nanostructures as a green nanocatalyst for Suzuki cross-coupling reaction

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The Suzuki-Miyaura cross-coupling reaction of Arylboronic acid with Aryl halides (C_{sp2}-X) has become a popular tool for selective construction of carbon-carbon bonds and mainstay of modern synthetic organic chemistry for the preparation of biaryl compounds[1].The use of copper-based alternatives in the cross-coupling reactions are taken into consideration, due to their orders of magnitude lower cost and harmfulness to the environment than other noble metals. Surprisingly, only a few copper-catalysed Suzuki cross-coupling procedures exist[2,3].In this work a new copper based catalytic system in Suzuki cross-coupling reaction was developed. For this purpose carbon stabilized well dispersed copper nanowires were synthesized as ligand free and inexpensive heterogeneous nanocatalyst. In fact,our aim has been to investigate application of the efficient, inexpensive, and ligand free copper based catalytic system with high activity for Suzuki cross-coupling reaction with minimum by-products in green media for first time. Soft hydrothermal/solvothermal reduction method under mild aqueous conditions have been exploited to fabricate copper nanowires/nanoparticles. To prevent aggregation of metal nanoparticles, a thick carbon layer coating was performed via hydrothermal method. This green nontoxic catalytic system reused at least 4 time in Suzuki reaction without significant loss of catalytic activity.

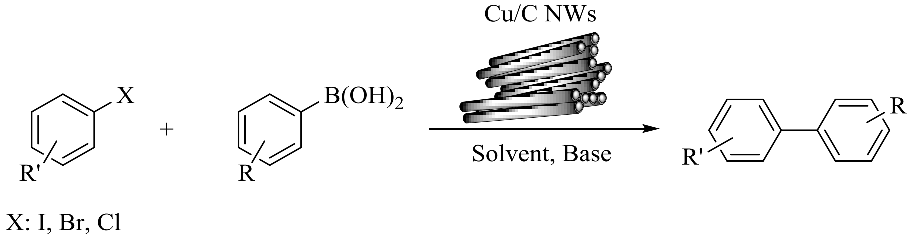

Figure 1. Schematic pathway for Cu/C NWs catalyzed Suzuki reaction.

References

[1] A. Suzuki, Chem. Commun.38,2005, 4759-4763.
[2] M. J. Jin, D. H. Lee, Angew. Chem. Int. Ed. Engl.49,2010, 1119-1122.
[3] S. Gu, J. Huang, X. Liu, H. Liu, Y. Zhou, W. Xu, Inorg. Chem. Commun.21,2012, 168-172.

Application of the Ugi reaction for the synthesis of novel 2-oxo-1-phenylethyl-N-phenylacetamide derivatives

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Multi-component reactions (MCRs) are powerful synthetic tools for the diversity-oriented synthesis (DOS) to generate combinatorial libraries [1]. They play a key role in drug discovery. MCRs are highly convergent and atom efficient generating high molecular complexity in a single-step process.Among MCRs, the Ugiand Passerini reactions, are the most popular approaches for the combinatorial chemistry [2,3].

In continuation of our recent research on development of novel multicomponent reactions, in this reaction we wish to report a simple and efficient One-Pot four-component reaction of, Aniline 1**,** Isocyanate 2**,** Aldehydes 3and Indomethacin 4 to yield novel 2-oxo-1-phenylethyl)-N-phenylacetamidederivatives. All products were confirmed by^{1}H NMR, ^{13}C NMR spectroscopy, melting point andFT-IR spectroscopy.

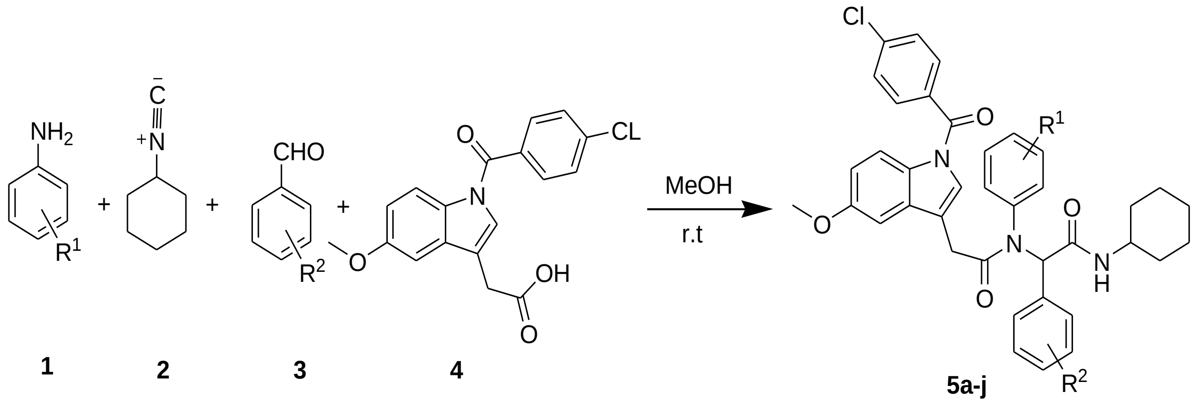

Figure 1.Synthesis of novel 2-oxo-1-phenylethyl)-N-phenylacetamide derivatives

References

[1] Domling, A.Chem. Rev. 2006, 106, 17.
[2] Kulsi, G.;Ghorai, A.; Chattopadhyay, P. Tetrahedron Lett.2012, 53, 3619.
[3] Reddy, B. V. S.; Dey, S. K.; Yadav, J. S.; Sridhar, B. TetrahedronLett. 2012, 53, 3676.

Microwave promoted synthesis of 4,5-dihydrofurans via three-component reaction in solvent-free conditions

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Dihydrofurans are the most important heterocycles commonly found in a wide range of biologically active synthetic and natural products [1]. The development ofresource and eco-friendly process in termsof sustainable chemistry for their synthesis remains an area of current interest, and various synthetic methods have been reported in literature. The use of microwave for the synthesis of organic compounds under solvent-free conditions proved to be efficient, safe and environmentally benign technique, with shorter reaction time, high yield, and easier work-up [2].

In continuation of our research on the development of new methodologies for synthesis of heterocyclic compounds and use of green chemical techniques [3], we herein disclose microwave assisted synthesis of 4,5-dihydrofurans 4 in good yields by three-component reaction of 3-(cyanoacetyl)indole1 with aromatic aldehydes 2 and *N*-phenacylpyridinium bromide 3 under solvent-free conditions (Figure 1).The structure of products is characterized on the basis of their elemental analysis, ^{1}H NMR and ^{13}C NMR, IR and mass spectra.

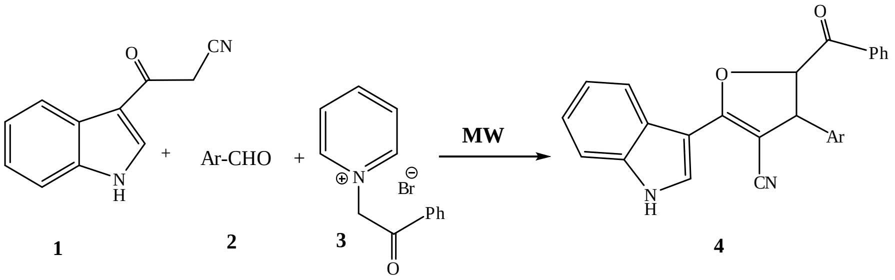

Figure 1.Synthesis of 4,5-dihydrofurans under microwave irradiation.

References

[1] C.P. Chuang, K.P. Chen, Tetrahedron 68 (2012) 1401.
[2] S. Majumder, M. Sharma, P.J. Bhuyan, Tetrahedron Letters 54 (2013) 6868.
[3] R. Baharfar, R. Azimi, Synthetic Communications 44 (2014) 89.

4-Sufophthalic acid as an efficient catalyst for the multicomponent One-Pot synthesis of substituted pyrazolones in aqueous media

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The research in multi-component reactions (MCRs) is a hot topic of organic chemistry because of their advantageous in the preparation of different heterocyclic molecules and in drug discoveryprocedures[1]. Although MCRs are efficient, environmentallyfriendly, fast, atom economic and time saving style. They supplyan effective tool for the preparation of various compounds withpharmaceutical and biological properties[2]. One type of thesereactions is the synthesis of pyrazolones which display biologicaland pharmacological properties.In order to develop a new method for the synthesis of Pyrazolones, we report here 4-sulfophthalic acid assisted synthesis of Pyrazolones, from the condensation of phenyl hydrazines, ethyl acetoacetate ,β-naphthol and benzaldehydes in water as solvent at in reflux condition.

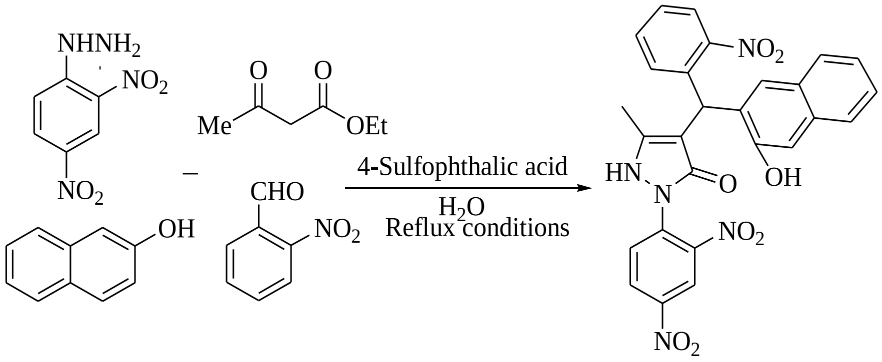

Figure 1.The reaction of 2,4-dinitrophenylhydrazine (1 mmol) and ethyl acetoacetate (1 mmol) aromatic aldehyde (1 mmol), 2-naphthol (1 mmol) as a model reaction.

References

[1] G. Cravotto, P. Cintas. Chemical Society Reviews 35 (2006) 180.
[2] J.T. Li, S.X. Wang, G.F. Chen, T.S. Li, Current Organic Synthesis 2 (2005) 175.

Synthesis of Bis(indolyl)methane Derivatives Catalyzed by 4-Sulfophthalic acid in Green Media

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In recent years, bis(indolyl)methanes(BIMs) have attracted considerable attention on account of their wide applications in the pharmaceutical and agrochemical sciences. Also, these heterocycles are important class of heterocyclic compounds in the pharmaceutical as well as synthetic chemistry. They are important antibiotics in the field of pharmaceuticals and also effective in the prevention of cancer [1-3]. In this simple research work, 4-sulfophthalic acidcatalyzed reaction of indole with different aryl aldehyde compounds in water yielded bis(indolyl)methane derivatives in high yield. The merits of this method are efficient, clean, easy work-up, and shorter reaction times.

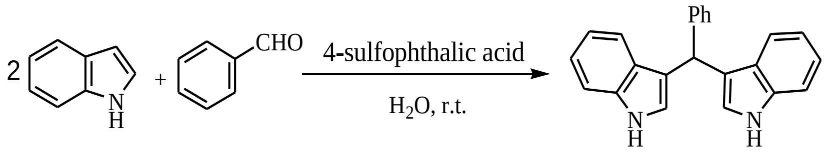

Figure 1.The reaction of Indole with benzaldehyde as a model reaction.

References

[1] Y.L. Yang,N.N. Wan,W.P. Wang,Z.F. Xie,J. D.Wang.Chines Chemical Letters *22*(2011)1071.
[2] K.Parvanak Boroujeni,K. Parvanak.Chines Chemical Letters22 (2011) 939.
[3] E.Kolvary,M. A. Zolfigol,H. Banary. Chines Chemical Letters*22*(2011)1305.

C-C bond cleavage of aziridines

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Aziridines exhibited intriguing and diverse reactivity, and thus have became unique and versatile synthons in organic synthesis. C–N/C-C bond cleavage of aziridine ring is a useful way to serve as three-atom synthons with extensive applications in organic synthesis. [1]

In contrast with ordinary solvents, such as Volatile Organic Compounds (VOC), DESs have a very low vapour pressure, and thus are non-flammable. The same reference mentions that DESs have a relatively high viscosities which might hinder their industrial applications as they might not flow easily in the process streams. DESs favorably possess low densities and can be liquid at a wide range of temperatures. Other studied properties for some DESs are their electrical conductivities, pH indices and surface tensions, which might be added to this article by any contributor.[3]

Unexpected regioselective oxidation of ketoaziridines to the corresponding aldehydes with choline chloride/thiourea is described. This regio-selective reaction presumably precedes via a domino sequence C-C/C-N cleavage of ketoaziridine ring. This metal-free method proved to be efficient for the oxidative cleavage of several ketoaziridines in moderate to good yields.

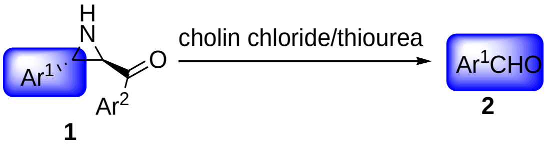

Figure 1.Regio-selective oxidation reaction of ketoaziridines

References

[1] H. A.; Samimi, M. Y. Bohari and F. Saberi, Synthesis, 2015, 47, 129.
[2] H. A.; Samimi and M. Y. Bohari, Tetrahedron Lett. 2016, 57, 223.
[3] G. García, S. Aparicio, R.Ullah and M.Atilhan,Energy Fuels, 2015, 2616.

Synthesis of chromene-3-carbonitrile and pyrano[2,3-d]pyrimidines, starting from cyclic active methylene compounds in the presence of novel deep eutectic solvents as promoter

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A simple and efficient protocol with environmental, has been developed for the One-Pot , multicomponent synthesis of fused six membered highly saturated chromene and pyrano[2,3-d]pyrimidines derivatives. These compounds have shown diverse medicinally [1] important effects such as anti-coagulant [2], anti-espasmodic [3], anti-bacterial[4], anti-cancer [5], The use of deep eutectic solvents for the preparation of organic molecules has been emerged as a vital and progressive area of research in recent years [6].

In the recent work, the condensation of various aldehydes, dimedone and mlononitrile in the ratio of 1: 1: 1.2 mmol respectively in the presence of three different deep eutectic solvents is reported. The eutectic solvents applied in this protocol include Choline chloride:urea (1:2), Choline chloride:L-proline (1:1) and Choline chloride:Glucose (1:1). The reactions were well performed at ambient temperatures (30-40^{o}C) and the 2-amino-7,7-dimethyl-8-oxo-4-phenyl-5,6,7,8-tetrahydro-4*H*-chromene-3-carbonitrile and pyrano[2,3-d]pyrimidine-3-carbonitrile products were easily separated from eutectic solvent by dissolving the reaction mixture in water and vacuum filtration. Relatively short reaction times, no need to extra harmful organic solvent, high yields and simple work-up procedure were among the other advantages of the present protocol.

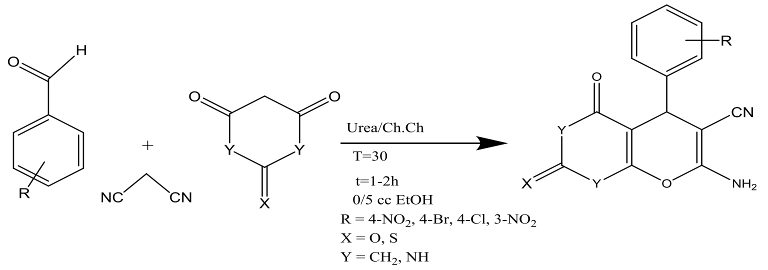

Figure 1.The synthesis of chromene and pyrano [2, 3-*d*] pyrimidine derivatives in the presence of deep eutectic solvent

References

[1] Li, F., Meng, Z., Hua, J., Li, W., Lou, H., Liu, L. Organic and biomolecular chemistry 13.20 (2015): 5710.
[2] Makarem, S., A. A. Mohammadi, and A. R. Fakhari. Tetrahedron Letters 49.50 (2008): 7194-7196.
[3] Lu, J., Fu, X. W., Zhang, G., Wang, C. Research on Chemical Intermediates (2015): 1-8.

Covalent Attachment of CyclometallatedPalladum(II) Complex to Functionalized Graphene Oxide as an Effective Catalyst for the Suzuki–Miyaura Reaction

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The Suzuki- Miyaura reaction has matured into a very powerful tool for the formation of new carbon – carbon bonds and is routinely used in fine chemicals research and pharmaceutical discovery laboratories.[1-3] In this study, a palladium supported catalyst has been synthesized by covalently bonding of a novel cyclometalatedorganopalladium(II) complex containing N-aromatic ligand onto the graphene oxide (GO) surface through coordination interaction with 3-(aminomethyl)pyridine (3-ampy) ligand spacers. The [Pd(C^N)Cl(3-ampy)]/GO nanohybrid, which C^N =N(1), C(2′)-chelated deprotonated 2-phenylpyridine, was characterized using Fourier transform infrared spectroscopy (FT-IR), Raman spectroscopy, energy dispersive X-ray analysis (EDAX), X-ray photoelectron spectroscopy (XPS), X-ray diffraction (XRD), and transmission electron microscopy (TEM). The supported catalyst showed enhanced catalytic performance towards Suzuki–Miyaura carbon–carbon coupling reaction compared with the homogeneous analogue, and it could be readily recycled and reused several times without discernible loss of its activity. The [Pd(C^N)Cl(3-ampy)]/GO nanohybrid showed highly improved catalytic activity toward aryl chloride derivatives as compared with other catalysts that have been reported. As shown in Figure 1, the catalyst/K_2CO_3 system was effective for the coupling of various aryl halides with phenylboronic acid in solvent toluene at room temperature.

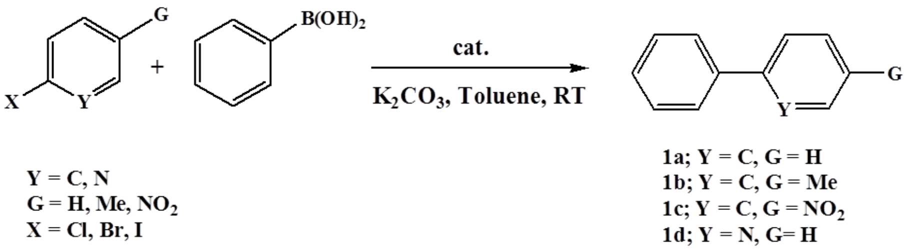

Figure 1.Suzuki–Miyaura cross-coupling reactions catalyzed by palladacycles.

References

[1] J. P. Corbet, G. Mignani.Chem. Rev 106 (2006) 2651.
[2] S. J. Hoseini, M. Dehghani, H. Nasrabadi.Catal.Sci. Technol 4 (2014) 1078.
[3] S. J. Hoseini, H. GhanavatKhozestan, R. HashemiFath.RSC Adv 5 (2015) 47701.

Synthesis of some imidazolopyridopyazine from pentachloropyridine

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In recent years, considerable attention has been given to the synthesis of benz- and bis-imidazole derivatives due to their various pharmacological activities [1,2]. 2-chloromethyl-1H-benzimidazole derivatives were prepared by condensing 2-chloromethyl-1H-benzimidazole with different aliphatic, aromatic, and heteroaromatic amines. Several papers have been reported the preparation of these important compounds [3,4]. In this paper, firstly we have established a new method for the synthesis of these compounds in a short reaction time with high yields under ultrasonic irradiation then the reaction of N-(1H- benzimidazole-2- ylmethyl) aniline 3with pentachloropyridine4in the presence of potassium carbonate in CH_3CN as a solvent at reflux gave 1,2,4-trichloro-5-phenyl-5,6-dihydrobenzo [4,5]imidazo [1,2-a]pyrido[3,4-e]pyrazine 5in good yields. The structure of products confirmed by IR, ^{1}H-NMR and ^{13}C- NMR.

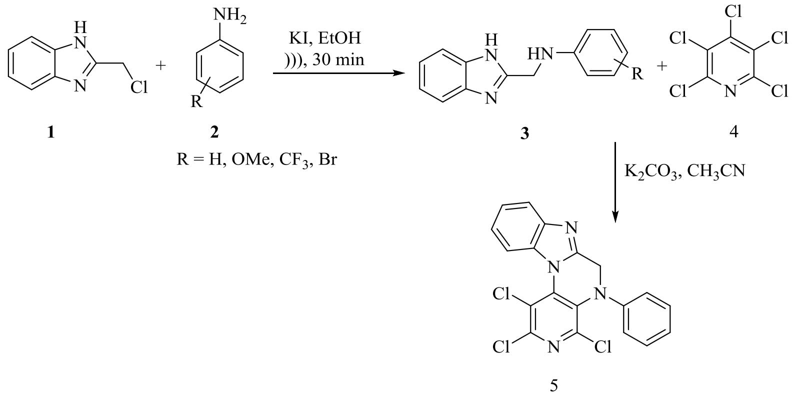

Figure 1. Scheme of the reaction.

Refrence

[1] E. Carlsson, P. Lindberg, S. Unge.Two of a kind.Chem. Britain 2002; 5:42-45.
[2] Singh AK, Lown JW. Design. Synthesis and antitumor cytotoxicity of novel bis-benz imidazoles.Anti. Cancer Drug 2000; 15:265-275.
[3] K.Petral, P. Parekh, P. Mehta, A.Kumari, A. Baro, Int. J. Pharm. Pharm.Sci, Vol 5, Issue 2, 115-119.

A novel Approach for the Synthesis of Spiroacenaphthelyne Pyrano-Pyrazole Derivatives

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Multicomponent reactions (MCRs) have recently emerged as valuable tools in the preparation of structurally diverse chemical libraries of spiro heterocyclic compounds. Spiro compounds are an important class of naturally occurring material characterized by highly significant biological properties.[1]

4*H*-pyrans derivatives have been considered because of their pharmacological activity like include spasmolytic, diuretic, anticoagulant, anticancer, and antianaphylactil anticancer, cytotoxic, anti-HIV, anti-inflammatory, antimalarial, antimicrobial, antihyperglycemic and anti-neurodegenerative disorders like Alzheimer's, Parkinson's, and Huntington's disease.[2,3]

We have developed the synthesis of spiroacenaphthylene in the reaction between acenaphthoquinone, pyrazolones and activated methylene compounds (like malononitrile derivatives) without using of catalyst in ethanol or water under mild reaction conditions. The structures of products were deduced from their IR, ^{1}H NMR, and ^{13}C NMR spectra. The mass spectra of these products displayed molecular ion peaks at the appropriate m/z values. The present procedure has the advantage that not only the reaction is performed under neutral conditions but also the reactants can be mixed without any activation or modification. The simplicity of the present procedure makes it an interesting alternative to complex multistep approaches.

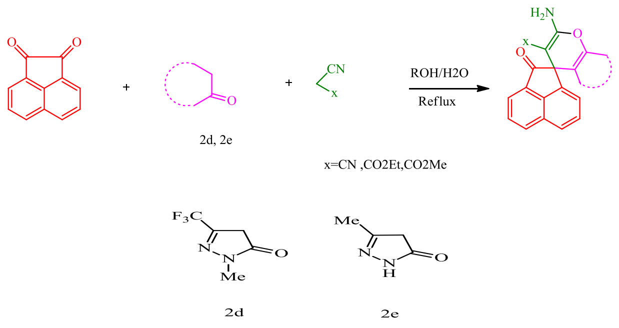

Figure 1. Schem of the reaction.

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[1] I. Ugi, Pure and Applied Chemistry. 73 (2001) 187-191. (b) B. B. Toure, D. G. Hall, Chemical Reviews. 109 (2009) 4439-4486. (c) A. Domling, W. Wang, K. Wang, Chemical Reviews. 112 (2012) 3083-3135.

[2] T. Raj, R. K. Bhatia, A. Kapur, M. Sharma, A.K. Saxena, M. P. S. Ishar, European Journalof Medicinal Chemistry. 45 (2010) 790-794.

[3] M. Rueping, E. Sugiono, E. Merino, Chemistry-A European Journal. 14 (2008) 6329-6332.

An Eficient Strategy for the One-Pot Multicomponent Synthesis of Spiroacenaphthelyne-Pyrazoloquinoline Derivatives

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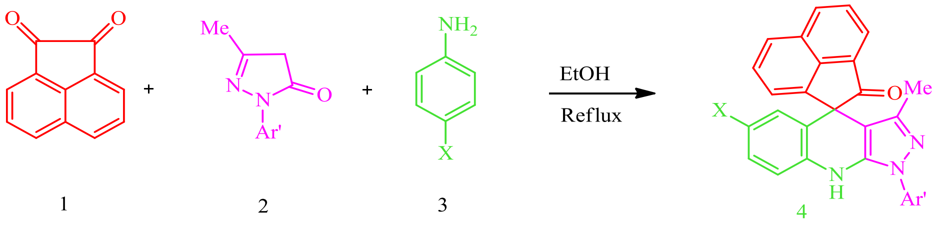
Over the past few years, multi-component reactions (MCRs) have been designed to be an efficient and potent tools and have become a significant area of research in organic chemistry. MCRs are used for the synthesis of biologically active compounds in medicinal chemistry and complex product from simple and readily available starting materials without isolation of intermediates in short time with high purity, maximum selectivity and in a minimum number of synthetic steps and good yields [1,2].

Pyrazolone derivatives have omnipresence applications in the development of acaricides, dyes, fungicides, herbicides, insecticides, inhibitors and reagents [3]. Herein, we report an efficient synthesis of spiroacenaphthelyne spiro[pyrazoloquinoline acenaphthylene] 4 based on a One-Pot three-component reaction of acenaphthoquinone 1, pyrazolone 2, arylamines 3 (Scheme 1). In this work, the structures of all compounds were deduced from their analysis, IR, ^{1}H NMR,^{13}CNMR spectra. The mass spectrum of 4 displayed the molecular ion peak at appropriate m/z value, which is in agreement with the proposed structure.



Scheme 1. Synthesis of spiroacenaphthelyne via three-component reaction.

References

[1] J. Zhu, H. Bienayme, Multicomponent Reactions, Willy-VCH, Weinheim, Germany, 2005.

[2] J. Zhu, L. E. Kalm, G. C. Tron, R. Lavilla, L. Banfi, A. Basso, V. Cerulli, G. Guanti, P. Lecinska, R. Riva, Advances in Experimental Medicine & Biology 35 (2004) 960.

[3] R. Bashir, S. Ovais, S. Yaseen, H. Hamid, M. S. Alam, M. Samim, Bio. & Med. Chem. Letters 21 (2011**)** 4301**.**

Environmental friendly synthesis of novel acyl hydrazide derivatives under solvent free conditions

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As we know, over the past decade, the environmental protection and waste prevention have been an increasing emphasis among researchers from both academia and industryfor elimination or reduce of volatile solvents in organic synthesis is a most important goal in Green chemistry [1]. Acyl hydrazides are suitable molecules in the synthesis of some imoportant products with pharmacologic activity such as β-Glucuronidase inhibitors [2], Indoles [3]. In this project, we report an eco-friendly method for the synthesis of new acyl hydrazide derivativesby direct alkylation of acyl hydrazides1 with dihaloalkanes 2 in the presence of base 1,4-diazabiscyclo[2,2,2]octane and organic salt tetrabutylammoniumbromide under solvent-free conditions (Figure 1).

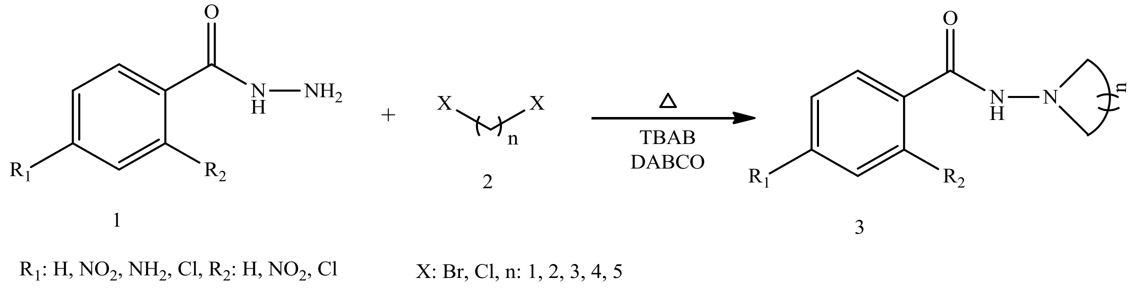

Figure 1. Addition of acyl hydrazide 1 to dihaloalkane 2 under solvent-free conditions.

The products were obtained in good to high yields within 18 h. TBAB was recovered and reused for three times without notable reduction in its catalyst properties. We used the ^{1}H NMR (400 MHz) and ^{13}C NMR (100 MHz), and IR technique to characterization of all products structure. In summary, we have described an efficient method for the synthesis new compounds that these potentially valuable products would make method practical and useful to synthetic chemists.

References

[1] V. Polshettiwar, R. S. Varma, Acc. Chem. Res. 2008,41, 629.
[2] KH. M. Khan, SH. Shujaat, SH. Rahat, S. Hayat, A. Rahman, Chem. pharm. Bull, 2002, 50, 1443.
[3] Kevin, G. J. Commeureuc, Z. Sheng-ze, A. J. Murphy. Tetrahedron Lett, 2009, 50, 3290.

Co/Alumina as an effective heterogeneous catalyst for selective oxidation of benzyl alcohols to carboxylic acids

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The oxidation of primary alcohols to carboxylic acids is an important reaction in both organic chemistry and industry.[1] Traditionally, this oxidation involves a two-step process involving oxidation of the alcohol to an aldehyde followed by further oxidation to the carboxylic acid. Given that the use of catalytic reactants with higher selectivity is one of the 12 principles of green chemistry, selective oxidation of alcohols to carboxylic acids can be important.

Owing to improved efficacy, homogeneous catalysis has grabbed more attention and interest than heterogeneous approaches.[2] Given the cost and sometimes toxicity associated with homogeneous methods, together with the loss of catalyst after one run, despite being widely used in academia, these approaches have scarcely been utilized in industry. To compensate for the deficiencies related to homogeneous catalysts, the use of either heterogeneous catalysis or heterogenized homogeneous catalystshas prevailed.[3] Today, heterogeneous catalysis has opened up a new avenue to chemists as a fundamental procedure from the standpoint of recovery and product purification, especially in the production of fine chemicals. It is also worth mentioning that the use of catalyst in more than one run is environmentally and economically advantageous.

Here, we are going to report the Co/Alumina as a heterogeneous and reusable catalyst for selective oxidation of alcohols to carboxylic acids. In this transformation, *tert*-butyl hydroperoxide (TBHP, 70 wt% in water) was employed as an external oxidant (Fig. 1).

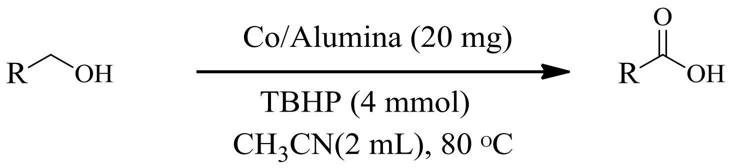

Figure 1. Synthesis of carboxylic acids

References

[1] A.C. Schmidt, C.B.W. Stark, Org. Lett.2011, 13, 4164.
[2] B. Cornils, W. A. Herrmann, Applied Homogeneous Catalysis withOrganometallic Compounds: A Comprehensive Handbook, VCH,Weinheim, 1996.
[3] J. M. Thomas, W. J. Thomas, Plat. Met.Rev.1996, 40, 8.

Synthesis and characterization of Ni-polystyrene sulfonic acid/CMK-8 nanocomposite and its application in direct reductive amination of aldehydes

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Industrial and biological importance of amines, made the researches to find an efficient approach for synthesis of these vital compounds. Elimination of unstable imine intermediate through catalytic direct reductive amination is one of the most useful methods. Heterogeneous and functionalized catalysts are one of the most beneficial ways to direct reductive amination of carbonyl compounds [1]. It has been proved that acidic condition of reaction can promote the efficiency of amination, therefore significance of bifunctional catalysts that are composed of acidic sites have been increased [2]. Recently different metal nanoparticles such as Pt, Pd, Au, Cu, and Ni have been used as hydride transfer catalysts in reduction of carbonyl compounds. However nanoparticle aggregation and activity depletion are one of the obstacles but regarding to recent researches metal nanoparticles embedded in mesoporous supports are one of the best crucial hydride transformers [3].

Hence, we synthesized polystyrene sulfonic acid containing Ni nanoparticles incorporatedin CMK-8 mesporous carbon as a novel acid-metal bifunctional heterogeneous catalyst. The catalyst was characterized by XRD, BET, FT-IR, SEM, TEM and XPS techniques.We investigated the effects of this catalyst for direct reductive amination of aldehydes (Figure 1).The reaction was carried out in the presence of $NaBH_4$as a reducing agent, ethanol as solvent, at room temperature and in short reaction time without producing any by-product. The stability of the catalyst was good and it could be reused six times without much loss of activity in reductive amination reaction.

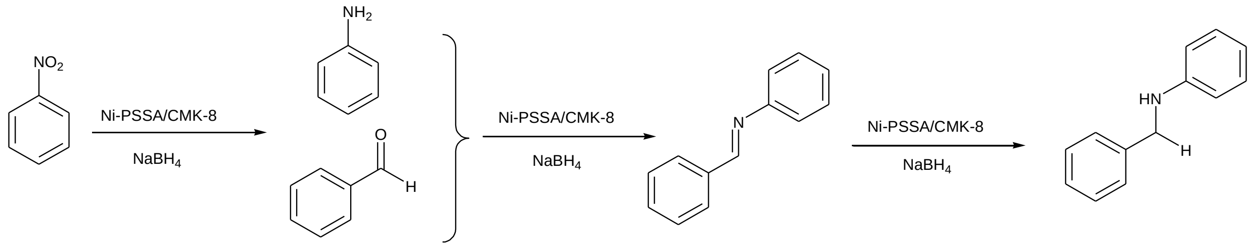

Figure 1. Reaction steps and intermediates proposed in the direct One-Pot reductive amination of aldehydes from nitro aromatic compounds

References

[1] F.I. McGonagle, D.S. MacMillan, J. Murray, H.F. Sneddon, C. Jamieson, A.J.B. Watso. Green Chem.15 (2013) 1159.
[2] O. Mazaheri, R.J. Kalbasi, RSC Adv. 5 (2015) 34398.
[3] D. shah, H. Kaur, J. Mol. Catal. A: Chem. 70 (2014) 381.

Unsymmetrial sulfides synthesis via cross-coupling reactions of thiols and aryl halids in the presence of MOF-199

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Organic sulfides are important compounds which widely exist in many biologically and pharmaceutically active molecules. Especially unsymmetrical sulfides moieties have been used in the treatment diseases such as Parkinson's, Alzheimer's, immune and inflammatory, diabetes, HIV [1,2].

Carbon-sulfur bond formation by cross-coupling reaction in the presence of transition metals has been widely investigated. Metal-organic frameworks (MOFs) have recently aroused much attention as a new class of nanoporous material that can used as an effective, heterogeneous, and recyclables in coupling reactions [3]

As a part of our current studies on the synthesis of Organosulfurs compounds, we report the results of our studies involving the reaction between iodobenzene and thios in the presence MOF-199 as a catalyst, KOH in wet PEG(400) at 120 °C under an N_2 atmosphere conditions. High yields were obtained and MOF-199 catalyst was easily isolated from the reaction mixture by simple filtration and reused with loss in activity.

$$\text{Ar-SH} \quad + \quad \text{Ar-X} \xrightarrow[\text{PEG, 120 } ^{0}\text{c}]{\text{Nanoprous MOF-199}} \text{Ar-S-Ar}$$

Ar : Aryl, Alkyl

X : Cl, Br, I

Figure 1.Scheme of the reaction.

Herein, a new application of MOF-199 as a heterogeneous catalyst in these type cross-coupling reactions is described. MOF-199 is as a porous, recyclable and chemoselective catalyst which is more efficient more economic, more comprehensive, and more environmentally friendly than previous catalyst.

References

[1] Li, Z.; Ke, F.; Deng, H.; Xu, H.; Xiang, H.; Zhou, X. Org. Biomol. Chem. 2013, 11, 2943-2946.
[2] Barba, F.; Ranz, F.; Batanero, B. Tetrahedron Lett . 2009, *50,* 6798–6799
[3] Soleiman-Beigi, M.; Sadeghizadeh, F. Rce Advances.2015,5,87564-87570

Synthesis of quinazolinone derivatives using 2-amino benzamides and aldehydes under ball-milling conditions

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2,3-Dihydroquinazolinone derivatives are an important class of fused heterocycles due to the broad range of potential biological activities [1]. The most popular method for the synthesis of 2,3-dihydroquinazolin-4(1H)-ones is based on the condensation of aromatic aldehydes and 2-aminobenzamide catalyzed by NH_4Cl,*p*-TSA and some other Lewis and Bronsted acids [2]. Most of these methods have certain limitations such as long reaction times, harsh reaction conditions, application of volatile organic solvents, toxic reagents and low yields of products. Recently, ball-milling has emerged as a powerful tool for effecting a chemical reaction in greener way [3].

In the present work, we report a new practical protocol for the synthesis of 2,3-dihydroquinazolin-4(1H)-ones by a simple One-Pot reaction of aldehydes and 2-aminobenzamide using heterogeneous acid catalysts under ball-milling conditions in the absence of solvents(figure 1).

This method was applied to various aromatic aldehydes and the corresponding products achieved in good yields. All the products were characterized by ^1H and ^{13}C NMR spectra, melting point and comparison with authentic samples.

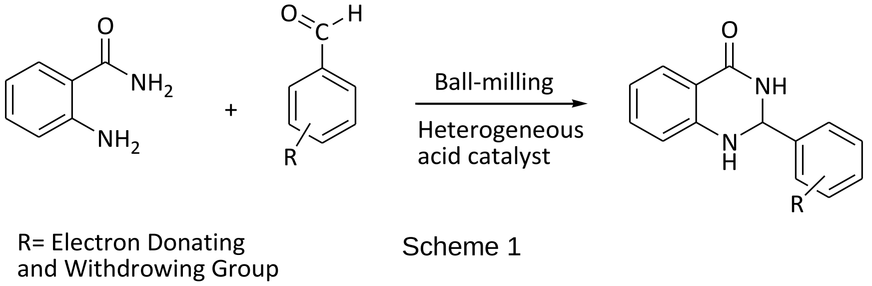

Figure 1.Scheme of the reaction.

References

[1] Y.H.Na, S.H.Hong, J.H. Lee, W. K. Park, D. J. Baek, H. Y. Koh, Y. S. Cho, H. Choo, A. N. Pae, Bioorganic & Medicinal chemistry Letter 16 (2008) 2570.
[2] A. Shaabania, A.Malekia, H. Mofakhama, Synthetic Communications38 (2008) 3751.
[3] N. Mukherjee, S. Ahammed, S. Bhadra, B. C. Ranu, Green Chemistry 15 (2013) 389.

Pd complex anchored onto MCM-41 as efficient and reusable nanocatalyst for the Suzuki reaction

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Zeolitic molecular sieves decorated with transition metals, mainly by the isomorphous substitution, had attracted great interest in redox catalysis because of their exceptional catalytic activity over various organic compounds [1–3]. Among them, because of the unique one-dimensional channel walls and better stability, synthesis and modifications in MCM-41 materials flourish more than in the other MCM-48 (cubic) and MCM-50 (lamellar) materials, as the former can enhance the reaction of sterically bulkier molecules by the suitable choice of surfactants/organic modifiers. Indeed, the greater flexibility of silica network enables the incorporation of various higher transition metals into the framework of MCM-41. In this work we have grafted 5-bromosalicylaldehyde ligand with palladium acetate salt onto MCM-41 successfully and the catalyst was analyzed by a series of characterization techniques such as. FT-IR, TEM. BET, SEM and TGA and it was applied as a heterogeneous catalyst for the formation of C-C bond from arylhalides and boronic acid (Figure 1).

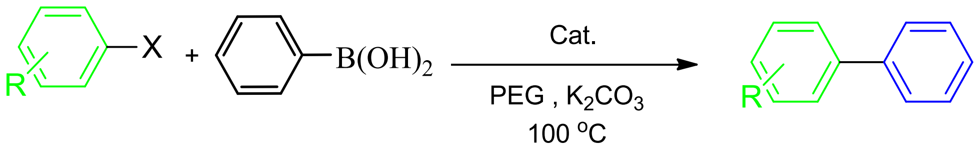

Figure 1.Formation of C-C bond in peresence catalyst.

References

[1] A. Tuel, Y.B. Taarit, Zeolites 14 (1994) 18.
[2] K. R. Reddy, A. V. Ramaswamy, P. Ratnaswamy, Journal of Catalysis. 143 (1993) 275.
[3] R. Joseph, M. Sasidharan, R. Kumar, A. Sudalai, T. Ravindranathan, Journal of the Chemical Society, Chemical Communications. (1995) 1341.

Palladium Schiff base complex supported on modified MCM-41: a reusable and efficient catalyst for Carbon-Carbon bond formation via the Heck coupling reaction

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Recently, the focus has shifted toward mesoporous MCM-41 as the major support because of the particular features that it possesses such as having large surface areas, variable pore diameters, and high-density surface silanol sites [1]. Mesoporous MCM-41 has provided the anchoring of valuable homogeneous catalysts/active organic moieties or the incorporation of redox metal ions into framework positions in a quite simple way, and thus increases their intrinsic catalytic activity as a result of the amorphous nature of the pore walls [2-4]. In the study, we try to report the synthesis Palladium complex was grafted into the functionalized mesoporous silica (MCM-41) to develop Palladium 5-boromosalicylaldehyde complex supported MCM-41 (Pd-5-Br-Salen@MCM-41) heterogeneous and reusable catalyst. It was used in coupling reaction between various aryl halides with n-butyl acrylate in the presence of base to provide the corresponding products in excellent yields. This catalyst was characterized by TGA/DTA, XRD, SEM/EDX, Fourier FT-IR, and TEM. The results indicated that the catalytic system could be recovered easily by simple filtration from the reaction mixture (Figure 1).

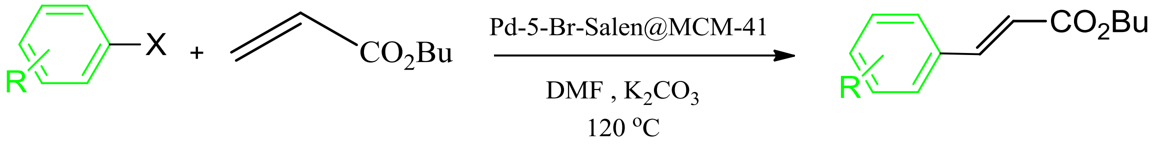

Figure 1. Synthesis of biphenyle using Pd-5-Br-Salen@MCM-41with Aryl hildes and n-butyl acrylate.

References

[1] E. Alacid, C.J. Najera. Journal of Organomet.Chem. 694 (2009) 1658−1665.

[2] B. Mu, T. Li. W. Xu, G. Zeng, P. Liu, Y. Wu. Tetrahedron Letter.63 (2007) 11475−11488.

[3] M.S. Saeedi, Sh. Tangestaninejad, M. Moghadam, V. Mirkhani, I. Mohammadpoor-Baltork, A.R. Khosropour.Materials Chemistry and Physics. 146 (2014) 113-120.

Diels-Alder Reaction of Styrylcyclohexenon Derivatives with Acrylo nitrile for Efficient Synthesis of New Substituted Dehydrodecalines

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Among important carbon-carbon bond formation reactions, the Diels-Alder reaction possesses a preeminent position. This cycloaddition process results in stereoselective formation of a cyclohexene ringhaving as many as four contiguous stereogenic centers.

By considering thi sprominence, Diels-Alder reaction in organic chemistry finds every day applications in synthetic methodologies and is used in many total syntheses.

We have recently reported the synthesis of several dehydrodecaline derivatives using styrylcyclohexyldienes which have been synthesized in Abaee's group[1-3]. This encouraged us to develop this cycloaddition process.

Thus, we examined the cycloaddition of these dienes with Acrylo nitrile. The figure 1 shows that after the cycloaddition occurs, the newly formed π bond rearranges to the more stable enone position.

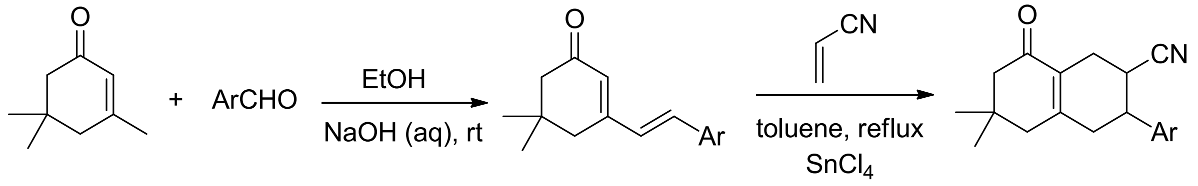

Figure 1.Scheme of the reaction

References

[1] M. M. Mojtahedi, M. S. Abaee, M. M. Zahedi, M. R. Jalali, A. W. Mesbah, W. Massa, R. Yaghoubi, M. Forouzani, Monatsh Chemistry 139(2008)917.

[2] M. S. Abaee, M. M. Mojtahedi, M. T. Rezaei, H. Khavasi,ActaChimicaSlovenica58 (2011) 605.

[3] M. S. Abaee, M. M. Mojtahedi, F. Saberi, G. Karimi, M. T.Rezaei, A. W. Mesbah, K. Harms, W. Massa,Synlett 23(2012)2073.

N,N-dihydroxypyromellitimide: a new and efficient organocatalyst for the Biginelli reaction under solvent-free conditions

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Solvent free condition is an area in modern organic synthesis. Biginelli reaction is one of the useful multi-component reactions due to it is an acid catalyzed condensation of b-ketoester with an aldehyde and urea/thiourea to yield 3,4-dihydropyrimidin- 2(1H)-ones (DHPMs) and their sulfuranalogs. These pyrimidinones have found to possess pharmacological activities such as antibacterial, antiviral, antioxidative as well as anti-inflammatory [1-2]. In this work, N,N-dihydroxypyromellitimide (DHPHI) was directly synthesized via reaction of phthalic dianhidride with hydroy amine hydrochloride in pyridine. Synthesis of 3,4-dihydropyrimidin-2(1H)-thiones using DHPHI under solvent free conditions leads to excellent yield. In the present methodology, the catalyst is inexpensive, readily available, efficient, recyclable and green. The three-component reaction of aryl aldehydes derived thiourea, and ethyl acetoacetate or acetylacetone occurs by means of 15 mol % of (DHPHI) insolvent-free reaction conditions. (Figure 1).

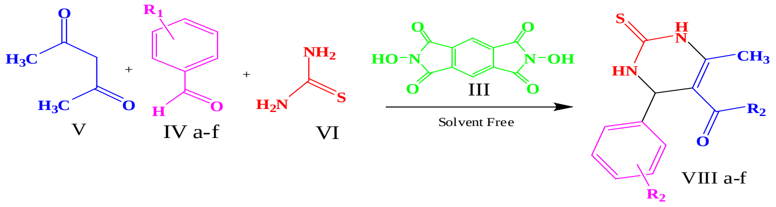

Figure 1. Scheme of the reaction

References

[1] Ashok M, Holla BS, Kumari NS (2007) Convenient One-Pot synthesis of some novel derivatives of thiazolo [2, 3-b] dihydropyrimidinones possessing 4-methylthiophenyl moiety and evaluation of their antibacterial and antifungal activities. Eur J Med Chem 42:380–385

[2] Magerramov AM, Kurbanona MM, Abdinbekova RT, FarzalievRzaeva IA, VM Allakhverdiev MA (2006) Synthesis and antioxidative properties of some 3, 4-dihyropyrimidin-2(1H)-ones (-thiones). Russ J ApplChem 79:787–790

Green synthesis of silver nanoparticles using aqueous extract of *Stoechas Lavandula*

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In green synthesis used extraction of plants for nanoparticles synthesis that could be advantageous over other environmentally benign biological processes.

Green synthesis is a useful method for synthesis of silver nanoparticles (AgNps) [1].AgNps is being the most investigated due to its wide application in the various field such as food, cosmetics, medicine and environmental [2]. In this study, the aqueous extraction of StoechasLavandula prepared and then silver nitrate used for reducing Ag^+ to Ag at room condition. The color of solution changed from yellow to dark brown.After 24 h of treatment, AgNPs were obtained. The structural parameters of AgNps were characterized by different methods [3], which include; ultraviolet-visible spectroscopy (UV-Vis), powder X-ray diffraction (XRD), scanning electron microscopy (SEM), transmission electron microscopy (TEM)and X-ray energy-dispersive spectroscopy (EDX). Characterization data demonstrated that AgNps are spherical shaped with diameter between 33- 45 nm. This route demonstrated a simple, cost effective and environmentally benign synthesis of AgNps.

References

[1] P. M.Gopinath, G. Narchonai, D.Dhanasekaran, A.Ranjani, N.Thajuddin. Asian journal of pharmaceuticals sciences 10 (2015) 138- 145.
[2] O. Zuas, N. Hamim, Y. Sampora, Materials Letters 123(2014) 156- 159.
[3] M. Ahamed, M. A. Majeed Khan, M. K. J. Siddiqui. Physica E 43 (2011) 1266- 1271.

A method for the synthesis of xanthenedione derivatives using Lithium triflate as a highly efficient catalyst

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Xanthenes are important class of heterocycles that are known to possess multiple biological activities. Although not widely found in nature, xanthenes exhibit a wide range of pharmaceutical activities such as anti-bacterial, anti-inflammatory, and anti-viral. Some xanthene based compounds have found application as antagonists for inhibiting the action of zoxazolamine and in photodynamic therapy. In addition, their derivatives can be used as dyes, pH sensitive fluorescent materials for the visualization of biomolecular assemblies and in laser technologies[1,2].

So, we would like to report synthesis of different xanthenedione derivatives by reaction of dimedone with different aromatic aldehydes at 85 °C under solvent free condition (figure 1).

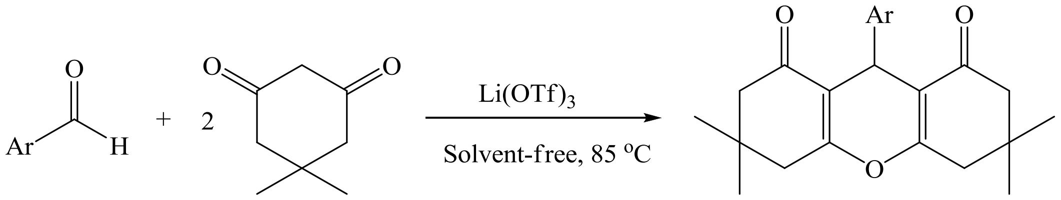

Figure 1. Synthesis of different xanthenediones by the Li(OTF)$_3$ catalyst

References

[1] A. Khazaei, M.A. Zolfigol, A.R. Moosavi-Zare, A. Zare, M. Khojasteh, Z. Asgari, V. Khakyzadeh, A. Khalafi-Nezhad, Organocatalyst tritylchloride efficiently promoted the solvent-free synthesis of 12-aryl-8,9,10,12 tetrahydrobenzo[a]-xanthen-11-ones by in situ formation of carbocationic system in neutral media, Catal. Commun., 20, 2012 , 54–57.

[2] M. Kidwai, A. Jahan, N.K. Mishra, A novel method for the synthesis of tetrahydrobenzo[a]-xanthen-11-one derivatives using cerium(III) chloride as a highly efficient catalyst, C. R. Chimie, 15, 2012 , 324–330.

Direct synthesis of Symmitrical disulfid from aril halydes with a novel sulfur source in the presence of copper nanoparticles

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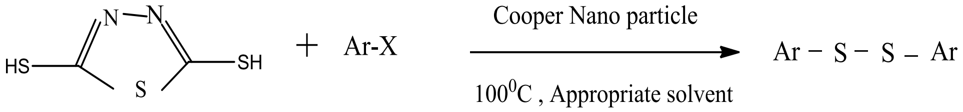
Organic sulfides are important compounds which widely exist in many biologically and pharmaceutically active molecules. Especially sulfides moieties have been used in the treatment diseases such as Parkinson's, Alzheimer's, immune and inflammatory, diabetes, HIV.The formation of carbon-sulfur bond has been widely examined and generally from nano particles catalyzed for coupling bond C-S have been used for the formation this bond.' For example disulfide bondes have been employed in stabilization of peptides in proteins, DNA cleaving and design of drug delivery systems [1].

Copper nanoparticles catalyst was easily isolated from the reaction mixture by simple filtration and reused with loss in activity Using nontoxic and nano catalyst, simplified operational process, short reaction times purification of the products without using chromatographic separation, and environmentally, and excellent yield [2].

As part of our current studies on the synthesis of organosulfurs compounds, we report the results of our studies involving the reaction between aryl halides with 1,3,4-Thiadiazol-2,5dithiol in the present of copper nanoparticles as a catalyst, KOH as a base at 100 ^{o}C in Wet Appropriate solvent . High yields were obtained and cooper nanoparticles catalyst was easily isolated from the reaction mixture by simple filtration and reused with loss in activity.



Ar: Aryl, Alkyl

X: Cl, Br,I

Figure 1.Scheme of reaction.

References

[1] Li, Z. Ke, F. Deng, H. Xu, H. Xiang, H. Zhou, X. Organic & Biomolecular Chemistry 11 (2013) 2943.
[2] Ranjbar-Karimi, R. Bazmandegan-Shamilia. A, Aslania. A, Kaviani. K, PHysica. B. Condensed Matter 405 (2010) 3096.

One-Pot synthesis of novel pyranocoumarins using 7-hydroxy 4-methyl-6-nitro coumarins, acetylenic esters and isocyanides

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Coumarins form an exceptional class of oxygen containing heterocyclic compounds, which exhibit significant biological activities, such as inhibitory of platelet aggregation [1], 1,2 inhibitory of steroid 5α-reductase, inhibitory of HIV-1 protease [2], antibacterial and anticancer activities [3]. In continuation of our general interest in the synthesis of heterocyclic compounds *via* three-component reactions, we have investigated the reactions of 7-hydroxy 4-methyl-6-nitro coumarins with acetylenic esters and isocyanides in tetrahydrofuran (THF) that afford the novel pyranocoumarins to high yields. The structures of the products were determined by ^{1}H, ^{13}C NMRand IR spectroscopy as well as mass spectrometry.

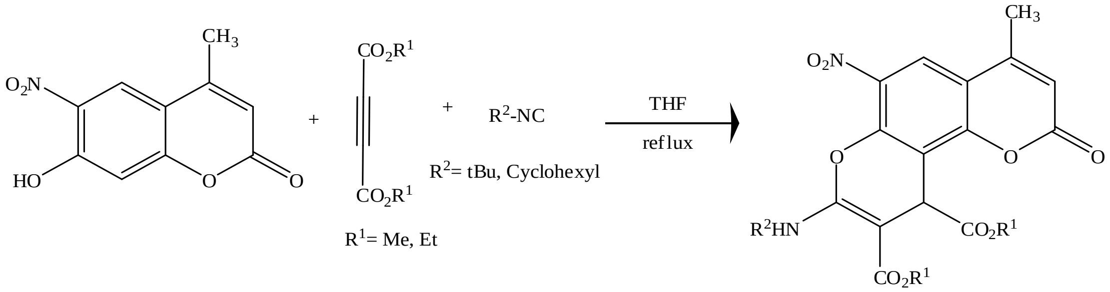

Figure 1.Scheme of the reaction

References

[1] A.K. Mitra, A. De, N. Karchaudhuri, S.K. Misra, A.K. Mukhopadhyay, J. Indian Chem. Soc. 5 (1998) 666.
[2] C.J. Wang, Y.J. Hsieh, C.Y. Chu, Y.L. Lin, T.H. Tseng, Cancer Lett. 183 (2002) 163.
[3] O. Kaysero, H. Kolodziej, Planta Med. 63 (1997) 508.

Cyclohexane-1,4-diyl bis(hydrogen sulfate): A highly biocompatible catalyst for synthesis of pyrimidines

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Pyrimidines have occupied an important place in organic and medicinal chemistry, mainly due to their diverse therapeutic and pharmacologicalproperties [1]. Among them, fused pyrimidines have been used as a common source for the synthesis of new therapeutic agents. Recent studies have shown that pyrimidine-fused heterocycles, particularly their oxo and thioxo derivatives, possess a wide range of biological activity and for this reason, they are extensively used in the design of new drugs [2].The synthesis of pyrimidine derivatives by a multicomponent reaction (MCR) is an attractive approach for the construction of this class of compounds [3]. It has been proven recently that this is a mild, worthwhile catalyst, which is efficiently and selectively catalyzes various organic transformations and synthesis. The catalyst was recovered activated and reused for two consecutive times with only slight variation in the yields of the products. Now, we report an efficient and convenient procedure for the One-Pot synthesis of aromatic aldehyde, barbituric acid and aromatic amine, by using homogeneous catalyst cyclohexane-1,4-diyl bis(hydrogen sulfate) [CDBH]to produce the pyrimidine-fused heterocycle derivatives in excellent yields (Figure 1).

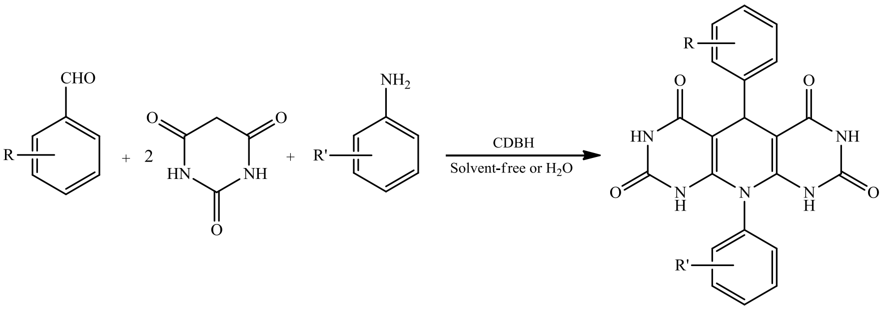

Figure 1. Preparation of 9,10-dihydropyrido[2,3-d:6,5-d']dipyrimidine derivatives through cyclo-condensation by using CDBH under solvent-freeconditionsand in the presence of water

References

[1] M. Radi, S. Schenone, M. Botta, Organic and. Biomolecular Chemistry 7 (2009) 2841.
[2] R. A. Lazarus, S. J. Benkovic, S. Kaufman, Journal of Biological Chemistry 258 (1983) 10960.
[3] H. Ohno, Y. Ohta, S. Oishi, N. Fujii, Angewandte Chemie International Edition 46(2007) 2295.

Applicationof Chiral Biphenyl Bisoxazoline Ligands in the present of HZSM-5 as Additive in Catalytic Asymmetric Allylic Oxidation of Cyclohexene

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The copper-catalyzed allylic oxidation of olefins with peresters has been the subject of numerous synthetic investigations. This reaction provides access to chiral allylic alcohols that are the key intermediates in natural product synthesis [1].

The literature survey shows that the chiral C_2-symmetric bisoxazolines (box's) are one of the most effective and popular classes of chiral ligands studied to copper-catalyzed allylic oxidations, and their application has made a major breakthrough with drastic improvement in enantioselectivity and yield [1, 2].

Herein, chiral biphenyl bisoxazoline ligands were synthesized from 2-amino benzoic acid and potential of these ligands for copper-catalyzed allylic oxidations of cyclohexenewas investigated in the Presence of HZSM-5 as additive [3].

In summary, HZSM-5 as additive was examined for oxidation ofcyclohexene, high catalytic activities, enantioselectivities up to 82% and 99% yield were obtained by using this combination of additives (Figure1).

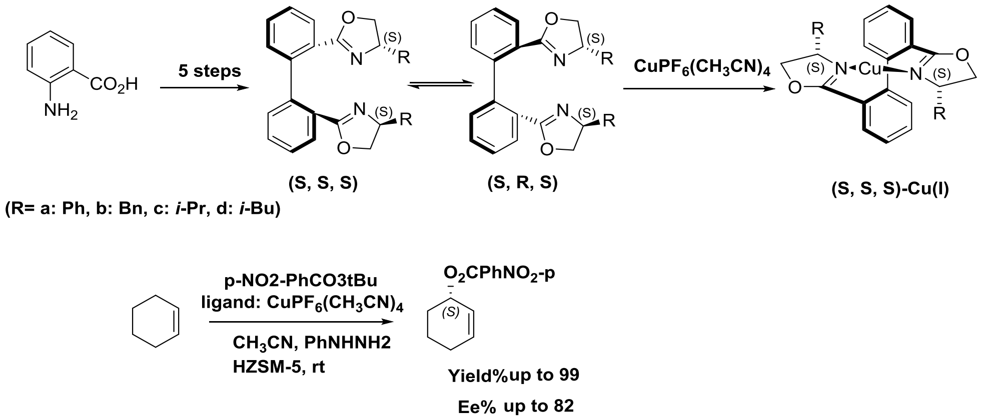

Figure 1. Copper complex of chiral biphenyl bisoxazoline ligands catalyzed allylic oxidation of Cyclohexene in the present of HZSM-5

References

[1] S.Samadi, K.Jadidi, B.Notash, Tetrahedron: Asymmetry 24 (2013) 269–277.
[2] G. Desimoni, G. Faita, K. A. Jørgensen, Chem. Rev. 106 (2006) 3561.
[3] P. Jalil, M. Kariapper, Z. Faiz, N. Tabet, N. Hamdan, J. Diaz, Z. Hussain, Appl. Catal. A. 290(2005) 159-165.

Synthesis of Chiral Oxazoline and Bisoxazoline Ligands, Immobilize of Some of them on MCM-41 and SBA-15 Nanoporous Silica and Investigation Their Potential in Heterogeneous and Homogeneous Phases in Asymmetric Allylic Oxidation of Cycloolefins

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Chiral bisoxazolines and oxazolines ligands are one of the most effective and popular classes of chiral ligands used for various metal-catalyzed asymmetric processes [1], such as allylic oxidation. The allylic oxidation of olefins using peresters in the presence of copper catalyst to give allylic esters is known as the Kharash-Sosnovsky reaction. This reaction has been the subject of great interest over the last decade and provides access to chiral allylic alcohols, which are key intermediates in natural product synthesis[2].

Some sort of chiral biaryl bisoxazolineligands 1, 2 andnew class of various chiral monodentate oxazoline 3 and bisoxazoline ligands 4 were conveniently synthesized in high yields and enantiomeric excess. The obtained organic chiral ligands 3, 4 have been covalently grafted on ordered mesoporous silicas MCM-41, SBA-15 and the resulting inorganic-organic hybrid materials such a chiral heterogeneous catalysts 5 characterized by TGA, DTA, powder X-ray diffraction, BET, BJH, EDX,CHN analysis, SEM and FT-IR. The catalytic and induced asymmetric effects of the chiral copper (I) complexes of these homogeneous and heterogeneous catalysts on the asymmetric allylic oxidation of cycloolefins were investigated under different conditions. Reactions using the catalyst exhibited good enantioselectivities up to 95% and high yields up to 99%.

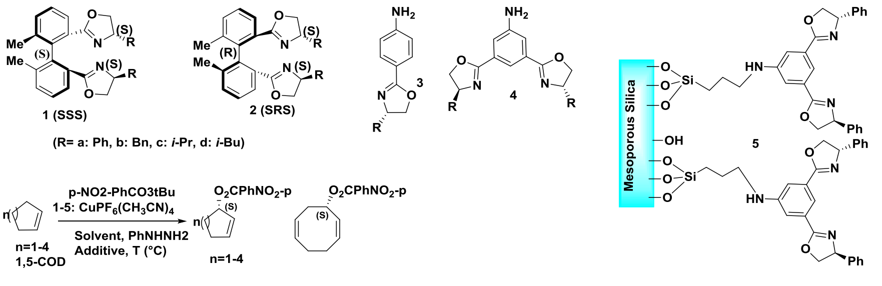

Figure 1. Allylic Oxidation of cycloolefins in the present of chiral catalyst **1-5**

References

[1] G. Desimoni, G. Faita, K. A. Jørgensen, Chem. Rev. 106 (2006) 3561.
[2] S.Samadi, K.Jadidi, B.Notash, Tetrahedron: Asymmetry 24 (2013) 269–277.
[3] a).T. P. B. Nguyen, J. Lee, W. G. Shim, H. Moon, Micropor. Mesopor. Mater.110 (2008) 560-569.
b).S.Samadi, K.Jadidi, B. Khanmohammadi, N. Tavakoli, J. Catal. 2016 (in press).

Study on the Mechanism of Aza-Diels-Alder Reactions of N-Aryl-Imin and Some Vinyl Dericatires

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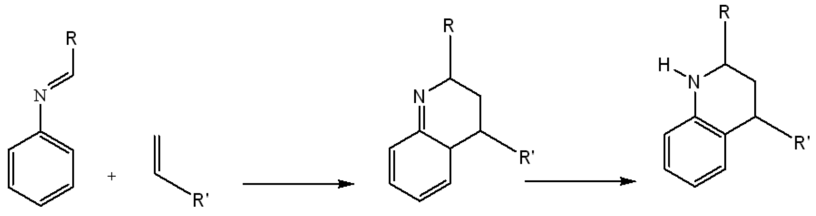
In its original form, the povarov reaction (PR) [1] involved a Lewis acid (LA) catalyzed aza-Diels-Alder (A-DA) reaction between a N-aryl imin and an electron rich dienophile, followed by a 1,3- hydrogen shift in the formal [4+2] cycloadduct 3 to yield a tetrahydroquindine 4 (Scheme 1). Over the past decade, various advances in the study of PR have been reported [2], including the broadening of its scope, progressing toward both the understanding of its reaction mechanism and its application in total synthesis [3].

In the present work,we perform a complete characterization of the reaction mechanism of the PR, as well as the main factors controlling the activation energy associated with the LA catalyzed A-DA reaction involved in these domino reactions. For this purpose a DFT study on these reactions were performed. At this computational level, the LA catalyzed A-DA reaction presents a two-step mechanism as a consequence of the large stabilization of corresponding zwitterion intermediate. The theoretical results indicated that the first step, which is associated with the nucleophilic attack of dienophiles in the imin carbon, constituents the rate-determining step of these A-DA reaction. Also analysis of the DFT-based reactivity indices of the reagents provides further explanation of the behaviors of the mechanism of the A-DA reaction involved in the povarov reaction.



1 2 3 4

Figure 1. Scheme of the reaction

References

[1] L.S.Povarov,Russ. Chem. Rev., 1967, 36, 656.

[2] For a review, see: V.A. Glushkov and A. G. Tolstikov, Russ. Chem. Rev., 2008, 77, 137.

[3] M. Hadden M. Nieuwenhuyzen, D. Osborne, P.J. Stevenson, N. Thompson and A.D. Walker, Tetrahedron, 2006, 62, 3977.

Magnetically recoverable gold nanorods as a novel nanocatalyst for the ultrafast reduction of nitroarenes in water

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The catalytic behaviour of noble metal nanoparticles, have been explored in various organic synthesis, which it is important for environmental protection, such as reduction of nitroarenes, CO oxidation, etc. Due to their high surface-to-volume ratio and high surface energy [1, 2]. The catalytic activity of noble metal NPs is mainly dependent on their size, shape, crystallinity, and the surface state. Since the potential binding sites presented by the atoms situated at the surface of NPs the catalytic properties have been changed with different size and shapes. The synthesis of gold nanorods in high yield and monodispersity has been developed, but only a few papers have been published related to their applications. The biological applications of high aspect ratio nanoparticles have been reviewed [3]. In this present report we demonstrated the efficiency of a novel designed gold nanorods loaded Fe_3O_4@Carbon core-shell nanocatalyst (FC-Au NRs) in the fast catalysis reduction of aromatic nitro-compounds. Herein, the Fe_3O_4@Carbon MNPs were first prepared using a glucose-based hydrothermal process, and the seed-less mediate as-synthesized gold NRs was then loaded on carbonaceous shell functional groups. The effect of several environmental parameters including initial nitroarene concentration, and $NaBH_4$ concentration as reducing agent on rate of 4-nitrophenol were investigated.

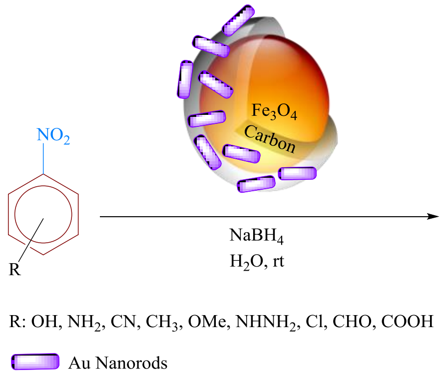

Figure 1. Schematic pathway ofFe_3O_4@C/Au NRs catalyzed reduction reaction.

References

[1] G. Schmid, in Nanoscale Materials in Chemistry, John Wiley & Sons, Inc. (2002) 15.
[2] C. Zhu, L. Han, P. Hu and S. Dong, Nanoscale, 4(2012) 1641.

Synthesis of 2-Aminothiophene Derivatives by Gewald Reaction Using Ultrasound Technique

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Multicomponent reactions (MCRs) serve as powerful tools for the synthesis of a broad range of molecules and biologically active compounds due to the simplicity and efficiency associated with MCR protocols [1,2].

Despite many efforts devoted to develop the Gewald reaction, many procedures are not practically justified due to environmental and safety restrictions they impose. In addition, some of the methods are not economically feasible sincethey require long time heating at elevated temperatures; give low yields of products, and some other problems [3]. In this project, a facile and practical method has been developed for the preparation of 2-aminothiophene derivatives via the Gewald reaction by using ultrasound technique in a reasonably short period of time.

Consequently, a series of 2-aminothiophenes were synthesized in high yields at room temperature. Under the conditions, several cyclic ketones react with malononitrile and sulfur to produce high yields of the respective products (Table 1).

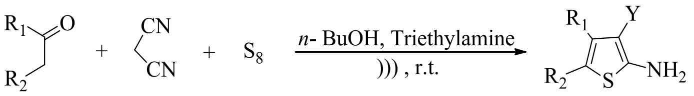
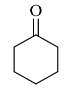
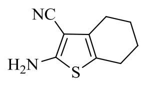
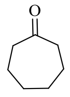
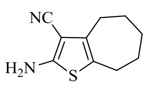


Figure 1.scheme of the reaction

Table 1. Ultrasound-Assisted Gewald Reaction at room temperature conditions.

Entry	Ketone	Product	Time (min)	Yield^a(%)
1a			8	96
2a			8	92

^{a}GC yields.

References

[1] H. N. Hafez, A. B. A. El-Gazzar,Bio. and Medicinal Chem. Letters 18 (2008) 5222.
[2] H. N. Hafez, H. A. R. Hussein, A. B. A. El-Gazzar, European Journal of Med. Chem. 45 (2010) 4026.
[3] H. Jiang, J. Shen, H. Liu, J. Tang, Synthetic Communications 35 (2005) 1351.
L.A. Bauer, N.S. Birenbaum, G.J. Meyer, J. Mater. Chem. 14(2004) 517.

Synthesis, Characterization and Spectroscopic Properties of Two New Azo Ligands Containing Salicyaldimine-based Ligand as Side Chains

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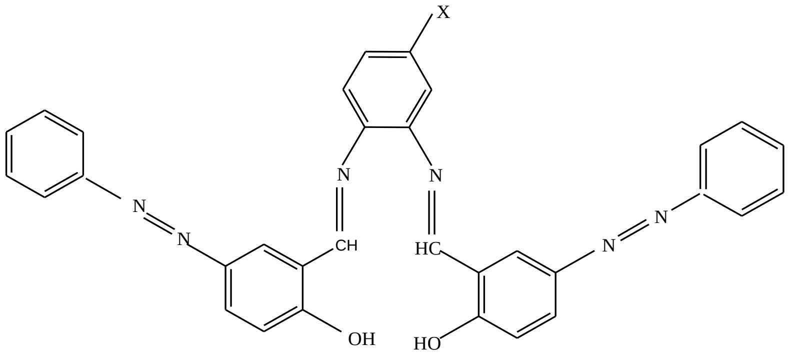
Azo ligands containing salicyaldimine-based ligand as side chains can be used in the production of chemical sensors because they show a significant change of color of the solution and maxima of the absorption band when they interact with transition metal ions or anions [1-3]. Therefore among the wide range of materials that may be suitable for the electronic and optical applications, salicyaldimine-based ligands are of particular interest.

In this work, two new azo Schiff-bases I and II were prepared from 1-(3-formyl-4-hydroxophenylazobenzene) and 4-nitro-1,2-phenylenediamine or 4-chloro-1,2-diaminobenzene in methanol solution. Two compounds were characterized with FT-IR, ^1H NMR and elemental analysis techniques. Also, optical properties of these compounds were investigated by UV-vis spectroscopy in the presence of some metal ion transitions.



X=NO_2 (I), Cl(II)

Figure 1.scheme of the reaction

References

[1] Z.Shaghaghi,Spectrochim.Acta A 131(2014) 67.
[2] B. Shaabani, Z. Shaghaghi, A.A. Khandar, Spectrochim. Acta A 98 (2012) 81.
[3] A.K. Mahapatra, S.K. Manna, P. Sahoo, Talanta 85 (2011) 2673.

A Theoretical Study on the Metal-free Triazole FormationThrough 1,3-Dipolar Cycloaddition of BenzylAzide and Oxanorbornadiene

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The development of selective and site-specific bioorthogonal conjugation methods is an important topic in chemical biology [1]. The term bioorthogonal chemistry refers to any chemical reaction that can occur inside of living systems without interfering with native biochemical processes [2].Strain-promoted [3+2] azide–alkyne cycloaddition is a bioorthogonal reaction which is modified by eliminating a cytotoxic copper catalyst [3].

In this work, we performed density functional theory (B3LYP and m06-2x) calculations on the possible 1,3-dipolar cycloaddition reaction pathways of benzyl azide with phenyl acetylene andoxanorbornadiene. The calculated activation energy of the “strain-promoted” cycloaddition reaction ofoxanorbornadieneis lower than the strain-free phenyl acetylene cycloaddition because of thesmaller distortion energy of the former reaction.The molecular mechanism of these reactions was established by ELF topological analysis of the changes of the electron density along the IRC.

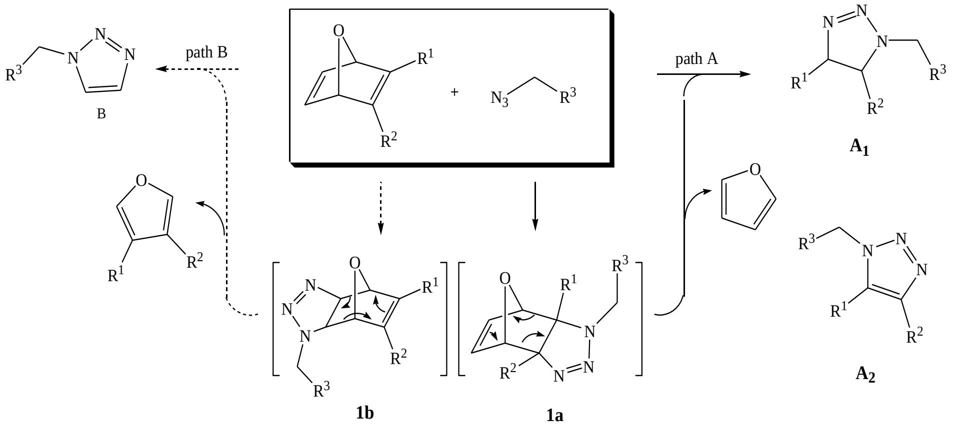

Figure 1.Reaction pathways for the formation of triazole compounds A1, A2, and B via triazoline intermediates Ia and Ib.

References

[1] S.S. Van Berkel, A.T.J. Dirks, M.F. Debets, F.L. Van Delft, J.J. Cornelissen, R.J. Nolte, F.P. Rutjes. ChemBioChem 8 (2007) 1504.
[2] E.M. Sletten, C.R. Bertozzi. AngewandteChemie International Edition 48 (2009) 6974.
[3] N.J. Agard, J.A. Prescher, C.R. Bertozzi. Journal of the American Chemical Society 126 (2004) 15046.

Synthesis and characterization of poly 2-(dimethyl amino) ethyl methacrylate/ZSM-5/KIT-6 as a novel bi-functional catalyst and its application in tandem reaction of deacetalization-Knovonagel condensation

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Recently, synthetic organic chemists have paid great attention to the development ofOne-Pot , sequential organic reactions owing to their comparably higher efficiencies, increased cost and reduced waste materials.Acid–basebifunctional catalyst is a popular concept quoted from enzyme catalysis reactions that contain two types of active centers of acid and base in catalytic systems. These catalysts may act in a cooperative way to activate both electrophiles and nucleophiles centers in reactions.However, most of these catalysts are hybrid organic-inorganic siliceous material that was prepared by grafting of organosilane compounds into the silica surface[1].However, there are several problems with these routes due to the use of highly toxic raw materials, high process cost, and complicated preparation procedures. Surface modification by polymers is one of the most effective methods due to the wide variety of functional polymers and can create many of functional group as reactions sites.Hierarchical zeolite is a new kind of zeolites that improve the performance of zeolite by combination of crystallinemicroporous frameworksand mesoporous materials(high thermal/hydrothermal stability of zeolites and fast mass transportation path of the mesoporous materials)[2].

In this study, we prepared a novel acid base bi-functional catalyst by in-situ polymerization of 2-(dimethyl amino) ethyl methacrylate in the micro/meso pores of hierarchical ZSM-5 zeolitewith low cost and simple route. In the catalyst structure, mesoporous ZSM-5 was used as a support which contains strong acid sites and poly 2-(dimethyl amino) ethyl methacrylate was used as a species which contains basic sites.The physical and chemical properties of the catalyst were investigated using FT-IR, XRD, BET, SEM, TEM and TGA techniques.Activity of the catalyst was tested in cascade reaction of deacetalization-Knoevenagel condensation (Figure 1).Excellent yields in a mild reaction condition, short reaction time and aqueous media were obtained. In addition, the results showed that the stability of the catalyst was excellent and could be reused 6 times without much loss of activity in the reaction.

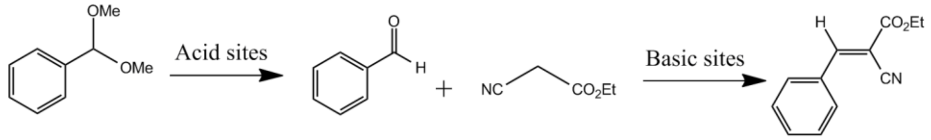

Figure 1.cascade reaction of deacetalization-Knoevenagel condensation over bifunctional catalyst

References

[1] S. Shylesh, W.R. Thiel, Chem. Cat. Chem. 3 (2011) 278.
[2] K. Na, M. Choi, R. Ryoo, MicroporousMesoporous Mater. 3 (2013) 166.

Synthesis, Antibacterial Activity of New Dihydropyrrol-2-one Derivatives Bearing Sulfonamide Groups

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The design and development of novel pharmaceuticalcompounds with a broad spectrum of activities is still a major challenge to medicinal chemistry researchers by reason the rapid appearance microbial resistance in humans and some animals. Dihydropyrrol-2-one derivatives are well known as the most important nitrogen-containing heterocyclic compounds due to their present in many natural products, synthetic pharmaceuticals, and molecular materials [1, 2].Sulfonamides have attracted much attention of chemical chemists because of pharmacological and biological activities [3, 4]. Due to the pharmacological and biological importance of sulfonamides, nitrogen-containing heterocyclic compounds in medicinal chemistry, the synthesis of compounds bearing sulfonamide moieties with the aim of outstanding biological properties has become interesting field in research.

A series of novel dihydropyrrol-2-one derivatives bearing sulfonamide groups in high yields via three-component reaction under catalyst-free and solvent-free conditions. The advantageous features of this methodology are high atom-economy, operational simplicity, shorter reaction time, and green procedure, catalyst-free and solvent-free conditions. Antibacterial results showed that most of the compounds displayed good antibacterial activity against P.aeruginosa bacteria.

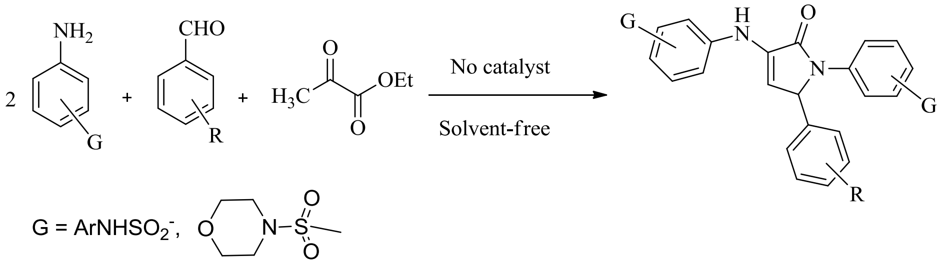

Figure 1. Scheme of the reaction

References

[1] B. Li, M. P. A. Lyle, G. Chen, J. Li, K. Hu, L. Tang, M. A. Alaoui-Jamali, A. Webster, J. Bioorg. Med.Chem 15 (2007) 4601.
[2] L. Zhang, Y. Tan, N. X. Wang, Q. Y. Wu, Z. Xi, G. F. Yang, Bioorg. Med. Chem 18 (2010) 7948.
[3] W. Boufas, N. Dupont, M. Berredjem, K. Berrezag, I. Becheker, H. Berredjem, N. E. Aouf, J. Mol. Struct. 1074 (2014) 180

Synthesis of a New Surfactant-like Triazine-functionalized Ligand for Carbon-Carbon and Carbon-Heteroatom Bond Formations

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Transition metal-catalyzed organic transformations are among the most important approaches in organic synthesis [1].In these reactions, the existence of an appreciate ligand is critical and many of the challenges in this field referred to the development of suitable ligands for fine chemical synthesis [2]. Triazine-based ligands have been considered as efficient ligands in transition-metal catalyzed organic reactions due to their many advantages in comparison with other ligands.There are some interesting reports in the literature on the use of 2,4,6-trichloro-1,3,5-triazine(TCT) in the synthesis of ligands for application in metal-catalyzed organic reactions. In fact, to synthesise these ligands, TCT was used as the starting material in order to generate a triazine moiety in the structure of an organic–inorganic hybrid material or polymer[3].

In the current study, our goal is to develop a novel catalytic system based on TCT and micellar concepts that enable the use of water as a solvent for the Pd-catalyzed coupling reactions. Our study was initiated by the synthesis of a surfactant-like triazine-functionalizedligand using the reaction of 3 equivalents ofdodecan-1-amine with TCT. In the structure of the ligand, thetriazine ring provides the nitrogencenter of ligand and the dodecyl carbon chain participates inthe surfactant part. The synthetic ligandwas characterized using elemental analysis, ^{1}HNMR and ^{13}CNMR. Next, the synthesized pseudo surfactant triazine-functionalized ligand was used in the carbon-carbon and carbon-heteroatom bond formation reactions.

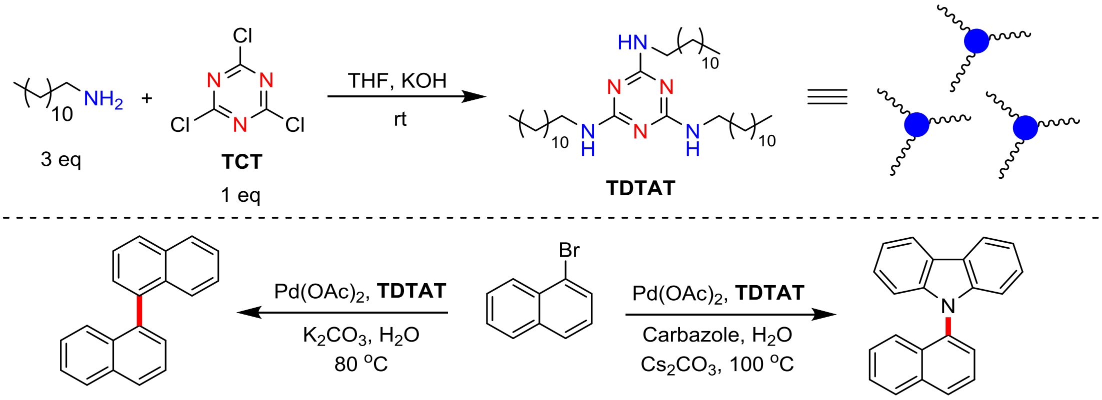

Figure 1.Scheme of the reaction

References

[1] K.M. Engle, J.-Q.Yu, J. Org. Chem. 78 (2013) 8927.
[2] G. Jindal, R.B. Sunoj, J. Am. Chem. Soc. 136 (2014) 15998.
[3] A. Modak, J. Mondal, M. Sasidharan, A. Bhaumik, Green Chem.13 (2011) 1317.

Melamine-$(H_2SO_4)_3$/Melamine-$(HNO_3)_3$ instead of H_2SO_4/HNO_3: A safe system for the oxidation/nitration reaction

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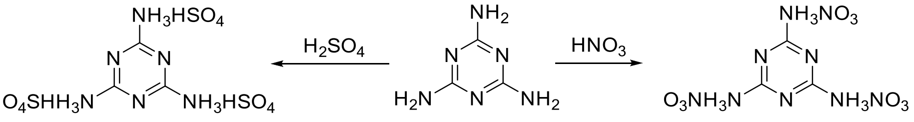
Solid acid reagents are unique acid catalysts/reagents that have become popular over the last two decades. They have proved to be useful to chemists in the laboratory and industry due to the good activation of adsorbed compounds, reaction rate enhancement, selectivity and easier work-up [1].

In continuation of our studies on the application of solid acids and oxidation of heterocyclic compounds [2] and nitration of phenols [3] we found that melamine readily reacts with concentrated sulfuric acid and fuming nitric acid to give melamine-$(H_2SO_4)_3$ (**I**) and melamine-$(HNO_3)_3$ (II). It is interesting to note that these exothermic reactions are fast, easy and clean not requiring any work-up (Figure 1).



I

II

Figure 1. Preparation of melamine-$(H_2SO_4)_3$ (**I**) and melamine-$(HNO_3)_3$ (**II**)

Mixture of these new solid acids acts as unique powerful system instead of hazardous H_2SO_4/HNO_3 system for the oxidation of urazoles and dihydropyridines as well as nitration of active aromatic rings under heterogeneous, solvent/metal-free and mild conditions.

References

[1] P. Salehi, M.A. Zolfigol, F. Shirini, M. Baghbanzadeh Curr. Org. Chem. 10 (2006, 2171.
[2] G. Chehardoli, M.A. Zolfigol, T. Faal-rastegar, S. Mallakpour, A. Ghorbani-choghamarani J. Chem. Sci.121 (2009) 441.
[3] G. Chehardoli, M.A. Zolfigol, S.B. Azimi, E. Alizadeh. Chin. Chem. Lett.22 (2011) 827.

Chemical cleaning of Sahand power plant turbine blades by biodegradable new liquor

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The unit 1 turbine of SAHAND power plant - 325 megawatt- is used to be hampering by silicate and oxide deposits. There are many methods for cleaning of turbine blades without shell opening. Some technics include: cleaning with superheated steam, CO_2, 10 percent base liqueur, dilute HCl and so on[1]. The num. 1 SAHAND power plant turbine was expected for cleaning just after the increasing in impulse pressure. Deposit analyzes showed that there is 56 percent is sodium silicates and 23 percent is iron oxides and 15 percent aluminum oxide, then some liquor were produced to dissolve this material completely. All of liquors were done for dissolving of turbine deposit and the best one chose. This three ingredient liquor can be degenerate by biomaterials.

After the cleaning and in 2 operation years, 11.6% increase in electricity production yield observed, also decrease of impulse pressure and 240 billion Rial excess in earning gained.

Refrences

[1] Betz Handbook of industrial ..sixth edit. , p 185

Palladium grafted dicarboxylic acid ligand supported on SBA-15 as an efficient catalyst for Suzuki- Miyaura reaction

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The cross-coupling reactions of aryl halides with arylboronic acids, often referred to Suzuki-Miyaura coupling reactions, are versatile methods for synthesizing unsymmetrical biaryls, which have a crucial role in natural products and pharmaceutical compounds [1].

Recently the heterogenisation of homogeneous catalysts and their investigation in synthesis of fine chemical has become a major area of research. 1,2- Bidentate carboxyl groups can form an efficient and stable chelates with transition metals [2]. Therefore, herein we wish to synthesis a heterogeneous Palladium catalyst coordinated to dicarboxylic acid ligand supported on SBA-15 and demonstrate its catalytic activity in Suzuki-Miyaura reactions.

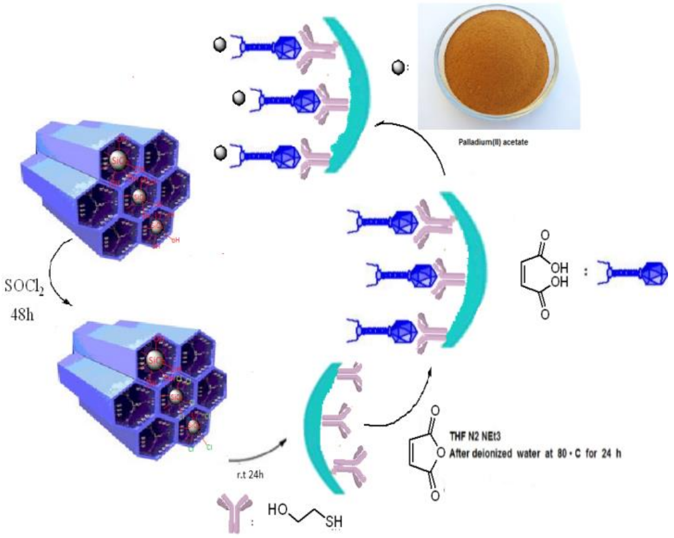

Figure 1.Scheme of the reaction

References

[1] S.W. Kim, M. Kim, W.Y. Lee, T. Hyeon, J. Am. Chem. Soc. 2002, 124, 7642.
[2] H. He, H. Xiao, H. Kuang , Z. Xie, X.Chen ,X. Jing, Y. Huang Colloids Surf., B 2014, 75,117.

One-Pot Three Compounds Synthesis of Spirooxindole Derivatives using $CuFe_2O_4$ Nanocatalyst in Water

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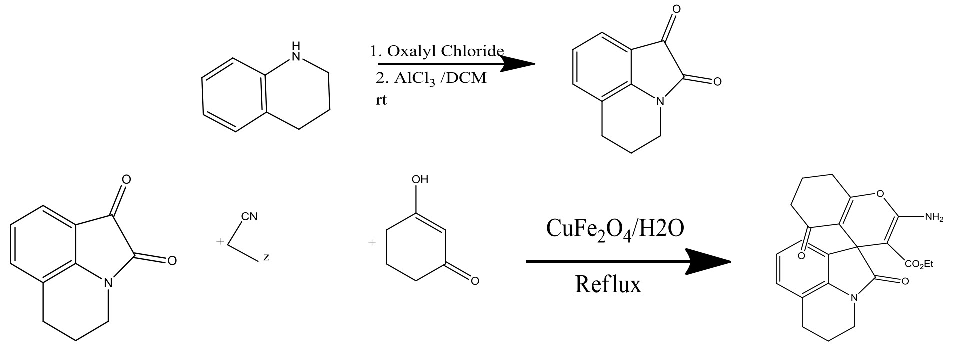
Interest in spiro[3,3′-oxindoles], i.e. having an oxindole nucleus but with a spirocyclic ring fused at C-3 [1], The unique structural features of spiroheterocycles and the presence of spiro linkage as a basic skeleton of antimicrobial, antitumor, hypotensive, antileishmanial, and local anesthetic agents [2] have increased their importance to a great extent. The multi component reaction or MCR strategy has been successfully adopted by many researchers for the synthesis of spirooxindoles [3].

In this study we report a simple and efficient method for the synthesis of spirooxindoles by the three component One-Pot condensation of 5,6-dihydro-1H-pyrrolo[3,2,1-ij]quinolone -1,2(4H)-dione, ethyl 2-cyanoacetate, and cyclic 1,3-diketones using $CuFe_2O_4$nanocatalyst as a green and reusable catalyst (Figure 1).



Z=COOEt,CN

Figure 1. Synthesis of spirooxindoles

References

[1] Baradarani, M.M., Khoshsirat, S., Moharampour, M., EbrahimiSaatlo, B., Rashidi, A., Różycka-Sokołowska, E. and Joule, J.A. 2016. Spiro[4H-pyran-3,3′-oxindoles] derived from 1,2,3,4-tetrahydroquinoline-Part 2. Journal of Heterocyclic Chemistry, DOI 10.1002/jhet.2658.

[2] Sarrafi, Y., Mehrasbim E., Vahid, A. and Tajbakhsh, M.2012. Well-ordered mesoporoussilica nanoparticles as a recoverable catalyst for One-Pot ulticomponentsynthesis of 4H-chromenederivatives. Chinese Journal of Catalysis, 33: 1486-1494.

[3] Singh, S.H.N.,Regati, S., Paul, A.K., Layek, M., Jayaprakash, S. et al. 2013. Cu-mediated 1,3-dipolar cycloaddition of azomethineylides with dipolarophiles: a faster access to spirooxindoles of potential pharmacological interest. Tetrahedron Letters, 54: 5448-5452.

Synthesis of some new 2-acetamido-*N*-(2-(cyclohexylamino)-2-oxo-1-phenylethyl)-*N*,3-diphenylacrylamidederivatives via Ugi reaction

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Combinatorial chemistry is now routinely applied to find outnovel biologically active compounds. In this context, multicomponentreactions (MCRs) are powerful tools in the modern drug discoveryprocess in terms of lead finding and lead optimization.Special subclasses are isocyanide-based MCRs (IMCRs).Today, most MCR chemistryperformed with isocyanides is related to the classicalreactions of Passerini [1] and Ugi [2].

Ugi reaction played an important role in organic and medicinal chemistry due to the importance of the resulting α-amino acyl amide and several bioactive natural products [3].

In continuation of our recent research on development of novel multicomponent reactions,[4] we report, herein a simple, facile, rapid, and efficient four-component for the preparation of some new 2-acetamido-N-(2-(cyclohexylamino)-2-oxo-1-phenylethyl)-N,3-diphenylacrylamide **5**via ugi reaction between alaldehyde 1, amines 2, isocyanides 3, and 2-acetamido-3-phenylacrylic acid4 for the first time.(Figure 1).

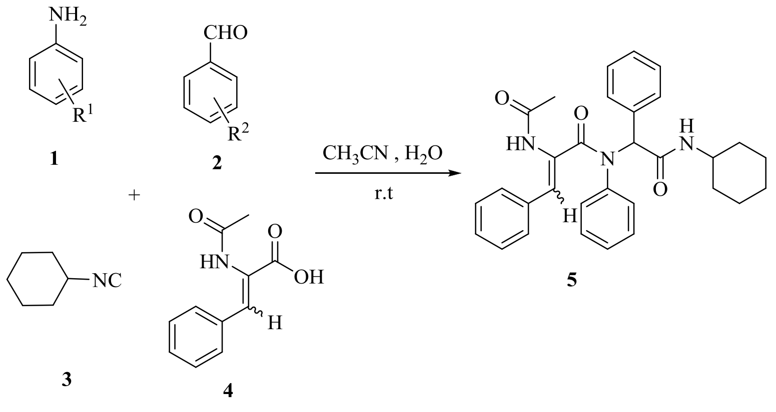

Figure 1.Scheme of the reaction

References

[1] Passerini, M.; Ragni, G. Gazz. Chim.Ital., 1931, 61, 964.
[2] (a) Ugi, I. Angew. Chem., Int. Ed. 1982, 21, 810.
[3] Pando, O.; Stark, S.; Denkert, A.; Porzel, A.; Preusentanz, R.; Wessjohann, L. A. J. Am. Chem. Soc. 2011, 133, 7692.

Bissulfamic acid-functionalized nanocatalyst as an efficient and retrievable catalyst for synthesis of 1,4-dihydropyridines

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As one of the known MCRs, Hantzsch reaction has attracted much attention on the synthesis of 1,4-dihydropyridines (1,4-DHPs) due to their significant biological and pharmacological properties such as antitubercular ,anticonvulsant, antitumour ,analgesic, anti-inflammatory and stress protective activities [1].

Hybrids of organic-inorganic materials are of great interest as heterogeneous catalysts in organic synthesis, since the functionality and flexibility of organic moiety as well as thermal and structural stability of inorganic solids are collected in these systems [2].Their large surface area per unit volume, a consequence of their small diameter, makes them interesting in the area of heterogeneous catalysis; Heterogeneous catalysis in the nano-scale takes advantage of a high exposure of the active species leading to a higher efficiency of the catalyst [3].

Considering the importance of MCRs and the diverse applications of 1,4-DHPs and the limitation with the previous synthetic routes and our earlier interest in green procedures of MCRs and recyclable organic-inorganic nanocatalysts [4], we wish to report an efficient and convenient methodology for the Hantzsch reaction by One-Pot cyclocondensation of aldehydes, ammonium acetate and ethylacetoacetate under mild and green conditions (Scheme 1).

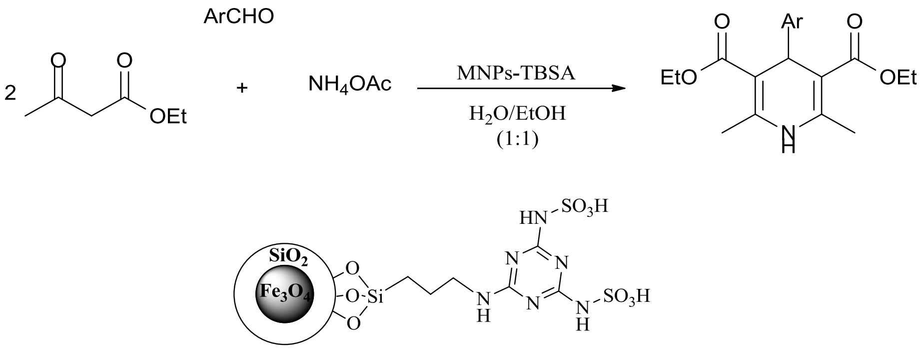

Figure 1. Synthesis of 1,4-dihydropyridines catalyzed by a novel MNPs

References

[1] S. Cihat, S. Rahime, Mini Rev. Med. Chem. 2006, 6, 747.
[2] L. Han, H. J. Choi, S. J. Choi, B. Liu, D. W. Park, Green Chem. 2011, 13, 1023.
[3] M. A. Nasseri, M. Sadeghzadeh, J. Chem. Sci. 2013, 125, 537.
[4] A. Mobinikhaledi, M. A. Bodaghifard, S. Asadbegi, Mol. Divers. 2016, 20, 461.

Highly dispersed magnetically recoverable carbon based palladium nanoparticles as a novel catalyst for room temperature Suzuki reaction

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It is well-known that palladium-catalyzed cross-coupling reactions are very important and powerful methodologies in synthetic organic chemistry [1].To improve the catalyst activity and lowering of the reaction temperature many efforts are focused on producing of the electron-rich homogeneous catalysts with special expensive ligands but only a few approaches have been reported for improving heterogeneous Pd-based catalysts, because the electron density of the Pd sites in heterogeneous scale could not be easily modified [2].Saikia and co-workers [3] concluded that the alkali metal hydroxides produced from interaction of water and WERSA act as internal bases to facilitate the Suzuki reactions. Based on this knowledge that introduction of special ligands leading to activation of homogeneous Pd-based catalysts we are interested in enhancing the activity of heterogeneous Pd-based catalysts by increasing their electron density via special amino acid as a novel ligand with high content of heteroatoms and polar medium by using of mixture of metal hydroxides. In this work, an efficient procedure based on amino acid-modified Fe_3O_4@Carbon magnetic nanoparticles (FCA MNPs) with highly dispersed Palladium nanoparticles (Pd NPs) was reported for room temperature Suzuki reaction. Fe_3O_4@C (FC) were first prepared by synthesis of Fe_3O_4 MNPs, and then stabilized by glucose carbonization in a Teflon-lined hydrothermal method. Pd^{II} ions was then loaded on amino acid modified surface of FCA MNPs and reduced for achieving the uniformly dispersed Pd NPs. The mixture of metal hydroxides as bases in water as a green non-toxic solvent in presence of FCA-Pd^X led to an efficient procedure for Suzuki reaction at room temperature.

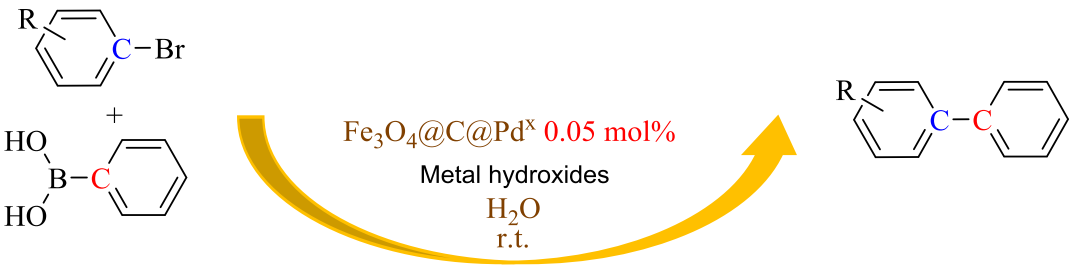

Figure 1. Studied pathways of Suzuki coupling.

References

[1] C. J. Li, Chem. Rev. 105 (2005) 3095-3165.
[2] A. Decottignies, A. Fihri, G. Azemar, F. Djedaini-Pilard and C. Len, Catal.Commun. 32 (2013) 101-107
[3] Boruah, P. R., Ali, A. A., Chetia, M., Saikia, B., & Sarma, D. Chem. Comm.51 (2015) 51 11489-11492.

Efficient synthesis of 3,6,6,9- tetra methyl-4,8-diazaundecane-2,10-dione dioxime as a radiotracer ligand

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Duringrecent years, numerous brain imaging radiopharmaceuticals have been synthesized including *N*-isopropyl-*p*-I--iodoamphetamine(IMP),*N*,*N*,*N*-trimethyl-*N*-2-hydroxy-3-methyl-5-I-iodobenzyl-1,3-propane-diamine(HIPDM)Tl-dimethyldithiocarbamate(DDC)Tc--*d*,*l*-hexamethylpropylene- amine (HMPAO) and Tc-*l*,*l*-ethylcystinatedimer (ECD) Ligands are very important as an excellent brain imaging agent[1].

In this report, an efficient One-Pot procedure for the synthesis of diazadioxime was described.Treatment of ketoxime with alkylamine followed by $NaBH_4$ in dry ethanol afforded the corresponding diazadioxime in good yield[2]. The procedure is easy to perform and does not require tedious purification procedures.All reagents are commercially available and inexpensive.This method is useful for commercial mass production[3,4].

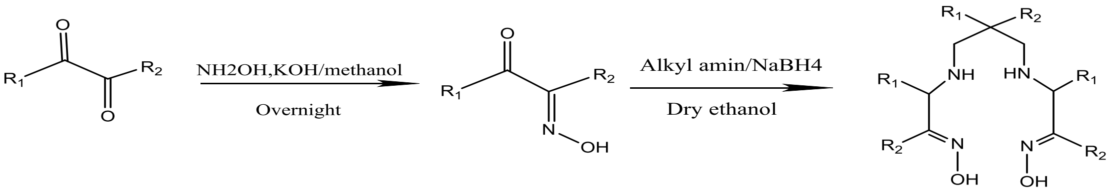

Figure 1.efficient One-Pot prodedure for the synthesis of 3,6,6,9-tetra methyl-4,8-diazaundecane-2,10-dione dioxim

References

[1] J. Ding Ying-Fong Huang, Chemg-ChyiTzeng.Bioorg. Med. Chem. Lett. 9 (1999) 3199-3202.
[2] Hueisch-Jy ding, Ying-Fong huang, Cherng-Chyitzeng, Si-Jung yeh, and Li-Lanwei., Chem. Pharm. Bull. 48(2) 288—289 (2000).
[3] S. Jurisson, E. O. Schlemper, D. E. Troutner, L. R. Canning, D. P. Nowotnik, and R. D. Neirinckx., Inorg. Chem. 1986, 25, 543-549.

A multi component access to novel Coumarin-3-carboxylicacid derivatives

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Isocyanide multicomponent reactions (MCRs) have proved to be extremely versatile entry points to a wide array of novel biologically active scaffolds[1] MCRs, by virtue of this simplicity and the diversity of potential individual components can permit the exquisite positioning of key pharmacophoric moieties in the correct chemical space to enable critical interactions within protein binding sites. Among MCRs,the Ugi and Passerini reactionsare the most popular approaches for the combinatorial chemistry[2,3]. In continuation of our recent research on development of novel multicomponent reactions,in this reaction we wish to report a simple and effient One-Pot four-component reaction of Aniline 1, Isocyanide 2, Aldehyde 3 and Coumarin-3-carboxylic acid 4 to synthesis of novel Coumarin-3-carboxylic acid derivatives 5a-5n.All product were confirmed by ^{1}H NMR,^{1}C NMR spectroscopy , melting point and FT-IR spectroscopy.

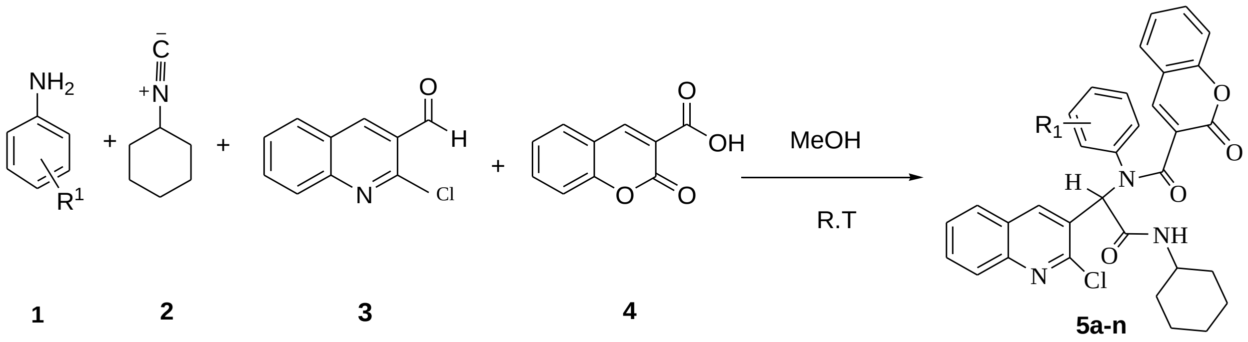

Figure 1. Synthesis of novel 2-oxoethyl-2-oxo-N-phenyl-2H-chromene-3-carboxamide.

References

[1] Dömling, A.; Wang,K.; Wang, w.Chem Rev.2012 , 6 ,3083
[2] Kulsi, G.; Ghorai, A.; Chattopadhyay, P. Tetrahedron Lett.2012, 53, 3619.
[3] Reddy, B. V. S.; Dey, S. K.; Yadav, J. S.; Sridhar, B. TetrahedronLett. 2012, 53, 3676.

Synthesis of 1,2-Diarylethylidenehydrazone Derivatives as Potential Antiseizure Agents

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A design of new antiepileptics is based on the existence of different pharmacophores that were established through the analysis of structural characteristics of clinically effective drugs as well as other antiepileptic compounds [1]. In the literatures [2] it is well documented that one of the important core fragments is defined by presence of: i) hydrogen donor/acceptor unit,ii) one electron donor atom and iii) a hydrophobic domain (aryl ring substituted/unsubstituted). This common template was found in the structures of first generation, however well-established antiepileptics such as carbamazepine or phenytoin, among the newest drugs e.g. Felbamate or in the second generation antiepileptic drugs and the drugs in clinical trial. Much efforts devoted in the recent years based on the pharmacophore model for the development of novel therapeutics resulted in the availability of several newer drugs (such astiagabine, lamotrigine) as promising antiepileptics[3].Therefore, continued search for novel antiepileptic drugs with less toxicity and more selectivity to be an area of investigation in the field of medicinal chemistry.

In this article the aim of synthesizing derivatives of 1,2-diarylethylidene hydrazone derivatives 4 by thioanisol 1 and aryl acetic acid derivatives 2during the two-step reaction as potential antiseizure agents (Figure 1). Structure of compounds and intermediates have been identified to instrumental analysis techniques such as Mass, IR, ^{1}H and ^{13}C NMR.

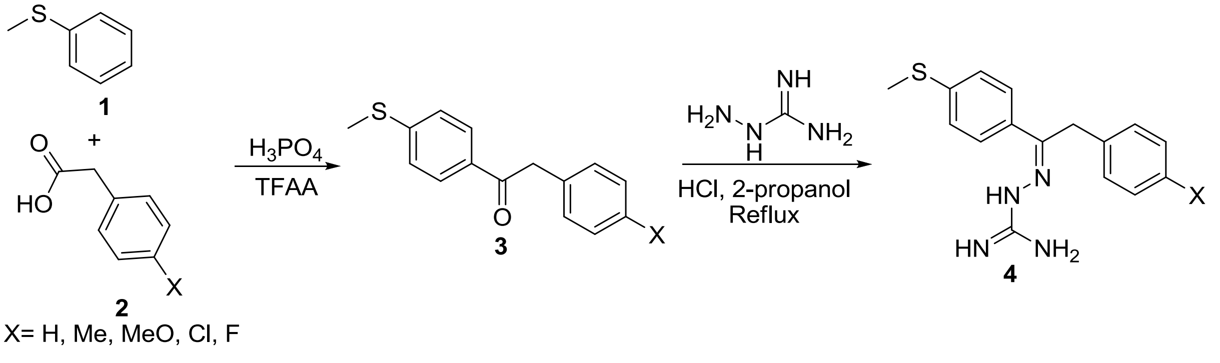

Figure 1. Synthesis of 1,2-diarylethylidenehydrazine derivatives

References

[1] X.Q. Deng, C.X. Wei, F.N. Li, Z.G. Sun, Z.S. Quan, Eur. J. Med. Chem. 45 (2010) 3080.
[2] L. Bruno-Blanch, J. Galvez, R. Garcia-Domenach, Bioorg. Med. Chem. Lett. 13 (2003) 2749.
[3] H. Stefan, T. Feuerstein, Pharmacol. Ther.113 (2007) 165.

(Z)-2-(1-(4-Methoxyphenyl)-2-henylethylidene)hydrazinecarboximidamide Derivatives as Antiseizure Agents

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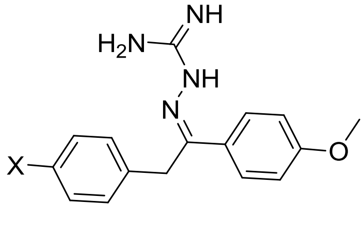
Epilepsy is a common neurological disorder characterized by recurrent seizures that affect about 1% of the world's population[1].Despite all the new antiepileptic drugs (AEDs) introducedin the last two decadesabout 30% of patients have uncontrolled seizures. Inaddition all AEDs have side effects. Consequently, there is a significant need to develop new more efficacious AEDs that will be more potent and with less side effects[2].

Hydrazones and their derivatives are known to exhibit a wide range of interesting biological activities like antioxidant, anti-inflammatory, anticonvulsant, analgesic, antimicrobial, anticancer, antiprotozoal, antioxidant, antiparasitic, antiplatelet, cardioprotective, anthelmintic, antidiabetic, antitubercular, trypanocidal, anti-HIV, and so forth. The present review summarizes the efficiency of hydrazones as potent antiseizure agents [3].

A series of novel (Z)-2-(1-(4-Methoxyphenyl)-2-henylethylidene) hydrazinecarboximidamides was prepared *via* two step reaction. A structure–activity relationship was established focusing on the influence of the substitution pattern in *para* position of the aryl moiety (Scheme 1). Some of the compounds proved to be as potential antiseizure agents.



X= H, Me, MeO, Cl, F

Figure 1. Structure of 1,2-diarylethylidenehydrazine derivatives

References

[1] J.O. McNamara, Nature 339 (1999)15.
[2] J.O. McNamara, L.L. Brunton, J.S. Lazo, K.L. Parker (Eds.), The Pharmacological Basis of Therapeutics, McGraw-Hill, New York, 2006, pp. 501 e526.
[3] S.K. Sridhar, S.N. Pandeya, J.P. Stables, A. Ramesh, Eur. J. Pharm. Sci. (2002) 129.

An efficient procedure for the synthesis of new silylthioalkyne-substituted 1,2,3-triazole derivatives using $LaMn_xCu_{1-x}O_3$ recyclable nanocatalyst in choline chloride/urea deep eutectic solvent

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Perovskites as mixed metal oxides have received wide attention, due to their low-cost, appropriate redox properties, stability of mixed oxidation, high thermal stability and high catalytic activity. This material is introduced by the general formula of ABO_3, where A is lanthanide or alkaline earth metal ion and B is a transition metal ion. The partial substitution of cations in both places A and B, provided multicomponent oxides with unusual valence in cation sites that usually increased catalytic activity of the perovskite systems [1]. However, few reports have been dedicated to mixed metal oxides in organic synthesis.On the other hand, some new approaches were hired to reduce waste and re-used materials, in order to the both environmental and economic issues. $LaMn_{0.3}Cu_{0.7}O_3$ nanoperovskite oxide was prepared by sol-gel procedure and was characterized by X-ray diffraction (XRD), scanning electron microscopy (SEM).

The catalyst was used in the 1,3-dipolar cycloaddition of benzyl halide, terminal alkyne and sodium azide. The $LaMn_{0.3}Cu_{0.7}O_3$ as an effective and inexpensive catalyst showed high catalytic activity at room temperature with low catalyst loading, especially in the presence of the choline chloride/urea(ChCl/urea 1:2)deep eutectic solvent [2] as a green medium.The catalyst and the DES could be recycled and reused at least five times without any significant effect on the results of the reaction. In continuous, a series of novel 1,2,3-triazole substitute thioalkynes was synthesized using carbon disulfide and tris(trimethylsilyl)methylithium [3].

These synthetic compounds are valuable intermediates in synthetic chemistry, chemical biology, and material science.

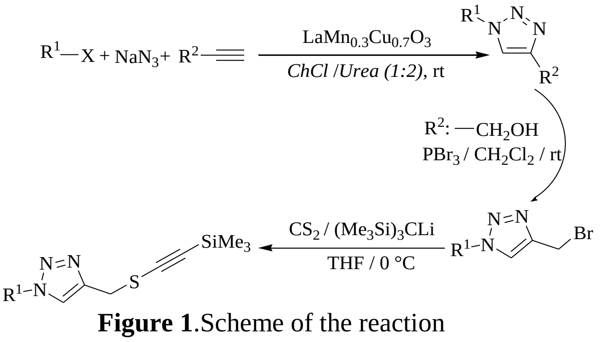

Figure 1.Scheme of the reaction

References

[1] (a) A. Civera, M. Pavese, G. Saracco, V. Specchia, Catal. Today. 83 (1-4) (2003) 199.b)H. Tanaka, M. Misono, Solid State Mater. Sci. 5 (2001) 381.
[2] Q. H. Zhang, K. D. Vigier, S. Royer, F. Jerome, Chem. Soc. Rev. 41 (2012) 7108.
[3] K. D. Safa, M. Alyari, Synthesis. 47, 2015, 256.

Synthesis of novel organosilylvinyl substituent bis-1,2,3-triazole derivatives having antibacterial activity

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The copper(I)-catalyzed 1,3-dipolar Huisgen cycloaddition (CuAAC) reaction of azides and terminal alkynes for the regioselective synthesis of 1,4-disubstituted 1,2,3-triazole derivatives is an important example of click chemistry. These compounds are useful as pharmaceutical agents, agrochemicals, dyes, corrosion inhibitors, photo stabilizers and photographic materials [1]. It is significant that modification of 1,2,3-triazole derivatives with organosilicon groups possibility provides biologically active compounds, which we investigated in this work.

Organosilicon compounds attract scientific attention for some reasons, especially due to a number of interesting results in the field of their biological action, as derivatizing and protecting reagents, intermediates in organic synthesis, and reducing agents. Recently, successful synthesis of a variety of organosilicon derivatives was reported in our laboratory [2].

The in vitro antibacterial activities of mono and di-1,4-disubstitude 1,2,3-triazoles and organosilylvinyl derivatives were tested on several Gram-positive and/or Gramnegative bacteria. The results exhibit the promising antibacterial activity for organosilylvinyl substituent bis-1,2,3-triazole derivatives**.**

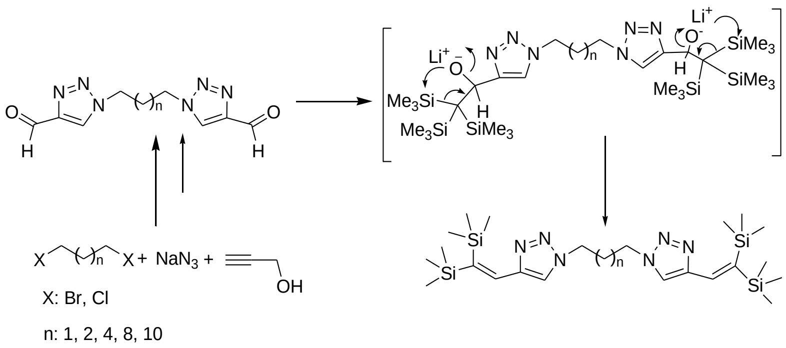

Figure 1.Scheme of the reaction

References

[1] a)M. Whiting, J. Muldoon, Y. C. Lin, S. M. Silverman, W. Lindstrom, A. J. Olson, H. C. Kolb, M. Finn, K. B. Sharpless, J. H. Elder, Angew. Chem. Int. Ed45 (2006) 1435.
b) H. C. Kolb, K. B. Sharpless, Drug Discov Today 8 (2003) 1128.
c) M. Balasubramanian, J. Keay, in: A. R. Katritzky, C. W. Ree, E. F. V. Scriven (Eds.), Comprehensive heterocyclic chemistry 2, Pergamon: Oxford, 1996, Vol. 5, p. 245.
[2] a) K. D. Safa, Y. M. Mosaei, J. Organomet. Chem. 695 (2010) 26.
b) K. D. Safa, M. Allahvirdinesbat, H. Namazi, Mol. Divers. 19 (2015) 29.

Synthesis of 2-aryl-1*H*-perimidinederivatives by reaction of 2-benzylidenemalononitriles andnaphthalene-1,8-diamine

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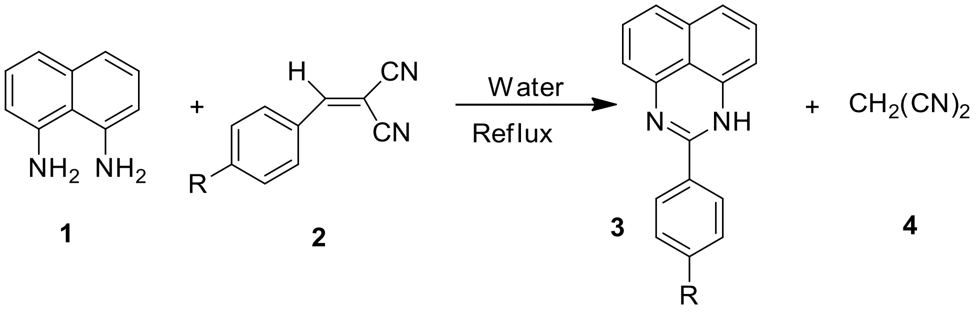
2-Aryl-1H-perimidines is a synthetic tricyclic compounds including double nitrogen atom on its structures. These chemical compounds and its analogs have been described as DNA-intercalating and antitumoral agents against several carcinogenic cell lines[1-3].

2-Phenyl-1H-perimidine is readily prepared, in high yield, by refluxing a mixture of 2-benzylidenemalononitrile and 1, 8- diaminonaphthalene in water. This reaction leads to products 3, 4. The structure of these productswere proved by ^{1}H-NMR, ^{13}C-NMR and IR spectral data(Figure 1).



R= 4-$CH_3C_6H_4$,4-ClC_6H_4 ,2,3-$(OCH_3)_2C_6H_3$,4-$NO_2C_6H_4$, 3-$NO_2C_6H_4$,
4-$OCH_3C_6H_4$, 2-ClC_6H_4 , 4-FC_6H_4 , 3-ClC_6H_4 , 4-BrC_6H_4

Figure 1.Scheme of the reaction

References

[1] F.D. Popp, A. Catala. J. Heterocycl Chem. 1 (1964) 108.
[2] W. Watsulko, A. Catala-Noble, F.D. Popp. J. Med. Chem. 9 (1966) 599.
[3] J.M. Herbert, P.D. Woodgate, WA. Denny. J. Med. Chem. 30 (1987). 2081.

Synthesis of 6-amino-2-oxo-4-aryl-4*H*-1,3-dithiine-5-carbonitrile derivatives by reaction of benzohydrazide, carbondisulfide and 2-benzylidenemalononitriles

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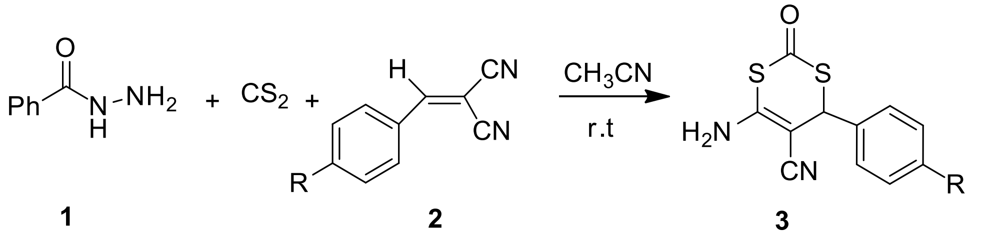
The development of simple, versatile, and environmentally friendly processes or methodologies forwidelyused organic compounds from readily available reagents is one of the major challenges for chemists in organic synthesis [1]. Organic sulfur compounds are widespread in numerous natural products and widely used as various artificial chemicals. These compounds are found in many products of biological and medical [2] relevance as well as in commercial drugs [3].

The mixture of benzohydrazide **1**, carbondisulfide in acetonitrile (7 ml) was stirred for 30 min and then 2-benzylidenemalononitrile **2** was added, and the mixture was stirred for 24 h. After completion of the reaction, determined by TLC, the solvent was removed under reduced pressure, and the viscous residue was purified by column chromatography (Merck 230–400 mesh) using n-hexane-EtOAc (2:1) as eluent to give 6-amino-2-oxo- 4-aryl-4H-1,3-dithiine-5-carbonitrile 3. The structure of these products were proved by ^{1}H-NMR, ^{13}C-NMR and IR spectral data(Figure 1).



R= 4-ClC$_6$H$_4$, 4-NO$_2$C$_6$H$_4$, 3-NO$_2$C$_6$H$_4$, 4-FC$_6$H$_4$, 4-BrC$_6$H$_4$, 2-ClC$_6$H$_4$, 3-ClC$_6$H$_4$

Figure 1.Scheme of the reaction

References

[1] A.Z. Halimehjani, K. Marjani, A. Ashouri. Green Chem. 12 (2010) 1306.
[2] A. Tyrkov, N. Urlyapova, A. Daudova. Pharm. Chem. J. 40 (2006) 377.
[3] T. Ariga, T. Seki. BioFactors 26 (2006) 93.

Solvent-free synthesis of dihydropyrimidinones by PTA@NTU-9 as efficient and reusable catalyst

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Synthesis of 3,4-dihydropyrimidin-2(1H)-one (DHPMs)are important for therapeutic and pharmacological properties.The Biginelli reaction,the three-component reaction betweenaldehydes, urea, and acetoacetate, is one of the most efficient waysto synthesize dihydropyrimidinone derivatives, which are important pharmacological compounds. Various classical methods such as using soluble transition metal salts and some homogeneous transition metal complexes include Schiff's base complexes, metal cyclam complexes and metalloporphyrins complexes are available for this reaction[1]. Heteropoly acids as known environmentally catalyst in green chemistry filed. These compounds are usually supported on a suitable carrier that improves the available surface area, sustainability in reaction medium and catalytic activity[2]. The heterogeneous catalytic systems provides an efficient approach for overcoming these problems. MOFs are a class of newly-developed inorganic–organic hybrid crystalline materials composed of organic linkers and metal nodes that have attracted much attention because they various potential applications, such as in catalysis, separation, gas storage and carbon dioxide capture.These carriers increases the surface area and stability of heteropoly acid in reaction conditions[3].

In this work, a novel heterogeneous catalyst that prepared with encapsulation of phosphotungstic acid ($H_3PW_{12}O_{40}$, PTA) into a Ti (iv)-based metal–organic framework (NTU-9). This compositehave been applied as heterogeneouscatalysts for the green synthesis of a variety of dihydropyrimidinone derivatives through the Biginellireaction and the desired products were obtained in high yields with short reaction time under mildsolvent-free conditions.

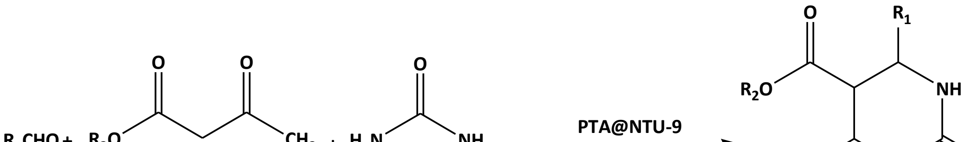

Figure 1. Synthesis of 3,4-dihydropyrimidin-2(1H)-one (DHPMs)

References

[1] A. Zare, Z.A. Nasouri, Journal of Molecular Liquids 216 (2016) 364.
[2] A.L. Cardoso, R. Augusti, M.J. Da Silva, Journal of the American Oil Chemists' Society 85 (2008) 555.
[3] H.C. Zhou, J.R. Long, O.M. Yaghi, Chemical Reviews112 (2012) 673.

Caffeine supported on boehmite nanoparticles: An efficient ionic liquid catalyst for synthesis of pyrazolopyranopyrimidines

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In the recent years, basic ionic liquids (BILs) have been successfully presented as catalysts to catalyze various reactions such as the Heck reaction, Michael addition reaction, and Markovnikov addition reaction[1-2].Although the catalytic ability of basic ILs has been successfully demonstrated in many reactions, the chemical industry still prefers to use heterogeneous catalysts due to their easy separation. Furthermore, it has been reported that supported ILs lead to more improvements in efficiency than homogenous ILs[3-4]. Therefore, it is highly desirable to support basic ILs onto solid supports.

The reaction of 3-chloropropyl boehmite nanoparticles (BNPs) with caffeine in acetonitrile afforded BNPs-3-propyl-imidazolopyridinium chloride [BNPs-Caff]Cl as a new BNP-supported ionic liquid (IL) catalyst. [BNPs-Caff]Cl proved to be an efficient heterogeneous catalyst for the synthesis of pyrazolopyranopyrimidines*via* a One-Pot four-component reaction of hydrazine hydrate, ethyl acetoacetate, barbituric acid, and an aldehyde.

The attractive features of this method are simple procedure, clean reaction, use of a reusable catalyst, easy workup, and performing a multi-component reaction (MCR) in water.

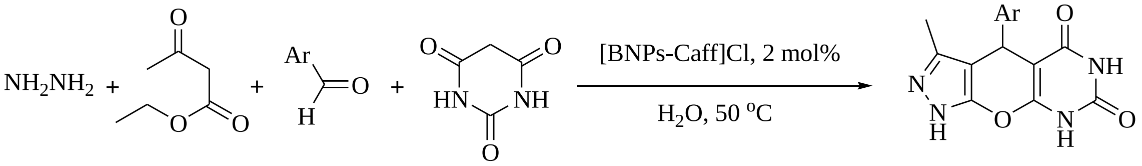

Figure 1.Scheme of the reaction.

References

[1] Y. Liu, M. Li, Y. Lu, G.-H. Gao, Q. Yang, M.-Y. He, Catal. Commun. 7 (2006) 985.
[2] S. Luo, X. Mi, L. Zhang, S. Liu, H. Xu, J.P. Cheng, Angew. Chem. Int. Ed. 45 (2006) 3093.
[3] L. Bian, J. Xu, L. Xie T. Ding, H. Zhang, W. Cao, Tetrahedron 69 (2013) 6121.

Boehmite nanoparticle supported–SO_3H as recyclable heterogeneous Catalyst for the efficient One-Pot synthesis of Pyrazolo [1,2-a][1,2,4]triazole-1,3-diones

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One-Pot multi-component reactions have proven to be more advantageous over conventional linear-type synthesis [1] since the multi-step reactions are usually subjected to compel isolation procedures and produce significant amounts of waste materials. In addition,multi-component processes provide rapid and efficient approach to organic transformations including diverse synthesis of polyfunctionalizedheterocycles. A wide range of naturally occurring compounds belongs to nitrogen-containing heterocyclic compounds. Many of these heterocycles are of significant biological and synthetic importance, which act as pharmaceuticals, agrochemicals, and polyfunctionalized fragments [2,3].

Among these heterocyclic compounds, 1,2,4 triazolidine-3,5-dione containing heterocycles, so-called urazoles, have received considerable interest in synthetic and industrial chemistry [4]. A facile and efficient One-Pot three component synthesis of pyrzolo [1,2-a][1,2,4] triazolo-1,3-diones *via* condensation reaction between aldehyde, 4-phenylurazole and malonitrile or ethylcyanoacetate in ethanol catalyzed byboehmite supported –SO_3H was developed. This method gave good to excellent yields, has short reaction time, operational simplicity and a recyclable catalyst.

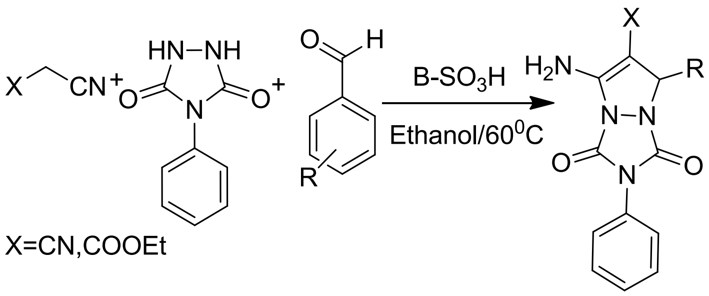

Figure 1.Scheme of the reaction.

References

[1] M. Yoshizawa-Fujita, K. Johansson, P. Newman, D.R. MacFarlanea, M. Forsyth, Tetrahedron Letters 47 (2006) 2755.
[2] M. Adharvana Chari, G. Karthikeyan, A. Pandurangan, T. Siddulu Naidu, B. Sathyaseelan, S.M. JavaidZaidi, A. Vinu, Tetrahedron Letters 51 (2010) 2629.
[3] A.P.M. Marcos, P.F. Clarissa, N.M. Dayse, Z. Nilo, G.B. Helio, Chemical Reviews 108(2008) 2015.

Synthesis of new amidoalkyl naphthol derivatives using Fe_3O_4@SiO_2 piperazine sulfuric acid as catalyst under solvent free conditions

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1-Amidoalkyl-2-naphtol derivatives are of significant importance since they have been frequently applied as hypotensive and bradycardiac agents [1]. 1-Amidoalkyl-2-naphtol can be converted to 1,3-oxazine derivatives [2]. 1,3-Oxazines have potentially different biological activities including antibiotic, antitumor, analgesic, anticonvulsant, antipsychotic, antimalarial, antianginal, antihypertensive, and antirheumatic properties.

1-Amidoalkyl-2-naphtol can be prepared by multi-component condensation of aryl aldehydes, 2-naphtols, and amide derivatives or acetonitrile in the presence of different Lewis or bronsted acids such as *p*-TSA, $ZrOCl_2$, $Yb(OTf)_3$/[Bmim]BF_4, $FeCl_3.SiO_2$, I_2, sulfamic acid [3]. However, many of the reported methods are associated with one or more of the following drawbacks: low product yield, expensive or air-sensitive reagents, long reaction time, harsh reaction conditions, the used of toxic, corrosive and non-reusable catalysts, and the use of large amounts of catalyst. Therefore, the development of more efficient procedures for the synthesis of 1-amidoalkyl-2-naphthols is still needed.

A simple and eco-friendly method for the preparation of amidoalkylnaphthols derivatives *via* the three-component condensation reaction of aldehydes, 2-naphtol, and amids in the presence of acidic catalyst is described (Figure 1).

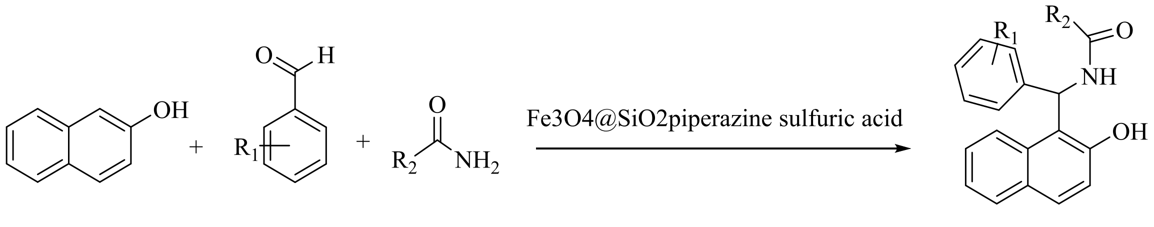

Figure 1. Synthesis of amidoalkyl naphtol by magnetic nanoparticles modified by piperazine sulfuric acid

References

[1] Shen, A.Y., C.T. Tsai, and C.-L. Chen, Synthesis and cardiovascular evaluation of N-substituted 1-aminomethyl-2-naphthols. European journal of medicinal chemistry, 1999. 34(10): p. 877-882.
[2] Damodiran, M., N.P. Selvam, and P.T. Perumal, Synthesis ofhighly functionalized oxazines by Vilsmeier cyclization of amidoalkyl naphthols. Tetrahedron Letters, 2009. 50(39): p. 5474-5478.
[3] Nagawade, R.R. and D.B. Shinde, Synthesis of amidoalkyl naphthols by an iodine-catalyzed multicomponent reaction of β-naphthol. Mendeleev Communications, 2007. 17(5): p. 299-300.

Isolation and purification of protocatechuic acid from *Rhuscoriaria* and synthesis of novel polymers consisted of gallic acid

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Rhuscoriaria Linn (*Anacardiacea*), commonly known as sumac, is an important crop widely used in iran as a food spice, andalso in folk medicine, due to its health-promoting properties.Sumac, has been used as a spice, condiment, appetizer, and as a souring agent for centuries. A broad range of nutritionally and medicinally significant phytochemical components have been identified from various parts of sumac as tannins, flavonoids, anthocyanins, organic acids, flavones, proteins, fiber, volatile oils, nitrates and nitrites. The plants also possesses minerals which are beneficial in the treatment of different disorders and contribute to various biological processes. In traditional system of medicine, this plant has been used in the treatment of diarrhea, dysentery, ulcer, haemorrhoids, hemorrhage, wound healing, hematemesis, hemoptysis, leucorrhea, sore ophthalmia, conjunctivitis, dieresis, animal bites, poison, pain, and liver disease.

Antioxidant activity and phenolic compounds of sumac extracts were investigated. Sumac was extracted in methanol and subjected to solvent–solvent partitioning to yield two fractions as ethyl acetate and aqueous. Methanol extract was further fractioned over Sephadex LH-20 column. Antioxidant activity of extracts and fractions were screened using ferric thiocyanate and DPPH radical scavenging methods. Phenolic composition of active fraction(s) was determined by HPLC–MS systems. Those fractions which exhibited strong antioxidant activity were rich in anthocyanins and hydrolysable tannins. While gallic acid was the main phenolic acid in the extracts, anthocyanin fraction contained cyanidin, peonidin, pelargonidin, petunidin, and delphinidinglucosides and coumarates. Pentagalloyl glucose was abundant in the hydrolysable tannin fraction. Effective scavenging concentration (EC_{50}) on DPPH radical was 0.70 μg/mL both in ethyl acetate and tannin fractions, and 5.33 μg/mL in anthocyanin rich fraction. Same extracts and fractions showed moderate lipid peroxidation inhibition effect compared with the synthetic antioxidants. The findings demonstrate that sumac can be used as a natural antioxidant.

References

[1] Abu-Reidah, I. M., Ali-Shtayeh, M. S., Jamous, R. M., Arráez-Román, D., & Segura-Carretero, A.)..Food Research International70 (2015) 74-86.
[2] Giancarlo S, Rosa ML, Nadjafi F, Francesco M ,Nat Prod Res 20 (2006) 882–886.
[3] Nimri LF, Meqdam MM, Alkofahi A, Pharm Biol 37 (1999) 196–201.

Preparation of CuNi and CuZn nano alloythin films supported on reduced graphene oxide and study of their applications in carbon-carbon cross-coupling

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Bimetallic nanoparticles have attracted remarkeble attention owning to their electronic and catalytic properties as compared to their monometallicnanoparticles [1]. The bimetallic alloy NPs comprising a noble metal and non precious transition metal such as cobalt, nickel, and copper show an enhancement in the catalytic activitiesdue to the synergistic effects between the two different metals [2].Graphen Oxidehave been used as thefavorablesupport for thin film nanoparticles because of its high surface area, electrical conductivity, high stability [3]. Herein, we report a facileand effective route for preparation of thin film nanoparticlesas catalyst. Catalytic activity ofthe as-prepared nanocatalyst was investigatedin carbon-carbon cross-couplings reactions. Thin film nanocatalystwas characterized by transmission electron microscopy (TEM),energy dispersive analysis of X-ray (EDAX) and X-ray diffraction (XRD).This catalytic strategy has shown significant advantages such as being recyclable, high yields and excellent catalytic activities.

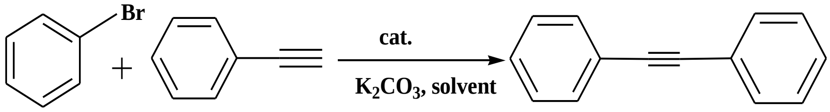

Figure 1.The Sonogashira coupling reaction of phenyl acetylene withbromobenzene

References

[1] D. S. Wang, Y. D. Li,*Adv. Mater*. 2011, 23, 1044−1066.
[2] Z.Niu, D.Wang, R.Yu, Q.Peng,Y,Li,*Chem. Sci*. 2012, 3, 1925-1929.
[3] S. J. Hoseini, M. Bahrami, M. Dehghani, *RSC Adv.*, 2014, 4, 13796-13804.

Modification of chemical control in thermo cycle of Sahand power plant

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The unit 1 turbine of SAHAND power plant - 325 megawatt- is used to be hampering by silicate and oxide deposits. There are many methods for modification of chemical control withoutchanging of equipment. Some technics are combined water treatment (CWT), All Volatile treatment (AVT), Phosphate equilibrium, congruent phosphate, and so on[1].

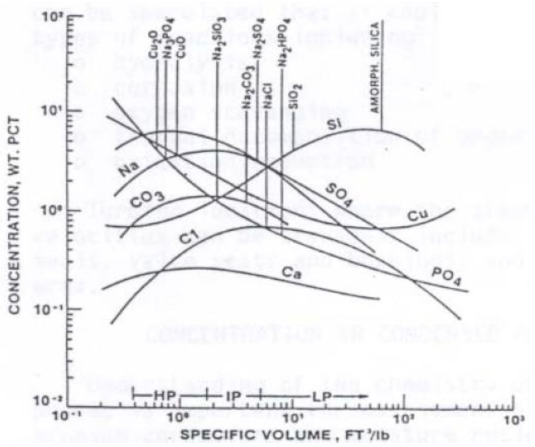

Figure 1

Figure 1 illustrate the condition that all dissolved material becoming through steam and settles on turbine blades. We changed the chemical condition of boiler and feedwater in Sahand thermal power plant to the modified one. This new condition include elimination of base from boiler,elimination of Aluminum fromcooling tower and drum, injecting of new reagents in boiler and feedwaterfor purpose to diminish conductivity, corrosion, carry over, foaming, silicate, deposits and overall result was the clean steam going on turbine. In this new condition we found that the efficiency of steam generator and turbine become better than previous condition.

References

[1] Betz Handbook of industrial ..sixth edit. , p 151.

Multicomponent Synthesis of some new 7-amino-8-(5-bromoquinoxalin-6-yl)-3,8-dihydro-2*H*-spiro[imidazo[1,2-a]pyrimidine-5,3'-indolin]-2'-one derivatives

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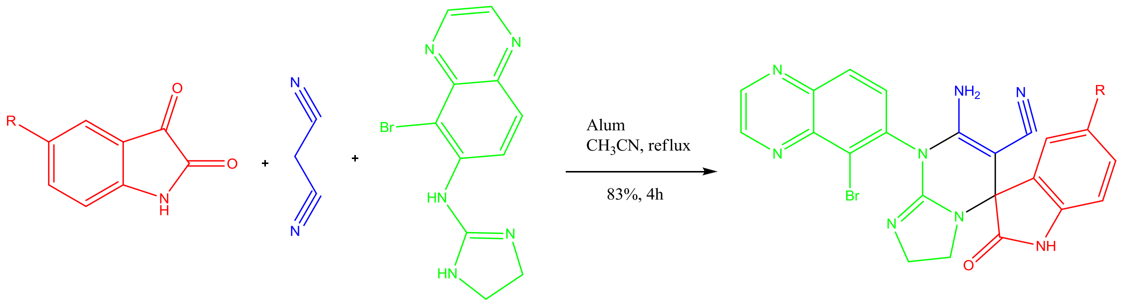
Multicomponent reaction (MCR) has emerged as a powerful strategy in modern synthetic organic chemistry, which allows molecular complexity and diversity needed in the combinatorial chemistry for the preparation of bioactivecompounds[1].

Much attention has been devoted towards dihydropyrimidine derivatives due to their significant therapeutic and medicinal properties. Alkaloids having the dihydropyrimidine core unit were found to show interesting biological activities such as antiviral, antibacterial and anti-inflammatory activities[2].

In continuation of our ongoing work on multi-componentreactions (MCRs) [3], we now wish to report afacile and rapid One-Pot three component reaction forpreparation of some novel 7-amino-8-(5-bromoquinoxalin-6-yl)-3,8-dihydro-2H-spiro[imidazo[1,2-a]pyrimidine-5,3'-indolin]-2'-one derivativesfrom isatines1, malononitrile 2 and brimonidine 3usingnontoxicand readily available $KAl(SO_4)_2.12H_2O$ as heterogeneouscatalyst (Figure 1**)**.



1 2 3 4

Figure 1.Scheme of the reaction.

References

[1] Hulme, C.; Gore, V. "Multi-component reactions: Emerging chemistry in drug discovery" 'From xylocain to crixivan'. Curr. Med. Chem. 2003, 10, 51-80.
[2] Kappe, C. O. Eur. J. Med. Chem. 2000, 35, 1043.
[3] A. A. Mohammadi, S. Taheri, S. Askari, R. Ahdenov. J. Heterocyclic Chem., 2015, 52, 1871.

One-Pot Three Component Synthesis of Some New Dihydropyrimidines Derivatives

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In recently years dihydro pyrimidines were attention of many chemists and biologists and their analogues have a wide range of biological activities, such as antiviral, antitumor and antimicrobial agents [1]. Several methods have been reported for synthesis of dihydro pyrimidines in different conditions [2].

In the context of our ongoing studies on synthesis of heterocyclic compounds[3],herein, we wish to report a novel, efficient, and One-Pot method for the construction of some new dihydro pyrimidines via condensation ofbrimonidine 1, malononitrile 2, and aldehyde 3 derivatives using the non-toxic and easily available Alum as a heterogeneous catalyst(Figure 1).

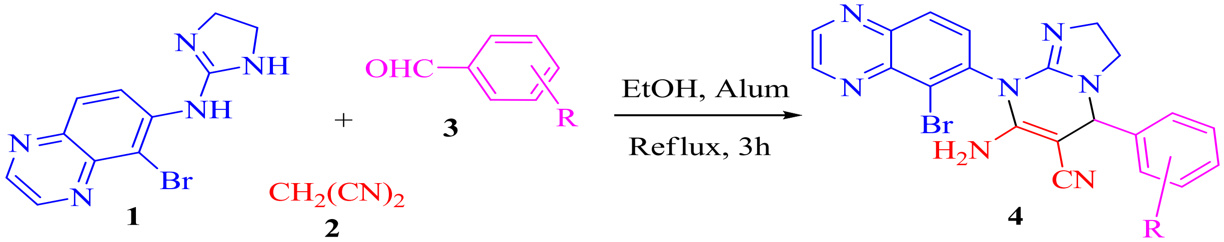

Figure 1. Scheme of the reaction.

References

[1] L. Dalla-Via, O. Gia, S.M. Magno, A. Da Settimo, A.M. Marini, G. Primofiore, F. Da-Settimo and S. Salaerno, Il Farmaco., 2001, 65, 159.

[2] Guang-Yong Lee, Kyung Hee Jung A, Hyunseung Lee, Mi Kwon Sona, JuHyeonSeoa, Sang-Won Honga, YujeongJeongc, Sungwoo Hong. Cancer Lett, 2013, 329, 59.

[3] A.A. Mohammadi, S. Taheri, A. Amouzegar, J. Heterocyclic Chem.,2016, 53, 805

Synthesis and structure of a new dithiazolopyridine as a novel fluorescent sensor of cyanide ion

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Recently, we reported the synthesis and characterization of the dithiazolopyridine 1 and studied its optical properties upon coordination to Cu^{2+} to give complex 1•Cu^{2+} [1]. We found that 1•Cu^{2+} displays high sensitivity, well reversibility and rapid response (<1 min) for recognizing CN^{-}in THF.

Figure 1.Scheme of the reaction.

Herein, the synthesis and characterization of dithiazolopyridine**2** is reported. In contrast to compound 1, probe 2 detected directly the cyanide ions without using of its metal complexes [Figure 1]. The practical application of the **2** for the detection of CN^{-} ions was realized by using solution coated silica strips (TLC plates).

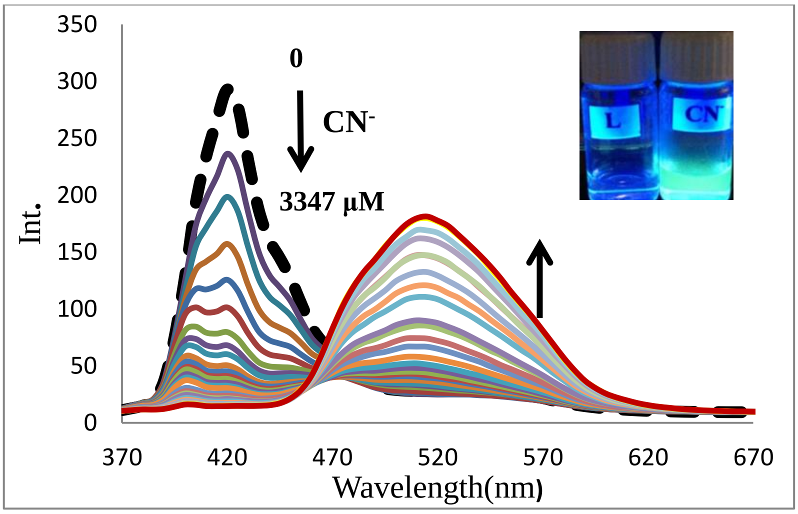

Figure 1. Compound 2 detected directly CN^{-}

Reference

[1] H. R. Darabi, et al.,Tetrahedron Letters 57 (2016) 256–259.

Synthesis of fluorinated coumarines via isocyanide-based multi component reactions

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The 3,4-dihydrocoumarin system is widely distributed in nature [1], and some derivatives have shown a wide range of biological activitiessuch as aldose reductase inhibition, antiherpetic, protein kinases, and a moderate estrogenic activity [2]. A variety of3,4-dihydrocoumarines were synthesized multi component reactions [3].

As a part of our current studies on the isocyanide-based multi component reactions, in this work,fluorinatedcoumarineshas been synthesized viafour-component reaction. A wide variety of pharmacologically significantand structurally interesting compounds were preparedviausing commerciallyavailablesubstituted 2-hydroxybenzaldehydes 1, Meldrum's acid 2, isocyanides 3,andfluoroalcohol4 inCH_2Cl_2 at room temperature without using any catalysts and activation in excellent overall yields (Scheme 1).Substituents could be independently varied at three different positions.

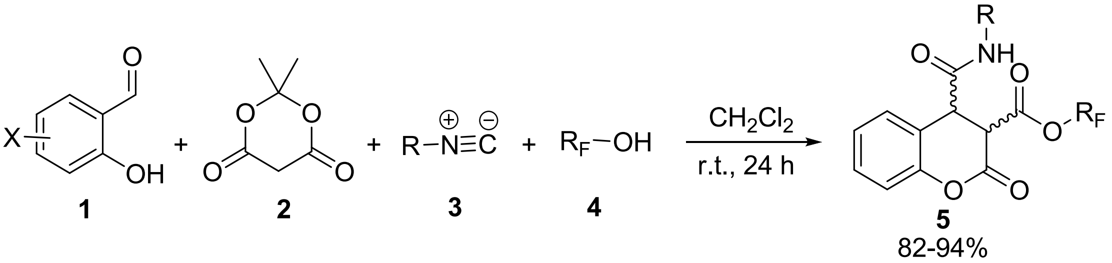

Figure 1. Synthesis of fluorinated coumarines

References

[1] J.Posakony, M.Hirao, S. Stevens, J.A.Simon, A.Bedalov, J. Med. Chem.47(2004), 2635.

[2] A.Kumar, B.K.Singh, R.Tyagi, S.K.Jain, S.K.Sharma, A.K.Prasad, H.G. Raj, R.C.Rastogi, A. C.Watterson, V.S.Parmar, Bioorg. Med. Chem. 13 (2005), 4300.

[3] A.Shaabani, A.Maleki, A.H.Rezayan, A.Sarvary, Mol.Divers. 15 (2011), 41.

PdCuFe/reduced-graphene oxide nanohybridthin film at oil/water interface suitable for catalytic reduction of *p*-nitrophenol

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The oil/waterinterfacial assembly strategy provides a powerful bottom-up approach for the nanofilm fabrication due to low cost and low environmental impact [1]. Most importantadvantages of this assembly strategy are the significant simplicity and universality found in almost all of the related low dimensional nanostructures. Recently, this techniquehas been used for the preparation of metal, semiconductor and oxide nanocrystals [2]. The method used to prepare thin films at the organic-aqueous interface involves dissolving the relevant precursor in the organic layer and injecting an appropriate reagent in the aqueous layer.Graphene oxide (GO) is widely usedas excellent carbon support for catalysts to achieve the desired activity and stability. It has been reported that graphene/GO-supported metal or metal oxide nanoparticles (NPs) could improve the performance of catalysts in the different ofreaction [3].

In this work, PdCuFe/RGO thin film was synthesized by the reduction of [$PdCl_2$(cod)], [Cu(acac)$_2$] and [Fe(acac)$_3$] complexes as palladium, copper and iron precursors at the toluene-water interface. The nanohybrid was characterized by X-ray diffraction (XRD), energy-dispersive analysis of X-ray (EDAX) and Transmissionelectron microscopy (TEM). Then we investigated the catalytic activityproperty of this nanostructure in the reduction reaction of *p*-nitrophenol.

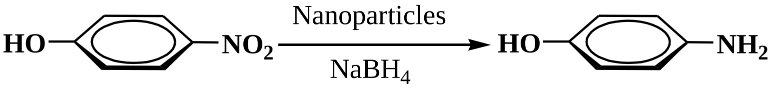

Figure 1.Scheme of the reaction.

References

[1] L. Hu, M. Chen, X. Fang, L. Wu, Chemical Society Reviews 41(2012) 1350.
[2] C. N. R. Rao, K. P. Kalyanikutty, Accounts of Chemical Research 41(2008) 489.
[3] Y. X. Huang, J. F. Xie, X. Zhang,L. Xiong, H. Q. Yu, ACS Applied Materials and Interfaces 6(2014) 15795.

Novel Economic Synthesis of Benzalkonium Chloride

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Benzalkonium chloride is a cationic surface-acting agent belonging to the quaternary ammonium group. It has three main categories of use: as a biocide, a cationicsurfactant, and phase transfer agent in the chemical industry [1]. These compounds have considerable chemotherapeutic properties. They possess antibacterial, antimycotic, antiprotozoal or antiproliferative activities [2, 3].

A highly efficient, two-step method to make Cetyl dimethyl benzyl ammonium chloride is described. First *N*,*N*-dimethyl benzyl amine was prepared via reductive methylation of benzylamine with *N*-methylpyrrolidine zinc borohydride (ZBHNMP) at pH 7 in THF. Then 1-chlorohexadecane reacted with *N*, *N*-dimethyl benzyl amine in dry ethanol under reflux conditions to excellent yield. After completion of the reaction, as indicated by TLC, the solvent was evaporated and the isolated product was recrystallized from acetone to give white crystals of cetyl dimethyl benzyl ammonium chloride. The product was characterized by IR, ^{1}H NMR, ^{13}C NMR and elemental analysis. The Cetyl dimethyl benzyl ammonium chloride was prepared by the general method shown in below Scheme.

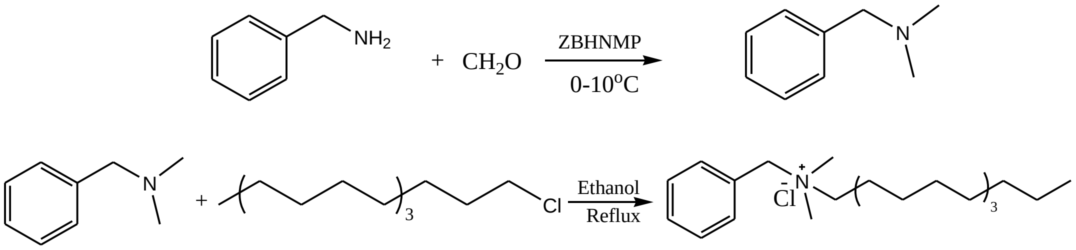

Figure 1. Scheme of the reaction.

In this work the efficient synthesis of valuable cetyl dimethyl benzyl ammonium chloride from inexpensive and commercially available precursor was described. Excellent yield, simple experimental procedure and easy product isolation are important features of this new protocol to prepare Benzalkonium chlorides.

References

[1] M. Lukác, M. Mrva, M. Garajová, EuropeanJournal of Medicinal Chemistry, 66 (2013) 46.
[2] J. Haldar, P. Kondaiah, S. Bhattacharya, Journal of Medicinal Chemistry, 48 (2005) 3823.
[3] J.E. LaDow, D.C. Warnock, K.M. Hamill, K.L. Simmons, EuropeanJournal of Medicinal Chemistry, 46 (2011) 4219.

Synthesis Procedure Optimization and Characterization of Sulfated Tungstate as a Heterogeneous Catalyst

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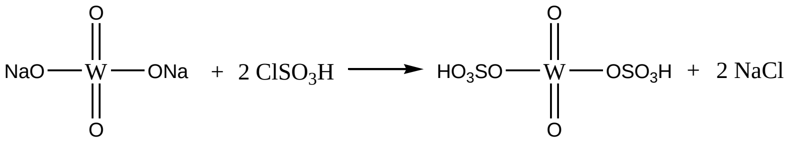
Development of green catalysts and catalytic reactions are the key demands for green chemistry and sustainability [1]. Sulfated tungstate is green catalyst and was demonstrated its effectiveness as catalyst in amidation, Ritter, Biginelli, and Strecker reactions [2]. Taguchi statistical experimental design has been widely employed in various chemical optimization procedures [3].

Sulfated tungstate was prepared via addition of anhydrous sodium tungstate to a stirred solution of chlorosulfonic acid at 0-5°C. The experimental process parameters for the synthesis of sulfated tungstate were optimized by the aid of Taguchi robust design using an OA_9 as orthogonal array design. The studied variables in this investigation were mole ratio of reagents, reaction time, temperature and solvent type. The morphology and chemical composition of the prepared catalyst is well characterized by TGA, X-ray diffraction, SEM and FT-IR spectroscopy.



$$NaO{-}W({=}O)_2{-}ONa + 2\,ClSO_3H \longrightarrow HO_3SO{-}W({=}O)_2{-}OSO_3H + 2\,NaCl$$

We have prepared sulfated tungstate as a stable, cost-effective and reusable solid inorganic acid catalyst useful for nitrone synthesis. The main parameters of the synthesis procedure were optimized by Taguchi statistical experiment design to obtain high yield and minimum particle size of sulfated tungstate.Catalytic activity of sulfated tungstate among the other solid acid catalysts for the preparation of the nitrones was evaluated.

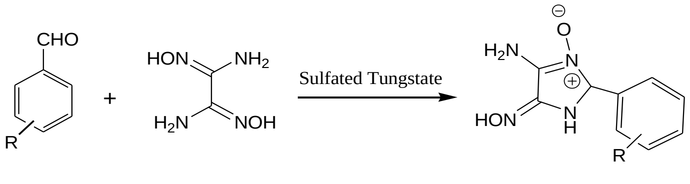


Figure 1. Scheme of the reaction.

References

[1] P. S. Chaudhari, S. D. Salim, R. V. Sawant, K. G. Akamanchi, Green Chemistry, 12 (2010) 1707.
[2] S. P. Pathare, R. V. Sawant, K. G. Akamanchi, Tetrahedron Letters, 53 (2012)3259.
[3] M. Rahimi-Nasrabadi, S.M. Pourmortazavi, M.R. Ganjali, A.R. Banan, Journal of Molecular Structure, 1074 (2014) , 85.

Preparation of Immobilized Tribromide on Fe_3O_4 Magnetic Nanoparticles (Fe_3O_4-Br_3) and its Utilization in the Knoevenagel Condensation Reaction andSynthesis of Polyhydroquinolines

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Polyhydroquinolines, as interesting and versatile N-heterocycles, have attracted much attention due to their pharmacological properties, such as antitumor, bronchodilator, antidiabetic, antiinflammatory, antibacterial, and antimalarial agents [1]. Consequently, many different synthetic methods for producing polyhydroquinolines derivatives have been reported using various catalysts.

The Knoevenagel condensation is one of the most powerful strategies for carbon-carbon bond formation in organic chemistry [2], and its products have numerous applications in thesynthesis of fine chemical, as well as carbocyclic and heterocyclic compounds of biological significance [3, 4].

In this work, we wish to report use tribromide immobilized on Fe_3O_4 modified magnetic nanoparticles as new, efficient and reusable catalysts for Knoevenagel condensation reactions and synthesis of polyhydroquinoline derivatives in mild conditions.The separation of catalyst from reaction mixture was performed without needed expensive centrifuges and process of filtering with using an external magnet and reused for several times without significant loss of its catalytic activity is advantaged this catalyst.

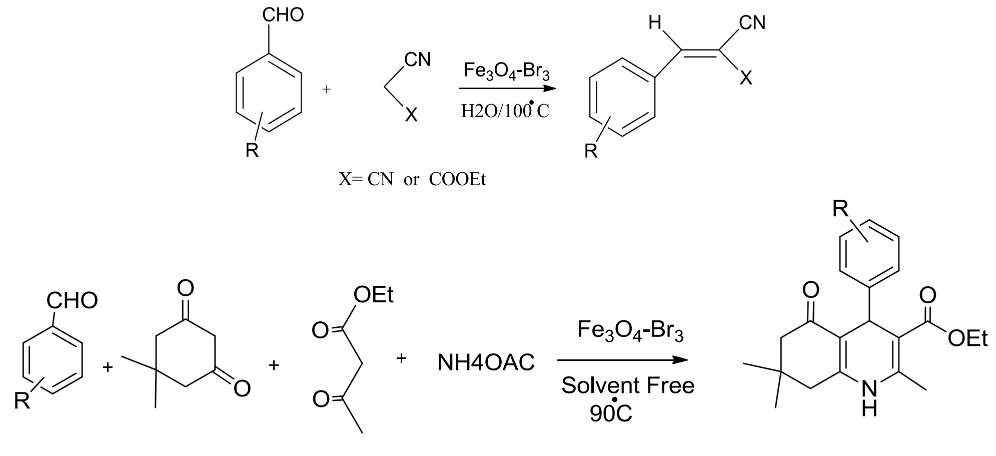

Figure 1. Scheme of the reaction.

References

[1] A. Sausins, G. Duburs, Heterocycles 27 (1988) 279.
[2] X. Z. Dong, Y. H. Hui, S. L. Xie, P. Zhang, G. P. Zhou and Z. F. Xie, RSC Advances3(2013) 3222.
[3] Y. M. Ren and C. Cai, Catalysis Letters 118(2007) 134.

Tribromide Immobilized on Modified Magnetic Fe_3O_4 Nanoparticles Used as Efficient and Reusable Nanocatalyst for the Synthesis of 2,3-Dihydroquinazolin-4(1*H*)-ones

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2,3-Dihydroquinazolinones are a class of heterocycles that attracted much attention because they have been reported to possess a wide range of pharmaceutical activities including antifertility, antibacterial, antitumor and antifungal [1]. Several methods have been reported for the synthesis of 2,3-dihydroquinazolinones. The typical procedure for the synthesis of 2,3-dihydroquinazolin-4(1H)-ones involves the condensation reaction of anthranilamide with aldehyde or ketone using acids as a catalyst under various conditions [2,3].

Organic reactions in aqueous media have attracted much attention because (i) water induces unique reactivity and selectivity that are not observed for reactions in organic media and (ii) water as solvent reduces the use of harmful organic solvents and may lead to the development of environmentally friendly chemical processes [4].

In this work, we report a simple and practical metal-free method for the synthesis of 2,3-dihydroquinazolin-4(1H)-ones by the cyclocondensation of anthranilamide withaldehydes using tirbromide supported on Fe_3O_4magnetic nanoparticles (Fe_3O4-Br_3) as arecyclable organocatalyst in water at 80 ^{o}Ctemperature.

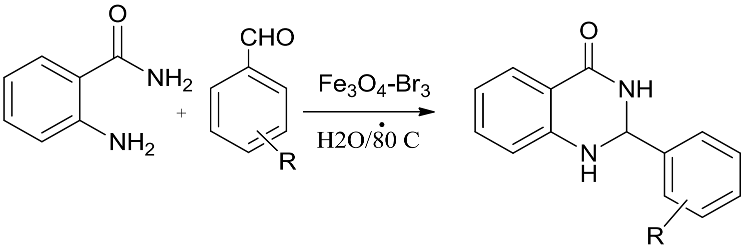

Figure 1.Scheme of the reaction.

References

[1] M. Hour, L. Huang, S. Kuo, et al. Journal Medicinal Chemistry.43 (2000) 4479**.**
[2] Rahman,M.; Ling, I.; Abdullah, N.; Hashim, R.; Hajra, A.RSC Advances 5 (2015**)** 7755.
[3] Ghorbani-Choghamarani, A.; Azadi,G. RSC Advances 5 (2015)9752.

Preparation and characterization of silver nanoparticle-containingsemi-interpenetrating network poly(acrylic amide)/poly(aspartic acid) hydrogels for antibacterial applications

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Hydrogels are three-dimensional hydrophilic polymer networks, that are able to swell when added to water or biochemical fluid.Interpenetrating polymeric networks (IPN) a new class of polymeric hydrogels provide great opportunity due to the additive effect of the polymers within the multicomponent polymeric system [1,2]. Interpenetrating polymer network (IPN)-based hydrogels can act as excellent nanoreactors for producingnanoparticles [3]. In the present study, we report for the first timeinterpenetrating polymer networks (IPN),based on polymer polyaspartic acid (PASP)-graphenehydrogel, into the poly(acrylamide) (PAm).This hydrogelserved as templates for producing stable silver nanoparticles (NPs) via in situ reduction of silver nitrate (AgNO3) using sodium borohydride ($NaBH_4$) as reducing agent.The chemical structures of IPN hydrogel–silver nanocomposites were characterizedby using X-ray diffraction (XRD), thermogravimetric analysis (TGA), scanning electron microscopy (SEM). Moreover, antibacterial ability and swelling properties of this hydrogelswerealso assessed.

References

[1] Sivagangi Reddy, N., Krishna Rao, K.; Eswaramma, S.; MadhusudanaRao, K., Soft Materials 2016, 14 (2), 96-106.

[2] Lim, S. L.; Tang, W. N. H.; Ooi, C. W.; Chan, E. S.; Tey, B. T.,. Journal of Applied Polymer Science 2016.

[3] Park, S.; Murthy, P. K.; Park, S.; Mohan, Y. M.; Koh, W.-G.,.Journal of Industrial and Engineering Chemistry 2011, 17 (2), 293-29.

Construction of drug carrier based on amylose grafted-poly(aspartic acid)

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The graft copolymers have been extensively investigated, due to specific morphology,and their widespread application in various fields, especially inpharmaceutical[1]. Graft copolymers are a branched copolymer where the components of the side chain are structurally different than that of the mainchain [2,3]. In this study, biodegradable and biocompatible copolymers of amylose/ethylenediamine-graftedpoly(aspartic acid) were successfully synthesized by aminolysis reaction of amylose and ethylenediamine ontopolysuccinimide.We using reductive amination reaction to the preparation ofend-functionalized amylose.The chemical structures of thiscopolymers were confirmed by FT-IR and^{1}H NMR spectroscopy andother analyzes.These copolymesr were then investigated for their ability as a drug carrier.

References

[1] J.-C., Yeh, H.-H, Yang, Y.-T., Hsu, C.-M., Su, T.-H., Lee, S.-L., Lou, Colloids and Surfaces A: Physicochemical and Engineering Aspects 2013, 421, 1-8.
[2] D.-E, Liu, H., Han, H., Lu, G., Wu, Y., J., Wang, , H., Ma, Gao, RSC Advances 2014, 4 (70), 37130-37137.
[3] J., Zeng, H., S., Huang, H., Liu, Xu, Huang, J., Yu, Colloids and Surfaces B: Biointerfaces 2013, 105, 120-127.

Preparation and characterization of 2,4-Dihydroxy benzoyl chitosan

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Recent studies of the chemical modification of chitin and chitosan are discussed from the viewpoint of biomedical applications. Special emphasis is placed on the role of individual functional groups in applications of modified chitosan. Among chitosan derivatives, quaternary ammonium chitosan, carboxyalkylchitosans and *N*-acyl chitosan and *O*-acyl chitosan, are some types of modified chitosans, which have been studied intensively in order to improve solubility, biological properties and find new applications [1,2]. Chitosan and its derivatives are useful as carriers in drug delivery systems, as antibacterial agents, and in other medical applications. In this work, 2,4-Dihydroxybenzoic acid covalently conjugated to chitosan *via* a 1-ethyl-3-(3-dimethylaminopropyyl)- carbodiimide-mediated (EDC-mediated) and *N*-hydroxylsuccinimide (NHS) reaction to generate chitosan derivatives. Modified chitosans were prepared under homogenous conditions in 1% acetic acid solution. The reaction occurs between the amino groups of chitosan and carboxyl groups of dihydroxybenzoic acid in the presence of EDC and NHS. EDC and NHS have been used as the activating agents for the amide bond formation. In the FT-IR analysis of chitosan, specific peaks of chitosan are observed at 1659 cm^{-1}, 1630 cm^{-1} and 1564 cm^{-1}, which are attributed to the C=O stretching vibration of amid I, N-H bending vibration of amine and N-H bending vibration of amide II, respectively[3]. Compared to the FT-IR spectrum of chitosan, the spectrum of CS-DH showed new peaks at 1654 cm^{-1} and at 1546 cm^{-1}, attributed to the carbonyl stretching vibration of amide I and N-H bending vibration of amide II, respectively. In the ^{1}H-NMR spectra of CS-DH, in addition of the protons of repeating unit of chitosan, protons of aromatic ring (H-arom) appear at 6.7 (H-8), 6.9 (H-7) and 7.3 (H-9), respectively.

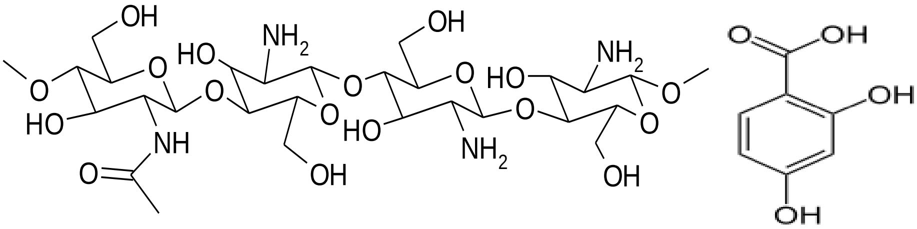

Figure1. Chemical structure of chitosan and 2,4-Dihydroxybenzoic acid.

References

[1] M.N.V. Kumar. Reactive and Functional Polymers 1 (2000) 46.

[2] C,H. Kim, J.W. Choi, H.J. Chun, K.S. Choi. Polym Bull 38 (1997) 387.

[3] C. Peniche, W. Arguelles-Monal, N. Davidenko, R. Sastre, A. Gallardoand J.S Roman. Biomaterials 20 (1999) 1869.

An Efficient Solvent-Free Synthesis of Spirooxindole-quinazolinediones using TiO_2/SiO_2 Nanocomposite Catalyst

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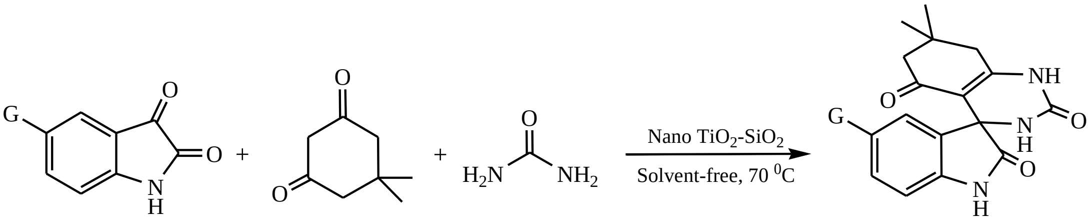
In the last decade, spirooxindoles has been identified as an important class of nitrogen containing heterocycles, which display wide range of biological properties such asantimalarial, antituberculosis, and growth hormone secretagogue [1]. Nanostructured metal oxides based their high physical and chemical abilities promote numerous organic transformations [2]. Nano titanium dioxide (TiO_2 NPs) is considered very close to an ideal of these highly efficient nanocatalysts due to its unique properties such as being non-toxic, inexpensive, moisture stable and reusable catalyst [3]. In addition, TiO_2 NPs over silica shells (TiO_2-SiO_2 nanocomposite) with improved the catalytic efficiency of TiO_2 NPs by an increase in the specific surface area, has been thought to be a new efficient catalyst. In the present study, I designed a new simple One-Pot three-component reaction of 1*H*-indole-2,3-diones (isatins) **1**, dimedone (**2**) and urea (**3**) to afford spiro[4.3']oxindole-3,4,7,8-tetrahydro-7,7-dimethylquinazoline-2,5-(1*H*,6*H*)-diones **4**, which was catalyzed by TiO_2/SiO_2 nanocomposite, under solvent-free conditions. This method in addition to its simplicity of operation has the advantages of high yields, easy work-up with avoidance of using harmful organic solvents, and recyclability of the catalyst.



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

Figure 1. Scheme of the reaction.

References

[1] N.R. Ball-Jones, J.J. Badillo, A.K. Franz, Organic and Biomolecular Chemistry 10 (2012) 5165.
[2] V.P. Reddy, A.V. Kumar, K. Swapna, K.R. Rao, Organic Letters 11 (2009) 951.
[3] M. Lakshmi Kantam, S. Laha, J. Yadav, B. Sreedhar, Tetrahedron Letters 47 (2006) 6213.

Copper(I) Iodide Nanoparticles Catalyzed Solvent-Free Synthesis of 4-arylacridinediones and 6-aryldiindeno[1,2-b:2,1-e]pyridinediones

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The importance of acridine core structure and other heterocycles containing its framework is well known, as they are found in numerous compounds with a variety of biological effects such as, antibacterial, antifungal, antimalarial, and anticancer properties. Many members of these compounds are used as chemotherapeutic agents against cancer cells [1]. Pyridine is also an important solvent and heterocyclic nucleusfor the design and synthesis of novel molecules with biological activities and properties. It occurs in several natural compounds which are used as a precursor in agrochemicals and pharmaceuticals [2]. The utility of nanostructured metal salts as catalysts in organic synthesis has drawn special attention due to their better properties compared to the bulk size. Nanosized copper iodide is one reusable Lewis acid catalyst which has revealed several catalytic activities for the synthesis of organic compounds and others [3]. I wish to report herein a solvent-free condensation between aromatic aldehydes **1**, ammonium acetate (**2**) and active methylene compounds including dimedone (**3**), or 1,3-indanedione (**5**), in the presence of CuI nanoparticles (CuI NPs) as an efficient and recyclable catalyst leads to 4-arylacridinediones **4**, and 6-aryldiindeno[1,2-b:2,1-e]pyridinediones **6**. The avoidance of using harmful organic solvents, production of pure products in high to excellent yields without any by-products, reusability of catalyst, and very simple operation are the advanteges of this novel and practical approach.

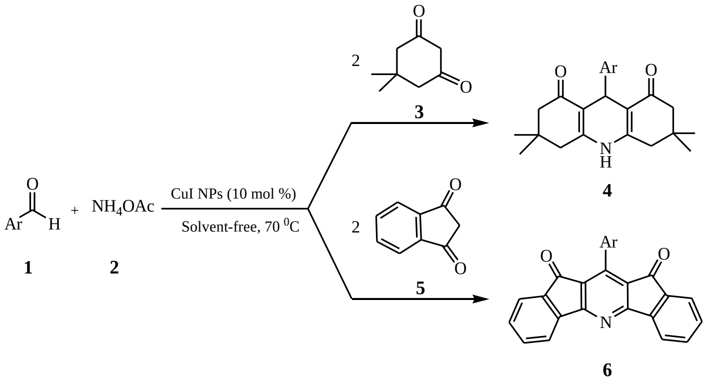

Figure 1. Scheme of the reaction.

References

[1] Adrienne, Current Medicinal Chemistry9 (2002) 1667.
[2] G.D. Henry, Tetrahedron 60 (2004) 6043.
[3] S.Abdolmohammadi, S. Karimpour, Chinese Chemical Letters 27 (2016) 114.

A new green method for synthesis of some novel derivatives uses Core-shell $Fe_3O_4@SiO_2$ nanoparticles as a reusable catalyst

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The preparation and the use of magnetic nanoparticles (MNPs) in organic synthesis has become a subject of intense investigation. which offer advantages in clean and sustainable chemistry as they can be non-toxic, readily accessible, and reusable. Additionally, the activity and selectivity of magnetic catalysts can be manipulated by its surface modification.[1] Thiopyran and indole core skeleton are important syntonic of heterocyclic compounds and are important class of structural motifs present in many natural products [2]. Thiopyrano sulfur compounds as well as have a many biological activity such as anti-bacterial, anti-hyperplasia and anti-cancer activities [3,4]. In this regard, we are reported a facile, green and high efficiency methodology for synthesis of some novel dihydrothiopyran derivatives from indolin-2-thion 1, malononitrile 2 and aldehyde 3. (Figure1) This catalytic system can be easily recovered and reused for at least three times without significant loss of its activity.

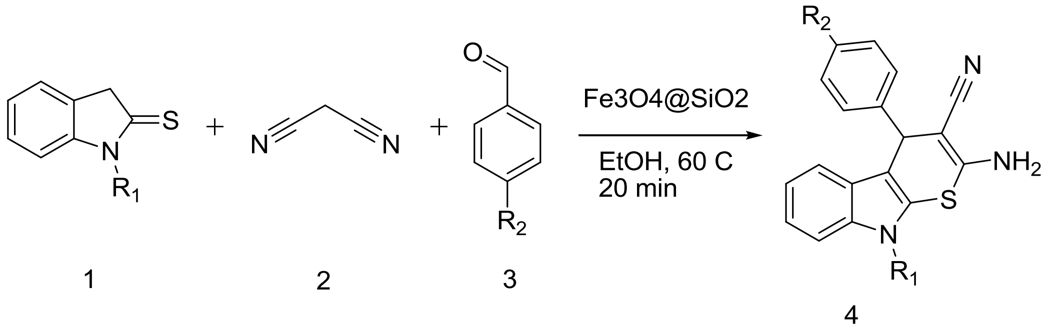

Figure 1. Scheme of the reaction.

References

[1] Zhijun Xu, Jiahua Lu, Qing Liu, Lian Duan, Aihua Xu, Qiang Wang and Yuguang Li, RSC Adv, 2015, 5, 76862.
[2] Taheri, S; Mohammadi, Ali. A; Ahdenov, R; Azarlak, R. JICS, 2016, 7, 1301.
[3] J.T. Li, S.X. Wang, G.F. Chen, T.S. Li, Curr. Org. Synth, 2005, 2, 415.

A Novel Magnetically Separable EDTA@$CuCl_2$ Functionalized Magnetic Nanoparticles for Synthesis of Benzamides

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Amides have been synthesized with minimal by-products in a one pot oxidative amidation of benzyl alcohols with amine hydrochloride salts. This greener amide formation was completed in the presence of Fe_3O_4@EDTA@$CuCl_2$ catalyst, base promoter and TBHP as an oxidant. The catalyst has been characterized by FT-IR, XRD, SEM, VSM, ICP and TG/DTA. After the completion of the reaction by aid of an external magnet, the catalyst could be removed from the reaction vessel and reused at least six times without significant loss of its activity. The measured content of Cu in Fe_3O_4@EDTA@$CuCl_2$ by inductively coupled plasma atomic emission spectroscopy (ICP-AES) was 0.4 mmol per gram of catalyst. Amide functional group has unique characteristics, including invariability, resistant to hydrolysis, high polarity, diversification of the conformation [1] and acts as prevalent functional group especially in pharmaceuticals and biologically activecompounds [2]. Amide bond formation was employed in the synthesis of 66% of drugs developed by pharmaceutical companies such as GlaxoSmithKline, Astra Zeneca and Pfizer[3]. Therefore, numerous methods for the synthesis of amides are in the great demand.

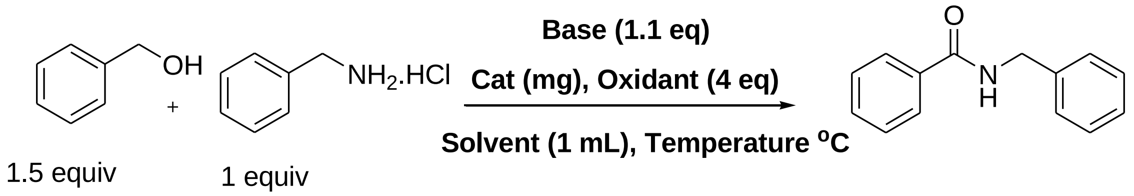

Figure 1. Scheme of the reaction.

References

[1] V. R. Pattabiraman, J.W. Bode, Nature 480 (2011) 471.
[2] Z.W. Chen, H.F. Jiang, X.Y. Pan, Z.J. He, Tetrahedron 67 (2011) 5920.
[3] R. García-Álvarez, P. Crochet, V.Cadierno, Green Chem. 15 (2013) 46.

Nitrosation reaction of aromatic compounds in presence of star-like three-dimensional nano structure as a catalyst and nitrosoniumion source reagent

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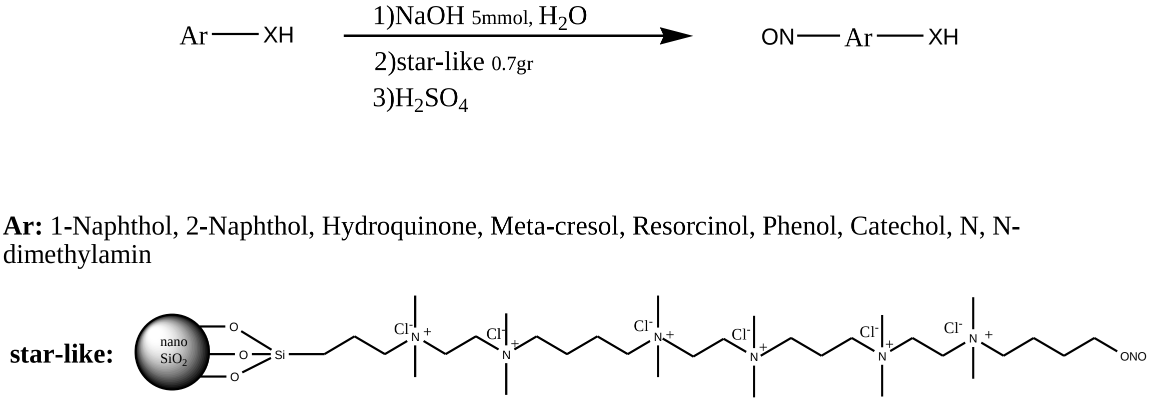
Nitrite functionalized star-like three-dimensional nano structure was synthesized and used as a highly efficient nitrosonium source and catalyst for nitrosation of active aromatic compounds such as 2-naphthol, 1-naphthol, hydroquinone, meta cresol, resorcinol, phenol, catechol and N,N-diethyl aniline at 0 °C and in short reaction time in excellent yields. Nitrite functionalized star-like three-dimensional nano structure plays dual roles as star-like three-dimensional nitrosonium source and catalyst because of its poly ionic characteristic. The catalyst can be easily recovered and reused without any change in its catalytic activity.



Ar: 1-Naphthol, 2-Naphthol, Hydroquinone, Meta-cresol, Resorcinol, Phenol, Catechol, N, N-dimethylamin

Figure 1. Scheme of the reaction.

References

[1] H. Feuer, The chemistry of nitro and nitroso groups. Part I, Interscience, New York, 1969.
[2] N.V. Zyk, E.E. Nesterov, A.N. Khiobystov, N.S. Zefirov, Russ. Chem. Bull. 48 (1999) 506

Catalytic application of {[HIMI]C(CN)$_3$}as a nano molten salt catalyst at the preparation of biologically active hena based compounds

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Naphthoquinone derivatives (NQs) are important class of heterocyclic compounds due to their pharmaceutically and biologically activities [1]. In addition, the naphthoquinone subunits are interested as privileged structural motif in the field of medicinal chemistry with numberless bioactivities such as antibacterial fungicidal, antimalarial, trypanocidal, and antitumoralapplicabilities [2]. In this research, we have explored the catalytic performance of 1*H*-imidazol-3-ium tricyanomethanide {[HIMI]C(CN)$_3$} as a novel, green and efficient catalyst for the preparation of a good range of naphthoquinone derivatives under mild and eco-friendly reaction conditions (Figure1). The scope and limitations of the described procedure will be presented.

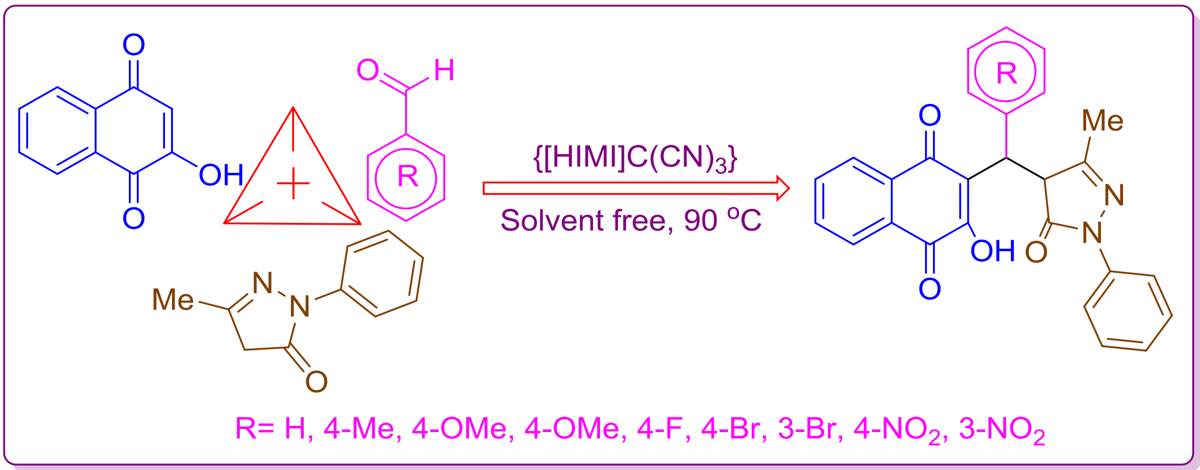

Figure 1. Synthesis of naphthoquinone derivatives under mild and eco-friendly reaction conditions

References

[1] P.J Arenas, Ethnopharmacol 21(1987) 279.
[2] S. L. Wang, J. Ding, F. Shi, Y. P. Liu, B. J. N. Ma, S. T. Tu, J. Heterocyclic Chem. 49 (2012) DOI 10.1002/jhet

$Fe_3O_4@TiO_2@O_2PO_2(CH_2)NHSO_3H$ as a novel nano magnetic catalyst: Application at the preparation of 2-amino-4,6-diphenylnicotinonitriles via anomeric based oxidation

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Nowadays, heterogeneous catalysis, due to the high capability in recycling and reutilizability, has surpassed the homogeneous catalytic systems, despite their benefits such as high activity and selectivity. On the other hand, magnetically recoverable catalysts (MRCs) have emerged as a potent and persuading option from the point of green chemistry view due to the meaningful merits like excellent catalytic performance and easy separation and recovery from the reaction mixture. Therefore, utilizing of the magnetic nano particles (MNPs) as suitable alternative support for the catalyst-supported materials in the designing and synthesis of magnetically recoverable heterogeneous catalysts are valuable as they are widely explored [1,2].

A new, green and reusable nano magnetic heterogeneous catalyst namely $Fe_3O_4@TiO_2@O_2PO_2(CH_2)NHSO_3H$was synthesized and fully characterized using suitable technics. Afterwards, the promoter applicability of the constructed heterogeneous core-shell catalyst was successfully explored at the synthesis of 2-amino-4,6-diphenylnicotinonitrile derivatives upon the reaction of a good range of aromatic aldehydes, acetophenone derivatives, malononitrile and ammonium acetate. The desired products were obtained with good to high yields in short reaction times under solvent free conditions. The suggested mechanism offers an anomeric based oxidation route to the products in the final step of the synthetic pathway (Figure 1) [3].

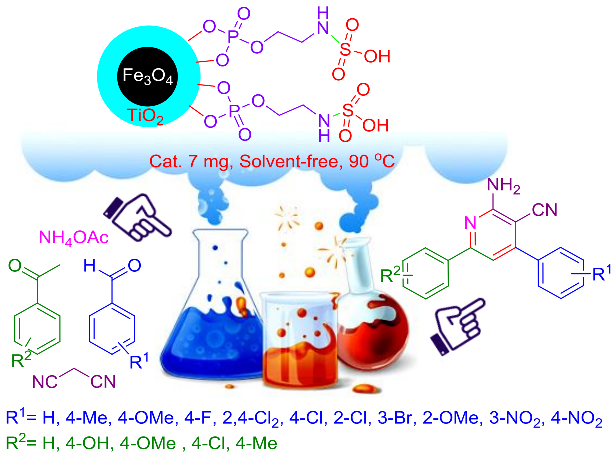

Figure 1. Synthesis of 2-amino-4,6-diphenylnicotinonitrile derivatives under mild an green conditions

References

[1] B. Karimi, F. Mansouri and H. M. Mirzaei, *ChemCatChem*., 7 (2015) 1736.
[2] T. Cheng, D. Zhang, H. Li, G. Liu, *Green Chem.*, 16 (2014) 3401.
[3] M.A. Zolfigol, M. Kiafar, M Yarie, A.Taherpour, M Saeidi-Rad,*RSC Adv*. 6 (2016) 50100.

Design, synthesis and catalytic application of a new ionic liquid functionalized silica coated magnetic nanoparticles as a reusable heterogeneous promoter for the synthesis of polyhydroquinolines

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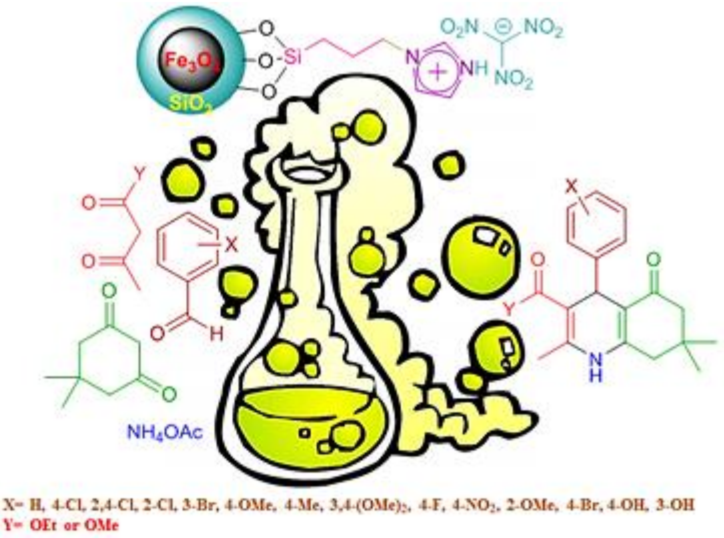
In recent times, development and expanding of the magnetic nano particles as versatile supports be revealed as an influential branch in the field of green chemistry due to the environmentally benign nature of these compounds. For the reason of easy separation of the magnetically based materials from the reaction system, manyattempts were focusedfor the surface modification of them in order to constructvaried heterogeneous magnetically recoverable promoters for the organic functional transformation [1].

Due to the varied pharmaceutical and biological applications connected to the polyhydroquinolines structural motif, huge attention have been paid for the production of these versatile organic compounds. Substituted 1,4-dihydropyridines are renowned as calcium channel modulators and they can be applied as a treatment for the therapy of the cardiovascular diseases [2].

Herein, we wish to introduce$\{Fe_3O_4@SiO_2@(CH_2)_3Im\}C(NO_2)_3$ as a novel, green and heterogeneous reusable catalyst for the four component preparation of the polyhydroquinoline derivatives under mild and eco-friendly reaction conditions (Figure 1).



X= H, 4-Cl, 2,4-Cl, 2-Cl, 3-Br, 4-OMe, 4-Me, 3,4-$(OMe)_2$, 4-F, 4-NO_2, 2-OMe, 4-Br, 4-OH, 3-OH
Y= OEt or OMe

Figure 1. Synthesis of polyhydroquinolines in the presence of $\{Fe_3O_4@SiO_2@(CH_2)_3Im\}C(NO_2)_3$

References

[1] T. Cheng, D. Zhang, H. Li, G Liu Green Chem., 16 (2014) 3401.
[2] A. Heydari, S. Khaksar, M. Tajbakhsh, R. Bijanzadeh, J. Fluor. Chem. 130 (2009) 609.

Encapsulation of phosphotungstic acid in interpenetrating amine-functionalized Zn(II)-based MOF as an efficient and reusable catalyst for epoxidation of olefins

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The epoxidation of olefins are an industrially useful process and attractive reaction in organic chemistrybecause the reaction products are extensively used as key intermediates in synthesis of pharmaceuticals, plasticizers, perfumes and epoxy resins [1]. Heteropoly acids, especially phosphotungstic acid ($H_3PW_{12}O_{40}$, PTA), as known environmentally catalyst in green chemistry filed [2]. Heteropoly acids was used to epoxidation of olefins but these compounds have low surface area (1–10 m^2/g) and high solubility in presence of solvents. To overcome these disadvantages, they are usually supported on a suitable carrier that improves the available surface area, sustainability in reaction medium and catalytic activity [2]. MOFs are a class of newly-developed inorganic–organic hybrid crystalline materials composed of organic linkers and metal nodes that have attracted much attention because they various potential applications, such as in catalysis, separation, gas storage and carbon dioxide capture [3].

In this work, epoxidation of alkenes is achieved with high to moderate yields under ultrasonic irradiation and reflux system. This process performed with a novel heterogeneous phosphotungstic acid ($H_3PW_{12}O_{40}$, PTA) catalyst that encapsulated into an amino-functionalized MOF (TMU-17 -NH_2). Comparison of these methods indicated that ultrasound irradiation could be used for the appropriate and rapid epoxidation of olefins. This heterogeneous catalyst characterized by various techniques such as PXRD, FT-IR spectroscopy, elemental analysis and TGA. Amount of encapsulated PTA was determined by ICP analysis.Epoxidation of cis-cycloocteneas model reaction was investigated to optimization of efficient parameters such as solvent, reaction time, type and amount of oxidant, amount of catalyst. Recycling experiments demonstrated that the PTA@TMU-17-NH_2 can be used several times without a significant decline in catalytic activity.

References

[1] P. Cancino, V. Paredes-García, P. Aguirre, E. Spodine, Catalysis Science & Technology 4 (2014) 2599.
[2] C. Kumar, K. Jagadeeswaraiah, P.S. Prasad, N. Lingaiah,,ChemCatChem 4 (2012) 1360.
[3] H. Furukawa, K.E. Cordova, M. O'Keeffe, O.M. Yaghi, Science 341 (2013) 1230444.

Synthesis of peptide nanofibers decorated with palladium nanoparticles and its application as an efficient catalyst for the synthesis of sulfides via reaction of aryl halides with thiourea or 2-mercaptobenzothiazole)

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In this work supported Pd nanoparticles on the peptide nanofiber (PdNP-PNF) has been prepared *via* fabrication of self-assembled woven nanofiberfrom peptide, subsequently immobilization of palladium nanoparticles on this nanostructural compound. To obtain self-assembled woven nanofiber, we designed and synthesized a peptide using arginine as building block. The C-terminus of amino acid was protected as ethylester. Coupling was mediated by dicyclohexylecarbodiimide-1-hydroxybenzotriazole (DCC-HOBT). TEM, SEM, XRD, ICP and FT-IR techniques were employed to characterize prepared nanofiber materials. In this work, the effect of phosphate buffer solutions (pH 8 and pH 11 (isoelectric point of arginine amino acid) on the structure of peptide nanofiber was investigated. Supported Pd nanoparticles on the peptide nanofiber (PdNP-PNF) were applied for the C–S coupling reaction using two different sulfur transfer reagents (thiourea and 2-mercaptobenzothiazole).

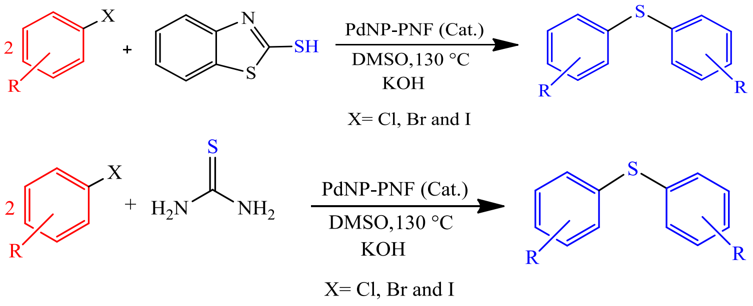

Figure 1. Synthesisof symmetrical sulfides *via* reaction of thiourea and aryl/alkyl halides catalyzed by peptide nanofibers decorated with Pd nanoparticles (PdNP-PNF)

References

[1] A. Ghorbani-Choghamarani, Z. Taherinia, Z. *RSC Adv.* 2016.

Synthesis and characterization of Cu(II)-imine-dopamine@Fe_3O_4 MNPs as a new catalyst for the selective oxidation of sulfides to sulfoxides

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Magnetic nanoparticles (MNPs) has been one of the most noteworthy catalyst support, offering the advantages of their easy preparation and functionalization, large surface area ratio, superficial recovery and easy separation by an external magnet, low toxicity and price [1]. The oxidation of sulfides to sulfoxides is great importance in organic synthesis. Chiral sulfoxide intermediates can be found in pharmaceuticals [2]. In recent years many transition metal catalysts systems have been reported for sulfoxidation but many of these systems suffer from one or more limitations, such ashard separation from the reaction mixtures, which lead to lower the purity of the products, leaching of metal and expensive materials [3]. In this light, herein we have proposed a highlyefficient method for synthesis of sulfoxides using H_2O_2 as green oxidant catalyzed by Cu(II)-imine-dopamine@Fe_3O_4 magnetic nanoparticles.

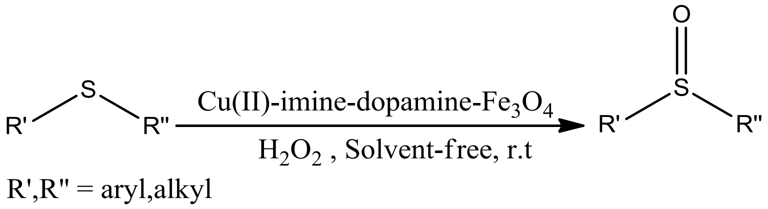

Figure 1.Oxidation of sulfides to sulfoxides.

References

[1] A. Ghorbani-Choghamarani, M. Nikoorazm, H. Goudarziafshar, M. Abbasi, B. Korean Chem. Soc. 32 (2011) 693.
[2] M. Hajjami, Z. Yousofvand, Catal. Lett. 145 (2015). 1733.
[3] H. Zhang, G. Wang, Tetrahedron Lett. 55 (2014) 56.

Ni(Π) Isatin/ Dopamine @ Fe_3O_4 as novel and effective nanocatalyst for the synthesis of 5-substituted 1H-tetrazoles in PEG

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During the past decades, advances in nanoscience and nanotechnology have pushed forward the synthesis of functional magnetic nanoparticles (MNPs), which is one of the most active research areas in advanced materials. MNPs that have unique magnetic properties and other functionalities have enabled a wide spectrum of applications. Iron oxide magnetic nanoparticles (Fe_3O_4-MNPs) are approximately 20–30 nm in size containing a single magnetic domain with a single magnetic moment and exhibit superparamagnetism. Magnetic nanocatalysts can easily be separated and recycled from the products by an external magnet [1].Tetrazoles are an important class of five-membered ring heterocycles broadly used in pharmaceuticals, agrochemicals, and material science [2]. In this study, we report Ni (Π) Isatin/ Dopamine@Fe_3O_4as a new heterogeneous catalyst for the synthesis of 5-substituted 1H-tetrazoles in PEG(Figure 1). This method is an efficient and rapid route for the synthesis of a wide range of substituted 1H-tetrazoles.

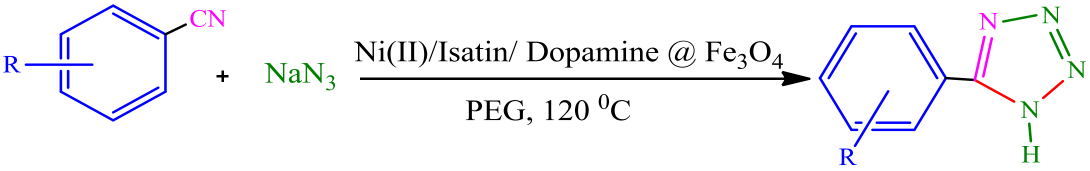

Figure 1. Synthesisof tetrazoles.

References

[1] M. Hajjami, B. Tahmasbi, Rsc Advances 5 (2015) 59194.
[2] R. Patouret, T.M. Kamenecka, Tetrahedron letters 57 (2016) 1597.

Chiral Poly(amide-imide) Bionanocomposites Containing L-Alanine Moieties Reinforced with ZnO Nanoparticles

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Composite materials having polymeric and inorganicunits have been attracting important attention as new materials because they have novel optical, mechanical, electronicproperties [1], as well as cosmetic and medicine applications [2,3]. Nanocomposites containing biocompatible polymer matrix and inorganic nanoparticle filler symbolize anew class of composite biomaterials for tissue engineering, scaffolds, and biomedical implants and devices [4,5]. Zinc oxide, ZnO, due to its numerous significant properties, such as catalytic, electrical, electronic, chemical stability, low dielectric constant, optical and effective antimicrobial, antibacterial and bactericide has drawn increasing concentration in recent years. ZnO is one of the most important n-type semiconductor materials with a 3.37 eV band gap at room temperature and a 60meV excitation banding energy that is in the UV region and makes this nanoparticle as an efficient UV absorber [6]. It also shows remarkable potential application in catalysts, electrical and optical devices, varistors, gas sensors, solar cells, cosmetic materials and so on. In addition, ZnO is nontoxic and environmentally friendly that is valuable for bio-applications [7]. In this study, apoly(amide-imide) (PAI) was synthesized via directpolycondensation reaction of*N*,*N*'-carbonyl-bis(phthaloyl-L-alanine) as dicarboxylic acid with diamine 4,4'-sulfonyl dianiline under green conditions using molten tetra-*n*-butylammonium bromide andtriphenylphosphite. Then, chiral PAI-based bio nano composites have been successfully prepared via ultrasonic irradiation technique using ZnO nanoparticles functionalized by 3-aminopropyltriethoxysilaneas a coupling agent to decrease aggregation of nanoparticles in the polymer matrix. The resulting bionanocomposites were characterized by FT-IR, X-ray diffraction, scanning electron microscopy (SEM), transmission electron microscopy (TEM) and thermo-gravimetric analysis (TGA). The TGA of the obtained nanocomposite sproves the enhancement in the thermal stabilitywith an increase in the percentage of ZnO nanoparticles. TEM and SEM images showed that the nanoparticles were uniformly dispersed in the polymer matrix.

References

[1] H. Deng, L. Lin, M. Ji, S. Zhang, M. Yang, Q. Fu, Prog. Polym.Sci., 39 (2014) 627.
[2] M. Sasidharan, K. Nakashima, Acc Chem. Res., 47 (2014) 157.
[3] Y. Xiao, S. Zhou, L. Wang, T. Gong, ACS Appl. Mater. Interfaces, 2 (2010) 3506.

Metals In Hair Colour Products: Implication For Human Health

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Hair colouring is widely used by women and men either to change their natural hair colour, to delay the onset of grey or to re-pigment already grey hair. A wide array of natural and synthetic hair-colouring agents is available.Vegetable and metallic dyes are natural colourants, but these have largely been replaced by synthetic organic dyes. [1] According to EU Regulation No. 1223/2009/EC cosmetic products for daily use can contain ‘technically unavoidable traces’ of metals. This definition is too vague. Authorities should set well-defined restrictions, considering the risks related with metal pollution of cosmetics such as hair color products [2]. Increased Pb, Cd, and Hg concentrations in the blood, urine or internal organs noted in individuals in whom the use of cosmetic products was the only source of excessive exposure to these metals confirms their absorption through the skin [3]. The study was undertaken in order to determine heavy metals content (As, Pb, Hg) in hair dyes both imported and locally manufactured which were produce under control of food & drug Administration. The target of this study was to determine the concentrations of heavy metals including in hair dyes sold in different shops with a view of assessing the potential risks that such cosmetic may cause to consumers. Table (1) gives a summary of the analysis of the concentrations of heavy metals in (20) hair dyes sampled.

sample	Origin	Pb	As	Hg
1	France	0.65	0.52	0.06
2	Italy	0.82	0.65	0.09
3	Italy	1.1	0.25	0.09
4	Iran	0.94	0.72	0.05
5	Iran	1.1	0.84	0.07
6	England	0.9	0.11	0.07
7	Germany	0.82	0.16	0.06

Table 1. Summary of heavy metals concentration in hair dyes samples

References

[1] S. Borowska, M.M. Brzóska, Journal Of Applied Toxicology 35(2015) 551.
[2] C. L. Vecchia, F. Turati, C. Pelucchi, C. Galeone, A. Decarli, Annals of Epidemiology 24 (2014) 151.
[3] B. Bocca, A. Pino, A. Alimonti, G. Forte, Toxic metals contained in cosmetics: A status report 68 (2014) 447.

Synthesis of Novel Fluorescein Derivatives for Protein Labeling

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Life is dependent on the chemistry of proteins. Proteins that are made up of 20 aminoacids, carry out fundamental reactions such as glucose and lipid break down. Therefore to be able to label proteins would give an enormous advantage in manipulating protein structure and function.In this work, we have aimed at using bioorthogonalchemistry to label proteins using fluorescein derivative in such a way that protein function and structure would not be altered dramatically [1]. In our preliminary experiment, we synthesis 5(6)-carboxyfluorescein with resorcinol and trimelliticanhydride [2]. We modified the 5(6)-carboxyfluorescein to 5(6)-acidchloridefluoresceinwith chlorinating agent. ^{1}HNMR were used to confirm the products. The product were used to label proteins in physiological conditions. The label protein was analysed via gel electrophoresis. Our future work, will focus on protein aminoacids that have reacted with fluorescein derivative. In addition, different proteomes will be used for binding new involving proteins.

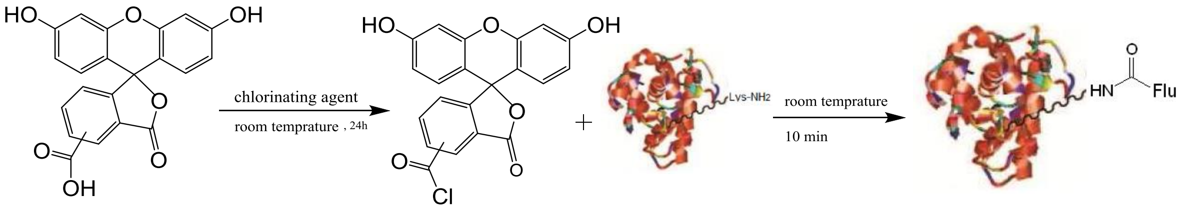

Figure 1. Synthesis of acid chloride fluorescein and its reaction with protein.

References

[1] Sletten EM, Bertozzi CR, Angew. Chem. Int. Ed. 2009, 48, 6974 – 6998
[2] J.V. McCullagh, K.A. Daggett, J. Chem. Ed. 2007, 84(11), 1799

Synthesis of Quinoxalines using silica-bonded imidazolium-sulfonic acid chloride (SBISAC) as a heterogeneous nano-catalyst

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Nowadays, heterogeneous catalysis, due to the high capability in recycling and reutilizability, has surpassed the homogeneous catalytic systems, despite their benefits such as high activity and selectivity. Therefore, knowledge base development of nano catalytic systems are more demand. On the other hand, quinoxaline derivatives are ofthe versatile class of nitrogen containing heterocycle compounds[1] and widely used in photochemical and electrochemical materials[2], dyes and pharmaceuticals[3]. Also these compounds are active against various transplantable tumors and have anticancer properties[1]. In this work, we used (SBISAC) as a highly efficient, heterogeneous and reusable nano-catalyst for the preparation ofquinoxalines via condensation reaction of benzene-1,2-diamines and benzil as 1,2-dicarbonyl compound in ethanol as the best solvent at room temperature. (**Figure 1**).

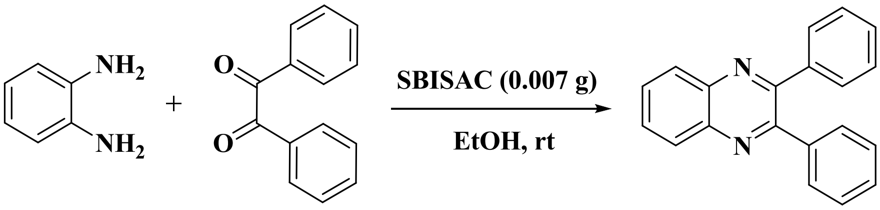

Figure 1. Preparation of quinoxaline derivatives via (SBISAC) as a heterogeneous nano-catalyst.

References

[1] S. Sajjadifar, E. Rezaee nezhad, E. Khosravani, Chemical Science Transactions3 (2014) 292.
[2] S. Dailey, J. W. Feast, R. J. Peace, I. C. Sage, S. Till, E. L. Wood, Journal of Material Chemistry11 (2001)2238.
[3] A. Gazit, H. App, G. McMahon, J. Chen, A. Levitzki, F. D. Bohmer , Journal of Material Chemistry39(1996) 2170.

Zirconium dioxide (ZrO_2) as an efficient catalyst for the Synthesis of Tetrahydrobenzo[*b*]pyran drivatives

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4*H*-pyran derivatives have useful pharmacological and biological properties such as, spasmolytic, anti-cancer, anti-coagulant, diuretic characteristics. 4*H*-Pyrans also occur in various natural products[1, 2]. Some of these derivatives have photochemical activities[3]. Various methods and catalysts have been reported for the preparation of 4*H*-pyrans such as TEBA[4], KF-basic alumina under ultrasound irradiation[5]. In this work, we have used zirconium dioxide (ZrO_2) as an efficient, commercially available, heterogeneous and recyclable catalyst for the preparation of 4*H*-pyrans via the One-Pot multi-component condensation of dimedone, aryl aldehydes, and malononitrile under solvent-free conditions (Figure 1).

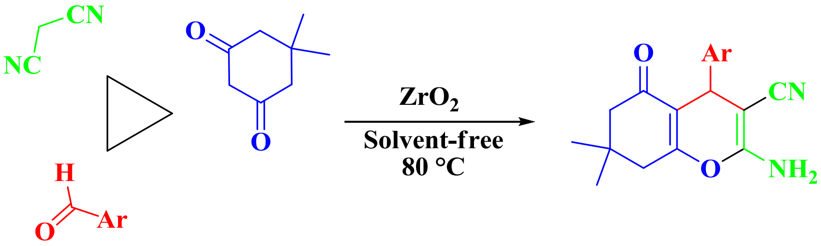

Figure1. The One-Pot multi-component preparation of 4*H*-pyrans catalyzed catalyzed by ZrO_2.

References

[1] W.O. Foye, Principal di Chemico Farmaceutica, Piccin, Padova, Italy (1991) 416.
[2] X.S. Wang, D.Q. Shi, S.T. Tu, C.S. Yao, Synthetic Communications, 33 (2003) 119.
[3] D. Armesto, W.M. Horspool, N. Martin, A. Ramos, C. Seaone, Journal of Organic Chemistry, 54 (1989) 3069.

N,*N*-Diphthalimide as Heterogeneous Recyclable Green Catalyst For Multi-component One-Pot Synthesis of 4-Aryl Substituted Dihydropyrimidinones Under Solvent-Free Conditions

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The One-Pot multicomponent reaction (MCR) was an attractive broad area ofresearch in the synthesis of N-containing heterocyclic scaffolds such as the 3,4-dihydropyridin-2-1H-(thiones) (DHPMs) and theirheterocyclic derivatives [1–۳].Organocatalysts possess advantages such as cost-effectiveness, ready availability, a metal-freeenvironment, relatively low toxicity, simple functionality, non-sensitivity to airand moisture, promotion of a variety of chemical transformations via variousactivation modes, mildness of the reaction conditions required, huge potential forthe development of large-scale production of Biginelli reaction [۳].In this work, *N,N*-Diphthalimide (DPHI) was directly synthesized via reaction of phthalicdianhidride with thiouera in solvent free. This reagent is found to be an efficient solid acidic organic catalyst in the Biginelli reaction. The three-component reaction of aryl aldehydes derivedthiourea, and ethyl acetoacetate or acetylacetone occurs by means of 10 mol % of (DPHI) insolvent-free reaction conditions. The present methodology is a green approach to access a series of 3,4-dihydropyrimidin-2(1H)-thiones in high yields. In addition, the use of DPHI as the catalyst offers several notable features such as simple operational procedure, no use of hazardous organic solvents, and recyclability of catalyst. (Figure 1).

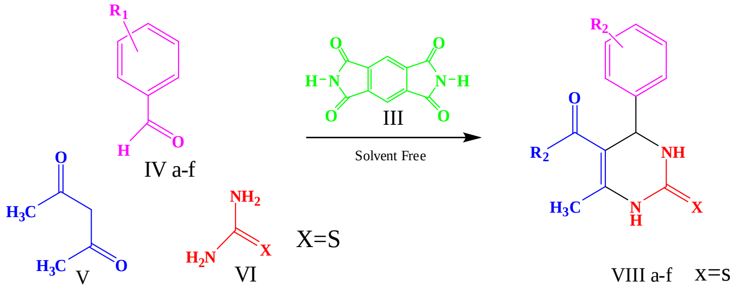

Figure 1.Scheme of the reaction.

References

[1] N. Li, X.-H. Chen, J. Song, S.-W. Luo, W. Fan, L.-Z. Gong, J. Am. Chem. Soc. 131, 15301 (2009)
[2] J.S. Suresh, Sandhu. Arkivoci 2012, 66 (2012)
[3] H. Kiyani, M. Ghiasi, Chin. Chem. Lett. 25, 313 (2014)

Water-Soluble Porphyrins as Novel Sensitizers for Photodynamic Therapy

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Photodynamic therapy (PDT) is a successful treatment method for various types of cancer, that leads to the selective destruction of tumor by cytotoxic singlet oxygen generated via visible laser light activation of photosensitizer [1, 2]. porphyrins are have been widely used clinically in PDT for cancer treatments because of their capability to generate singlet oxygen efficiently and their tendency to accumulate in tumor tissue, However, porphyrin structure is unsuitable for biomedical application [3]. Novel water-soluble 5,10,15,20-tetrakis(4-N-carbonylacrylic aminophenyl)porphyrin was designed and synthesized for the first time as the tetrasodium salts by via reaction of tetrakis(4-aminophenyl)porphyrin(NH_2-TPP) with maleic anhydride. 4-Nitrobenzaldehyde was employed in order to synthesize tetrakis(4-nitrophenyl)porphyrin (NO_2-TPP) and then it was converted to NH_2-TPP by $SnC1_2$. The structure of the porphyrin was thoroughly studied by a variety of techniques such as NMR, FT-IR and UV-visible spectrophotometer. In this work, the efficiency of porphyrin as photodynamic therapy (PDT) systems was investigated. The production of reactive singlet oxygen, cytotoxity and phototoxicity of it was assessed. The study showed that the singlet oxygen production ability of porphyrin can be well controlled by irradiation. We tested on A453 cells to compare effectiveness. This photosentesizer exhibited cell viability over 97% and good photocytotoxity, indicating it is promising photodynamic photosentesizer for cancer therapy.

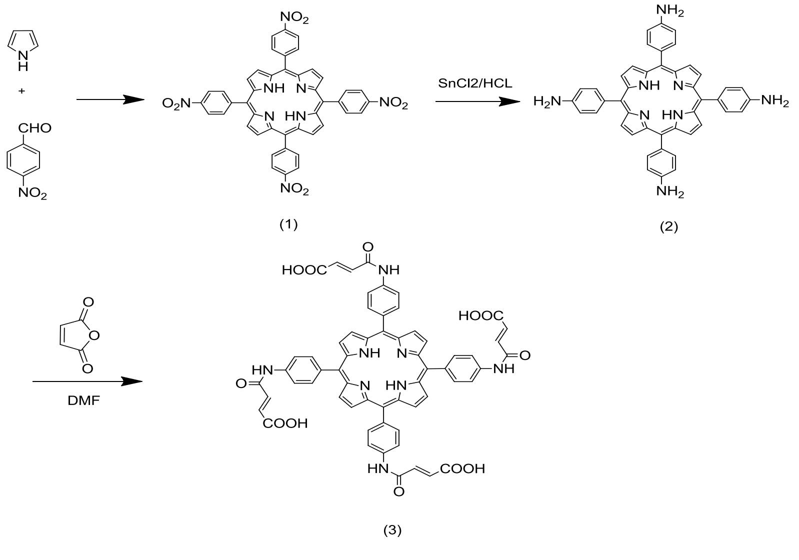

Figure 1.Scheme of the reaction

References

[1] M. Kempa, et al. Spectrochimica Acta Part A, 146 (2015) 249.
[2] K. Haedicke, et al. Acta Biomaterialia, 14 (2015) 197.
[3] J. Luo, et al. Inorganic Chemistry, 53 (2014) 4184.

Synthesis andapplication of Poly(N،N´-dibromo-N،N´–bis(4-(bromo(methyl)amino)phenyl) naphthalene- 2،7-disulfonamide) as an efficientreagent for the synthesis of benzimidazole derivatives

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In recent years, preparation of Benzimidazoles has been an interesting subject. Benzimidazole and its derivatives have been used as the antiulcerative esomeprazole (1) .Benzimidazoles are remarkably effective compounds against various strains of microorganisms.N-Bromo compounds are inexpensive and nonhazardous reagents and also they are widely applicable in industrial processes for the synthesis of drugs, pharmaceuticals and agrochemicals (2,3) . This method has some advantages including easy handling, short reaction times, high yield and simplicity of the product isolation(2,3). In this work, Poly(*N*،*N*´-dibromo-*N*،*N*´–bis(4-(bromo(methyl)amino)phenyl) naphthalene- 2،7-disulfonamide)catalyst was used for the synthesis of Benzimidazoles derivatives by the condensation reaction between *O*-phenylenediamine and various aldehydes at 80°C under solvent-free conditions .Figure 1.

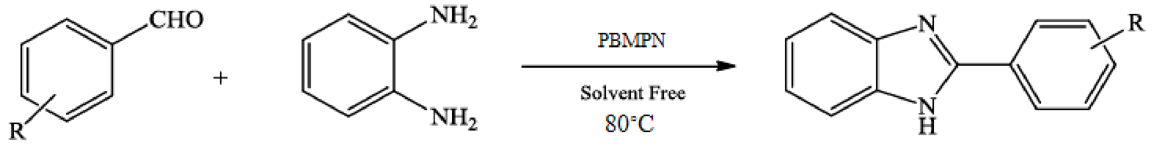

Figure 1. Synthesis of benzimidazoles in the presence of PBMPN

References

[1] Karimi-Jaberi, Z.;Amiri, M “An efficient and inexpensive synthesis of 2-substituted benzimidazoles in water using boric acid at room temperature,” E-Journal of Chemistry ., 2012 , 9: 167–170.

[2] Khazaei, A.; Saednia, Sh.;Roshani, L.; Kazem-Rostami, M .;Zare, A “Synthesis, characterization and application of poly(N,N□-dibromo-Nethylnaphthyl-2,7-disulfonamide) as an efficient catalyst for the acetylation and deacetylation reactions,” Letters in Organic Chemistry ., 2014 , 11: 159–167.

[3] Khazaei, A.; Rostami, A.; Raiatzadeh, A.; “Poly (N-bromo-Nethylbenzene-1,3-disulfonamide) and N,N,N'',N'tetrabromobenzene- 1,3-disulfonamide as efficient reagents for synthesis of quinolines” Journal of the Chinese Chemical Society ., 2007, 54: 1029–1032.

Synthesis and Characterization of β- substituted Trimethine Cyanine Dyes

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Cyanine dyes and their derivatives constitute an important class of organic compounds, which possess numerous applications in many areas (chemistry, physics, biology, etc.) [1–2]. seven novel trimethine cyanine with various substituents in βposition of the methine chain were synthesized via a three-step procedure with1-metheyl -2- phenyl-1H-indole and 2-Heteroaryl-substituted trimethinium salts. The visible spectral behavior of these trimethine cyanine dyes was examined in DMSO. Elemental analysis, IR, 1H-NMR, 13C-NMR, and mass spectral data confirmed the molecular structure of the newly synthesized compounds.

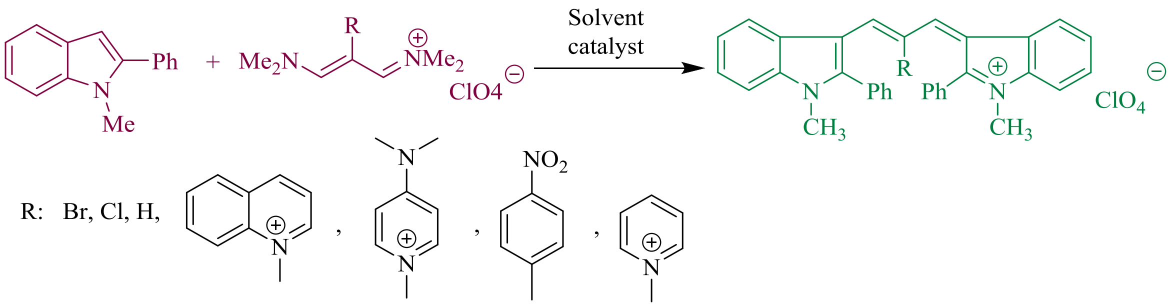

Figure 1. Synthesis of β- substituted Trimethine Cyanine Dyes

References

[1] M. Y. Losytskyy, K. D. Volkova, V. B. Kovalska, Makovenko, et al, J Fluoresc 15 (2005) 849.
[2] G. Patonay, J.Salon, J. Sowell, L. Strekowski, Molecules 9(2004) 40.

Synthesis of Substituted Pyridines via Annulation of Ketones with Vinamidinium Salts

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For the past century, classical methods for the formation of pyridines have been used extensively. Such methods include the condensation of enaminoketones or β-ketoesters with 1,3-diketones[1]. The Hantzsch pyridine synthesis from β-dicarbonyl compounds in the presence of an aldehyde and ammonia,2 and the related Knoevenagel cyclization of β-aminoacrylates with β,α-unsaturated carbonyl compounds [3]. Despite the numerous studies and applications that have appeared in the literature [4]. Most methods are still severely limited in their use by the lack of generality, the harsh reaction conditions involved, the poor yields, or the formation of complex mixtures of side products. New methodologies alleviate some of these limitations. They include the inverse electron-demand Diels-Alder cycloaddition of triazines with electron-rich alkenes. The cycloaddition of azadienes with Fisher carbenesand the sequential reaction of metalated phosphonates with nitriles and unsaturated carbonyl compounds.

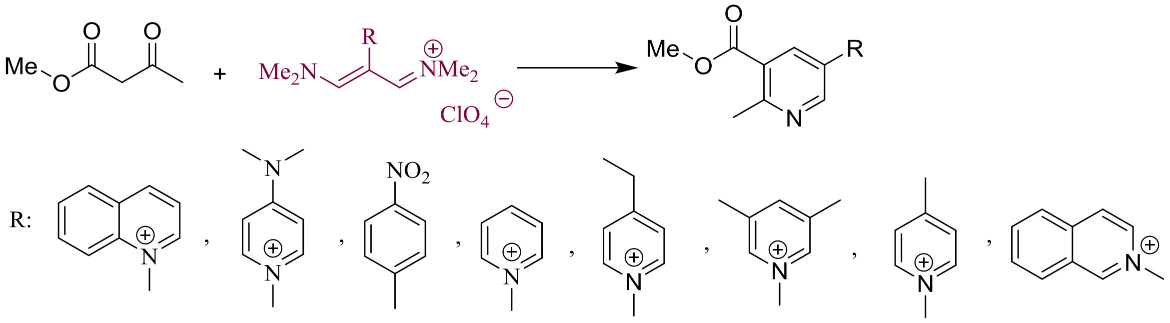

Figure 1. Synthesis of substituted Pyridines via Annulation of Ketones with Vinamidinium salts

Reference

[1] P. Friedla¨nder, C. F.Gohring, Ber 16(1883)1833.
[2] A. Hantzsch, Liebigs Ann. Chem.215(1882)1.
[3] E.Knoevenagel, A. Fries, Ber. Dtsch. Chem. Ges.31(1898)761.
[4] For an extensive review on the preparation of pyridines and their benzo derivatives, see: G. Jones, In Comprehensive HeterocyclicChemistry; A. R.Katritzky, C. W. Rees, Eds.; Pergamon Press: Oxford, 2 (1984)395-510.

A simple and highly efficient procedure for the synthesis of 3-(benzylthio)-9b-hydroxy-9b*H*-imidazo[5,1-*a*]isoindole-1,5-dion derivatives

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Developing new synthetic methods for novel nitrogen-containingmolecules is an important area of organic synthesis[1]. As a privileged fragment, the isoindole core is a ubiquitous subunit in many natural and synthetic products with remarkable biological activities. Members of this family have wide applications in medicinal chemistry, being used as antibiotic and antitumor agents[2]. Isoindolinones and many derivatives containing this heterocyclic unitembedded in their skeleton have attracted a great deal of interest, since they represent the common building block of a wide range of naturally occurring and/or bioactive substances.Within this family, 3-hetero-substituted isoindolinones occupy a special place as witnessed by a great number of papers emphasizing their pharmaceutical and medicinal bioactivities[3].

Here, we introduced a novel, convenient, and practical procedure for the synthesis of highly functionalized isoindol derivatives**3***via* oxidative cleavage of 2-(benzylthio)-3a,8a-dihydroxyindeno[2,1-*d*]imidazoles**2**with lead(IV) acetate in acetic acid at room temperature (Figure 1).The 3a,8a-dihydroxyindeno[2,1-*d*]imidazoles**2**were easily synthesized from the additionreaction of ninhydrin and isothiouronium halide**1**. These new compounds were undoubtedly characterized by IR, ^{1}HNMR,^{13}CNMR and Mass spectroscopic data.Consequently,the combination of highyields, short reaction times, and mild reaction conditions makes this methodhighly efficient.

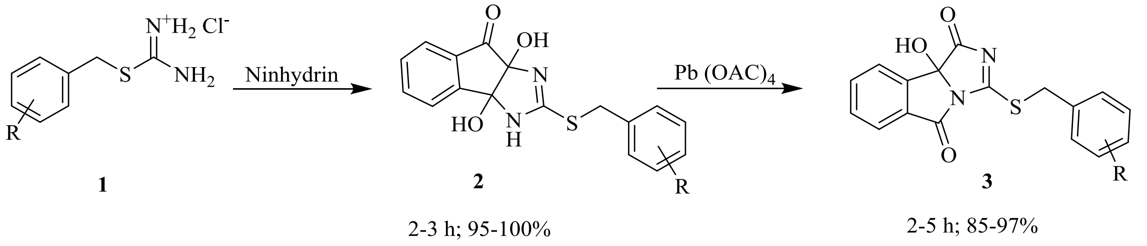

Figure 1.highly efficient synthesis of isoindols3*via* oxidation of 3a,8a-dihydroxyindenoimidazoles 2

References

[1] A. Deiters, S. F. Martin. Chemical Reviews 104 (2004) 2199.
[2] Y. Deng, D. C. Yang, Y. Shen, Y. G. Zhong. Chinese Chemical Letters 18 (2007) 7.
[3] A. Moreau, A. Couture, E. Deniau, P. Grandclaudon. Journal of Organic Chemistry 69 (2004) 4527.

The synthesis of aryl benzoate derivatives by using of copper(II) oxid nanoparticles

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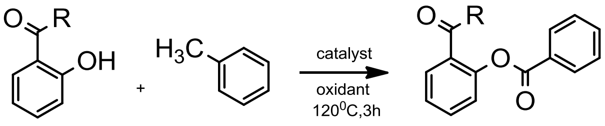
In recent years,the hetrogenization of homogeneous catalysts has attracted immense attention[1]. Although many homogeneous catalysts demonstrate high selectivity and can be used to control the stereo chemistry and regio chemistry of the reaction products[2]. Recovery and reusability of catalysts are highly desirable from both economic and environmental standpoints. Copper remains one of the most important metal catalysts for this purpose because of the ability of the copper atom to act as a single –electron and or a two-electron mediator and as a lewis acid. Moreover,copper can act as either an electrophile or nucleophile,depending upon its oxidation state and the reaction conditions. Oxidatives C-O cross-coupling is a one of the most important methods for the synthesis of various oxygen-bearing organic compounds,such as ethers, esters, oxazoles or carbamates. In this paper our work on heterogeneous catalysts and C-O cross-coupling reactions.Initially silica-coated feriitenanoparticles ($Fe_{3-}O_4$@SiO_2) treatedwith (3Aminopropyl)trimethoxysilane(APTMS), isatoic anhydride and copper(II) acetate in solvent give the new magnetic catalyst.The magnetic catalyst was charactrized by FT-IR, XRD, VSM, EDX, SEM. We examined new magnetic catalyst for synthesis of aryl benzoate derivatives.Finally the products were characterized by FT- IR and ^{1}H NMR.



R=H,CH3

Figure 1. Scheme of the reaction.

References

[1] Minakata,S.; Komatsu,M.Chem.Rev.2009,109,711.
[2] (a) Hagen, J. Industrial catalysis: A Practical Approach; Wiley-VCH: Weienheim, 1999. (b) Cole-Hamilton, D. J. Science 2003,299,1702.

Synthesis and characterization of pH/temperature stimuli-responsive nanogels by direct polymerization and ultrasound polymerization methods

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The term “nanogel” usually defines aqueous dispersions of hydrogel particles formed by physically or chemically cross-linked polymer networks of nanoscale size [1]. Nanogels with the semi interpenetrating polymernetworks (semi-IPNs) structure have attracted increasing attention due to their multiresponsive properties and potential application in agrochemical and biomedical areas [2]. Better mechanical properties can be achieved by preparing semi-IPNs by a free radical polymerization method [3]. In this work, wereport on a novel dual responsive semi-IPN nanogel copolymersusing biocompatible, biodegradable and hydrophilic materialswith thermo- and pH- responsivity. Therefore, HPC-poly(IA-co-MAA) nanogels were prepared viafree radical polymerization of monomers in the reaction system comprised of hydroxypropyl cellulose (HPC) polymer, itaconic acid (IA) and methacrilic acid (MAA)monomers andN,N′-methylenebisacrylamide (BIS) crosslink agent in the presence of H_2O_2/Ascorbic acid initiator system (Figure 1). The prepared nanogels werecharacterized by FT-IR, UV-Vis spectrophotometer, dynamic light scattering (DLS),zeta-potential, X-ray diffraction (XRD), transmissionelectron microscopy (TEM), andatomic force microscopy (AFM). Moreover, we developed new nanogelcontaining encapsulated cationic anticancer drug (doxorubicin) and evaluated pH and thermal depending drug release at pH=5 and 7 at desiredtemperatures (T=37 and41°C). Also,present research is a preliminary report on the synthesis of thesemi-IPN copolymer HPC-PIA nanogels by using ultrasound assisted free radical polymerization in viscous glycerol aqueous solution of IA monomer contain HPC and BIS in an open system with 20 kHz ultrasound, 58Wcm^{-2}.In summary, these nanogels might find potential application in intelligent drug delivery system for cancer therapy optimization.

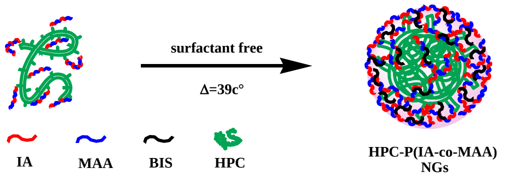

Figure 1. Synthesis of HPC-Poly(IA-co-MAA)nanogels with semi-interpenetrating polymer network structure.

References

[1] A.V. Kabanov, S.V. Vinogradov, Angewandte Chemie International Edition, 48 (2009) 5418-5429.
[2] D. An, D. Zhao, X. Li, X. Lu, G. Qiu, K.J. Shea, Carbohydrate polymers, 134 (2015) 385-389.
[3] P. Cass, W. Knower, E. Pereeia, N.P. Holmes, T. Hughes, Ultrasonics sonochemistry, 17 (2010) 326-332.

Synthesis of Polyhydroquinoline Derivatives Via Hantzsch Condensation using SulfuricAcid Supported on Modified Magnetic Fe_3O_4 Nanoparticles ($MNPs-OSO_3H$) as Catalyst under Solvent-Free Conditions

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One- pot reaction in which three or more starting materials react sequentially and lead to product(s) that retain all or most of the atoms of the starting materials are called multicomponent reactions (MCRs) .These reactions are characterized by their convergence, ease of execution, high yields, efficiency and atom economy [1].

Polyhydroquinolines (PHQs) are one of the most important classes of heterocyclic scaffolds providing major ligands for biological receptors. PHQs are the source of some valuable drugs which are very important in pharmacy. For instance, they demonstrate activity for the treatment of angina pectoris and hypertension [2]. Therefore, developing more efficient methods working under mild conditions using more environmentally acceptable catalysts is in high demand [3].

In this work, we present a facile and highly efficient protocol for the synthesis of polyhydroquinolines via Hantzsch multicomponent condensation of dimedone, aldehydes, ethylacetoacetate and ammonium acetate by using sulfuric acid supported on magnetic nanoparticles ($MNPs-OSO_3H$) as a nano-magnetic heterogeneous catalysts. This method has several advantages such as high yield, short reactiontime, simple workup, easy separation of the catalyst and its reusability.

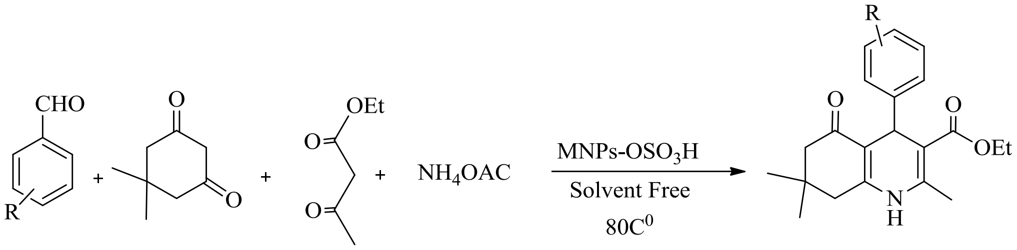

Figure 1. General reaction for the synthesis of polyhydroquinoline.

References

[1] M. Domling, I. Ugi, angewandtechemie 39 (2000) 3168.
[2] M.G. Dekamin, S. Ilkhanizadeh, Z. Karimi. RSC Advances 4 (2014) 56658.
[3] M.J.Climent, A. Corma, S. Iborra. RSC Advances2 (2012) 16.

Sulfuric Acid-Functionalized on Magnetic Fe_3O_4 Nanoparticles as an Efficient Reusable Catalyst for the Synthesis of 2,3-Dihydroquinazoline-4(1*H*)-ones and Knoevenagel Condensation Reactions

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Heterogenization of homogeneous catalysts has been an interesting area of research from the industrial point ofview; this combines the advantages of homogeneous catalysts (high activity and selectivity, etc.) with the engineering advantages of heterogeneous catalysts (easy catalyst separation, long catalytic life, easy catalyst regenerability, thermal stability and recyclability) [1]. In this present work, we wish to report a new green approach for the synthesis of2-aryl-2,3-dihydroquinazolin-4(1H)-ones throughcyclocondensation of 2-aminobenzamide with aromatic aldehydesand Knoevenagel condensation reactions using MNPs-OSO_3H as catalyst (Figure 1,2).

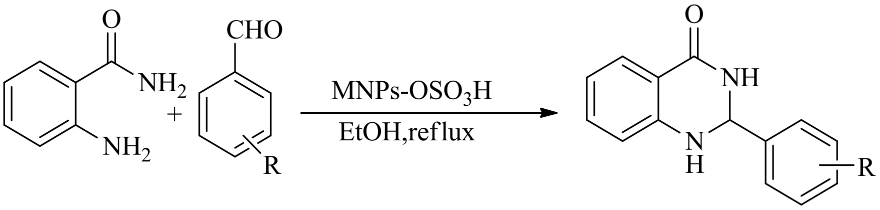

Figure 1. Synthesis of 2, 3-dihydroquinazolin-4(1H)-ones catalyzed by MNPs-OSO_3H

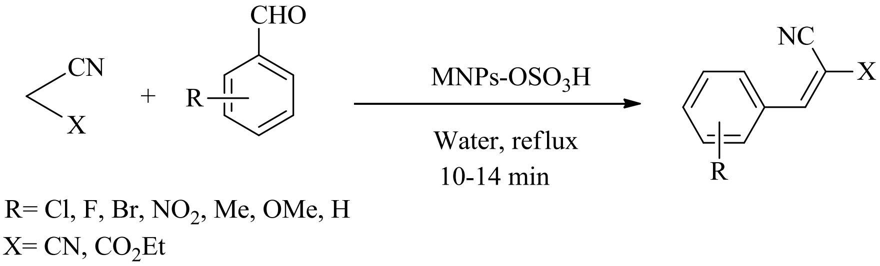

Figure 2. Knoevenagel condensation (KC) of active methylene compounds with aldehydes catalyzed by MNPs-OSO_3H.

References

[1] D. Choudhary, S. Paul, R. Gupta, J.H. Clark, Green Chem. 8 (2006) 479

The Copper-Catalyzed N-Arylation of Nitrogen Containing Heterocycles

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N-Aryl amines arevaluable compounds which are found in natural products, pharmaceuticals, and material chemistry [1].A recent approach to the synthesis of N-aryl amines is the copper-catalyzed Ullman type reaction in the presence of bidentate ligands which allowed these reactions to progress faster and under milder conditions [2]. The tridentate 4'-(4-methoxyphenyl)-2,2':6',2"-terpyridines (Mtpy) have been of great interest over the last few years, mostly because of their ability to chelate transition metals. As part of our ongoing effort directed towards copper-catalyzed C-X (X=S, Se-Te) bond-forming reactions [3], here we report a simple and efficient catalytic system (CuI/Mtpy) for N-arylation of various nitrogen nucleophiles with a vast array of functional groups including electron-withdrawing and donating substituents on the aryl halides (Figure 1).

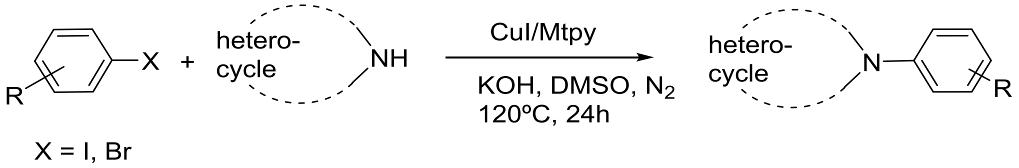

Figure 1. Scheme of the reaction

References

[1] D. A. Horton, G.T. Bourne, M. L. Smythe, *Chem. Rev.*, *103* (2003) 3, 893. b) M. Liang, J. Chen, Chem**.** Soc. Rev., 42 **(**2013) 3453
[2] Carlo Sambiagio, Stephen P. Marsden, A. John Blacker, Patrick C. McGowan,Chem. Soc. Rev., (2014) 43, 3525.
[3] B. Movassagh, Z. Hosseinzadeh, Synlett, *27* (2016) 777.b) B. Movassagh, A. Yousefi, B. Z. Momeni, S. Heydari, Synlett, *25* (2014) 1385.

Novel triethylenetetramine functionalized absorbent from polyacrylonitrile for heavy metal ion adsorption

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The contamination of water recourses by heavy metal is a serious worldwide environmental problem[1]. Recently, much attention has been paid to the synthesis and applications of chelating sorbents based on natural and synthetic materials in removal of harmful contaminants from aqueous media. Polyacrylonitrile is one of the promising candidates because it can be easily obtained and many derivatives can be prepared using hydroxyl or amine residue [2]. Several functional groups such as diethylene-triaminetetraacetic, monoethanolamine, diethylenetriamine and Ethylenediaminetetraacetic acid have been used for metal ions adsorption[3]. In this study we have developed a simple method for functionalizing of polyacrylonitrile (PAN) with two volume percent (50 and 100) of triethylenetetramine (PAN–TETA 50 and 100). The evolved surface characteristics and surface reactions of PAN–TETA and their metal complexes were investigated by FT-IR and scanning electron microscope. The prepared resins were applied to remove Zn (II) from aqueous solutions. The optimization of experimental conditions and parameters including initial pH, adsorbent dose, contact time, initial metal ion concentration for the removal of Zn (II) were investigated. Adsorption increased with increasing metal ions concentration, initial pH, and temperature. Pseudo first-order, pseudo-second-order models were considered to evaluate the rate parameters. The adsorption followed pseudo-second-order kinetic model with correlation coefficients greater than 0.993. Attempts were made to fit the isothermal data using Langmuir, Freundlich and Temkin equations. The maximum adsorption capacity of 102.16 mg g−for zinc ions were achieved in pH=6. Thermodynamic parameters of ΔG°, ΔH° and ΔS° indicated the adsorption process was spontaneous and endothermic.

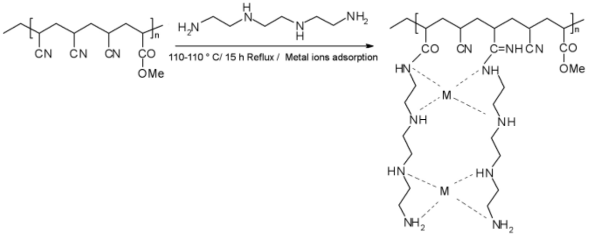

Fig. 1. Figure of PAN–TETA resins synthesized and interaction with metal ions.

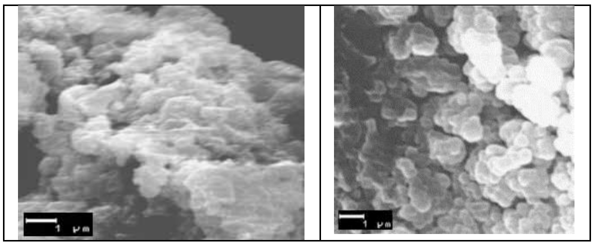

Fig. 2. SEM images of (a) PAN–TETA resin , (b) PAN-TETA Zn (II)

References

[1] T.K. Naiya, A.K. Bhattacharya, S.K. Das. Journal of Colloid and Interface Science 325 (2008)
[2] G.R. Kiani , N. Arsalani. Iranian Polymer Journal 15 (2006) 727.
[3] G.R. Kiani, H. Sheikhloie and N. Arsalani, Desalination 269 (2011) 266.

Removal of Zn (II) from Aqueous Solution using Halloysite Nanotubes: Optimization of Process by Taguchi Method

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Environmental pollution caused by toxic heavy metals is one of the most serious problems in many densely populated cities worldwide [1]. The adsorption process is arguably one of the more popular methods for the removal of heavy-metal ions because of its simplicity, convenience, and high removal efficient [2]. Taguchi optimization technique is a unique powerful optimization discipline that allows optimization with minimum number of experiments [3].In this paper, Taguchi method was applied to determine the optimum conditions for Zn (II) removal from aqueous solution by Halloysite Nanotubes (HNTs). An orthogonal array experiment design ($L_{16}(4^5)$ which is of five control factors (pH), t (contact time), m (sorbent mass), T(temperature)and C_0 (initial concentration of Zn (II)) having four levels was employed. Sorption capacity (mg/g) and percent removal (%) were investigated as the quality characteristics to be optimized. In order to determine the optimum levels of the control factors precisely, range analysis and analysis of variance were performed. And for percent removal, the optimum condition was found to be pH=6, T=35°C, w=0.4 g, and C_0=50 mg/L. Under these optimum conditions, sorption capacity and percent removal can reach 132.16 mg/g and 99.76%, respectively.

Process parameter	Designation	Level 1	Level 2	Level 3	Level 4
PH	A	3	4	5	6
Temperature (°C)	B	20	35	50	65
Contact time (min)	C	10	40	70	100
Sorbent mass (g)	D	0.1	0.2	0.3	0.4
Initial Zn (II) conc. (mg/L)	E	50	80	110	140

Table. 1. Controllable factors and their levels

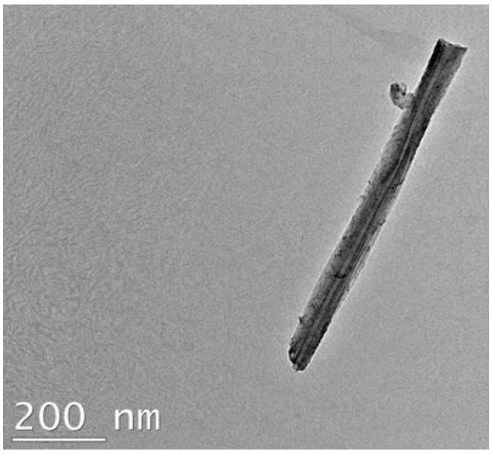

Figure1. TEM image of HNTs.

References

[1] B.A. Shah, A.V., Shah, N.B. Patel, R. Singh, Environ. Prog. Sustainable Energy 30 (2011) 59.
[2] G.R. Kiani, M. Dostali, A. Rostami, A.R. Khataee, Appl. Clay Sci. 54 (2011) 34.
[3] C.S. Chou, R.Y. Yang, J.H. Chen, S.W. Chou, Powder Technol 199 (2010) 264.

Cellulose supported acidic ionic liquid: an efficient and eco-friendly catalyst for the synthesis of quinoxaline derivatives in green media

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In recent years, green chemistry has focused mainly on environmentally friendly reactions, sustainable resources and reusable catalysts.Ionic liquids (ILs) have attracted extensive research interest as environmentally benign solvents due to their excellent properties such as negligible vapor pressure, solvating ability and non-flammability[1]. Compared to pure acidic ILs, IL-based heterogeneous catalysts offer more advantages. They are required in small amounts, areeasy to separateand have a competent catalyst recovery[2]. The immobilization process aims to transfer the desired catalytic propertiesof the liquids to a solid catalyst.Cellulose is themost abundant renewable bio-macromolecule in the naturewhich is widely produced in industrial scale. It has properties including biodegradability and non-toxicity which make it superior supportfor catalytic applications over conventional organic orinorganic ones.

In continuation of our interest to develop environmentally benign synthetic methods in organic chemistry[3], we report herein an efficient and green protocolfor the synthesis of substituted quinoxalines using acidic ionic liquid immobilized on cellulose(Cell-[pmim]HSO_4) as a catalyst in aqueous media(Figure 1).

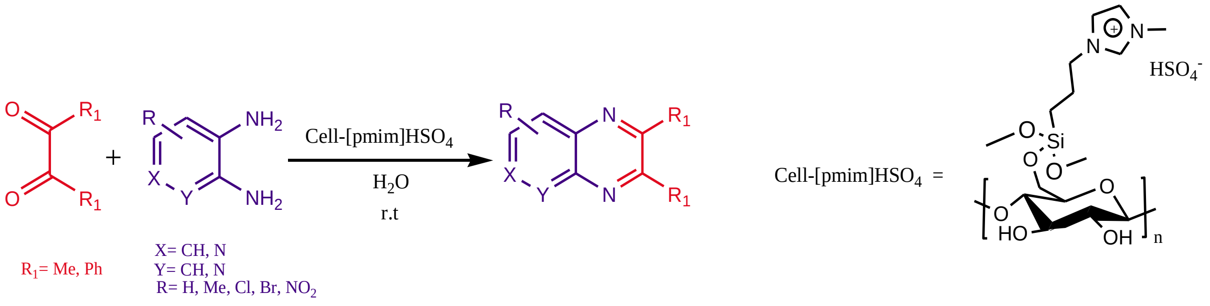

Figure 1. Synthesis of quinoxalines in aqueous media using Cell-[pmim]HSO_4.

References

[1] P. Wasserscheid, W. Keim, Angewandte Chemie International Edition, 39 (2000) 3772.
[2] H. Zhou, Y.-M.Wang, W.-Z.Zhang, J.-P.Qu and X.-B.Lu, Green Chemistry, 13 (2011) 644.
[3] H. Valizadeh, M. Amiri, E. Khalili, Molecular Diversity 16(2012)319.

Production of Fine Chemicals by Selective TEMPO-Oxidation of Lignin Models

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Lignin, an important aromatic biopolymer, is a major component of biomass. As a promising alternative to fossil resource[1], lignin has attracted much attention in recent years. It is considered to be the unique renewable aromatic resource and therefore represents a potentially valuablefeedstock for the production of organic fine chemicals[2]. Because of the complex and variable starting material, the valorization of lignin are often proceed through model compounds withβ-O-4linkage, which represents the most common substructure inlignin[3]. Herein we report the production of aldehydes by selective oxidation of 1° aliphatic alcoholin model compounds. TEMPO-mediated oxidation system, which composed by TEMPO (10% mol, TEMPO= 2,2,6,6-tetramethylpiperidine-N-oxyl) in combination with KBr (10% mol) and NaClO, was found effectively converting the primary hydroxyl groups of dilignols to carboxyl groups followed by retro-aldol bond cleavage.This catalyst system can also be applied for other lignin model compounds andorganosolv lignin.

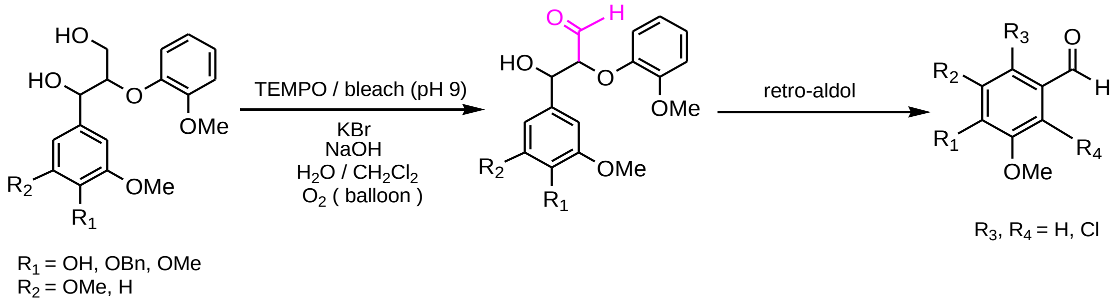

Figure 1. Selective oxidation of primary hydroxyl group in lignin models.

References

[1] W.Boerjan, J.Ralph, M.Baucher, Annual Review of Plant Biology, 54 (2003)519.
[2] S. R. Collinson, W. Thielemans, Coordination Chemistry Reviews ,254 (2010) 1854.
[3] J. Zakzeski, P. C. A. Bruijnincx, A. L. Jongerius, B. M. Weckhuysen, Chemica. Review, 110 (2010) 3552.

Nano ZSM-5 Catalyzed Groebke Condensation: An Efficient Protocol for the Synthesis of 3-Aminoimidazo[1,2-*a*]pyridines

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The imidazo [1,2] annulated nitrogen heterocycles bearing pyridine, pyrimidine, and pyrazine moieties constitute an important class of biologically active compounds such as sedative-hypnotic drugs Alpidem and Zolpidem. In 1998, an isocyanide-based multi component reactions (I-MCRs) was reported for the synthesis of imidazo[1,2]azines by condensation of an aldehyde, an isocyanide, and a 2-aminoazine [1]. Several methods have been developed for the synthesis of imidazoazines *via* above I-MCRs in the presence of the [bmim]Br ionic liquid, bio-supported catalyst cellulose sulfuric acid, *p*-toluenesulfonic acid, silica sulfuric acid, ammonium chloride, or tin(II) chloride at room temperature [2]. In this work,the ability of nano zsm-5 as an acid catalyst to promote the three-component condensation reaction from a diversity of aromatic aldehydes 1, 2-aminopyridines 2, and isonitriles 3 at room temperature is described. This methodology affords a number of 3-aminoimidazo [1,2] pyridines 4 in the presence nano zsm-5 (Figure 1) as a new and mild acid catalyst in the multi-component reaction in reasonable yields and short reaction time without any significant optimization of the reaction conditions.

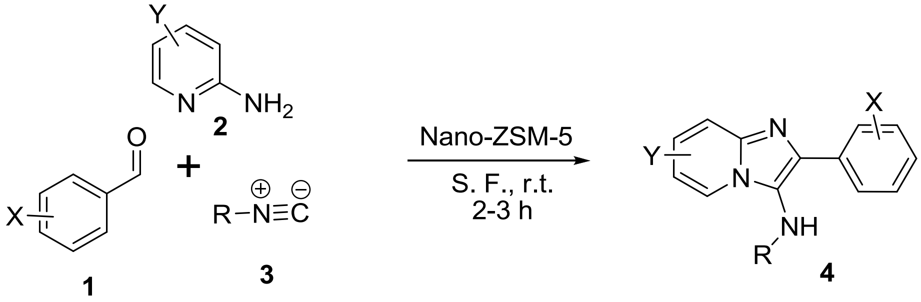

Figure 1. Nano ZSM-5 catalyzed Groebke reaction

References

[1] K. Pericherla, P. Kaswan, K. Pandey, A. Kumar,Synthesis47 (2015), 887.
[2] A. Shaabani, A. Maleki, A.H. Rezayan, A. Sarvary,Molecular Diversity15 (2011),41.

The Use of Single Wall Carbon Nanotubes (SWCNTs) as a Supported for Mesalazine drug As a Potential Method for Drug Delivery

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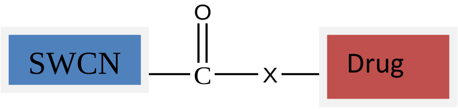
Drug delivery systems based on grafting of drugs to the single-walled carbon nanotube (SWCNT) give an improved treatment with lower toxicity and decreasing the drug dose consumption and can be used for the treatment of different diseases (1-2). the grafting of drugs to the SWCNT was attained bythe initial conversion of carboxylic groups in SWCNT to corresponding acyl chlorides (3). In vitrodrug release studies were performed from the grafted SWCNT–drug than is indeed a hydrolysis reaction, which involves breaking of amide bond in a predefined volume of buffer (pH 1.3) at 37 °C. The quantity of released drugs was measured by UV-Vis spectrophotometer



X = O, NH, NR
Drug: Amantadine, Metformin, Gabapentin,
Betahistine, Dipyridamol, Lisinopril, Atorvastatin

Figure 1. Covalent grafting of various drugs to the SWCNT.

References

[1] Khazaei, A.;Saednia,Sh.; Saien,J.;Kazem-Rostami,M.;Sadeghpour,M.;Kiani Borazjani.M.;and Abbasi,F.; J . Braz. Chem. Soc.2013:1-7

[2] Hornyak, G. L.;Dutta, J.;Tibbals,H. F.;Rao,A. K.,″In Introduction to Nanoscience″ ,Taylor and Francis Group, Boca Raton, 2008p.223.

[3] Khazaei, A.; Navid soltani rad, M.; Kiani Borazjani, M.;Int J. Nanomed.2010:5

Nano triethanolammonium trichloroacetate as new catalyst for the synthesis of 1*H*-pyrazolo[1,2-*b*]phthalazine-5,10-dione derivatives

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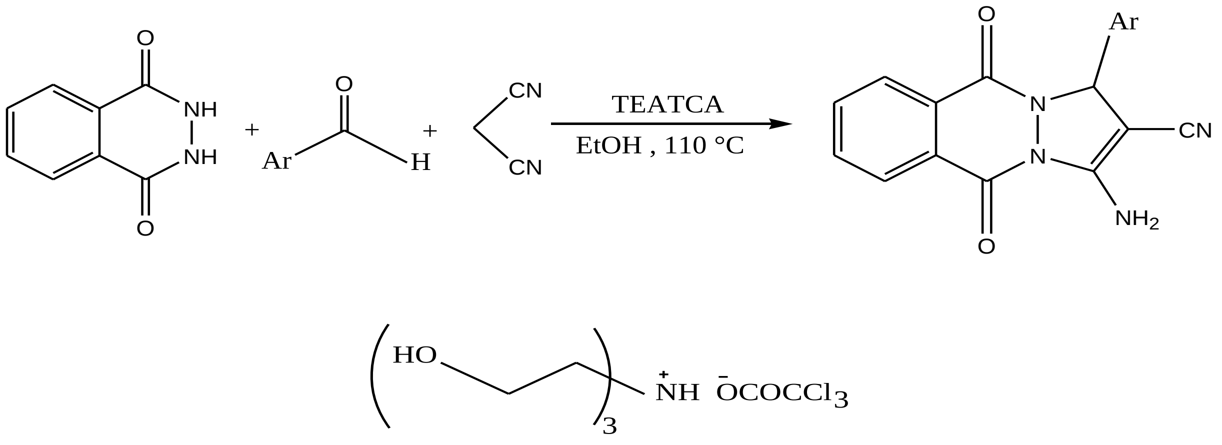
Nitrogen-containing heterocyclic compounds are widespread in nature, and their applications to biologically active pharmaceuticals, agrochemicals, and functional materials are becoming more and more important[1]. The development of new efficient methods to synthesize *N*-heterocyclic with structural diversity is one major interest of modern synthetic organic chemists [2-3]. Herein, we wish to report a novel three-component synthesis of 1*H*-pyrazolo[1,2-*b*]phthalazine-5,10-dione derivatives using nano triethanolammonium trichloroacetate [TEATCA] as catalyst for condensation reaction of phthalhydrazid, malononitrile, and aldehydes in EtOH at 110 °C(FigureI). This method offers several advantages such as inexpensive catalyst, easy synthetic procedure, use of greener solvent (EtOH), high yield.



TEATCA

Figure1. Synthesis of 1*H*-pyrazolo[1,2-*b*]phthalazine-5,10-dione in EtOH, at 110°C.

References

[1] R.Ghorbani-Vaghei, S. Noori, Z. Toghraei-Semiromi, Z. Salimi, RSC Adv. 2014, 4, 47925-47928.

[2] (a) E. C. Franklin, Chem. Rev. 1935, 16, 305-361; (b) F. W. Bergstrom, Chem.Rev. 1944, 35, 77-277.

[3] (a) A. G. Waterson, Curr. Org. Chem.2000, 4, 175-203; (b) R. V. A. Orru, de Greef, M, Synthesis2003, 1471-1499; (c) Kirsch, G.; hess, S.;Comel, A, Curr. Org. Chem. 2004, 1, 47-63.

Nano triethanolammonium trichloroacetate as new catalyst for the synthesis of tetrahydrobenzo[*b*]pyran derivatives

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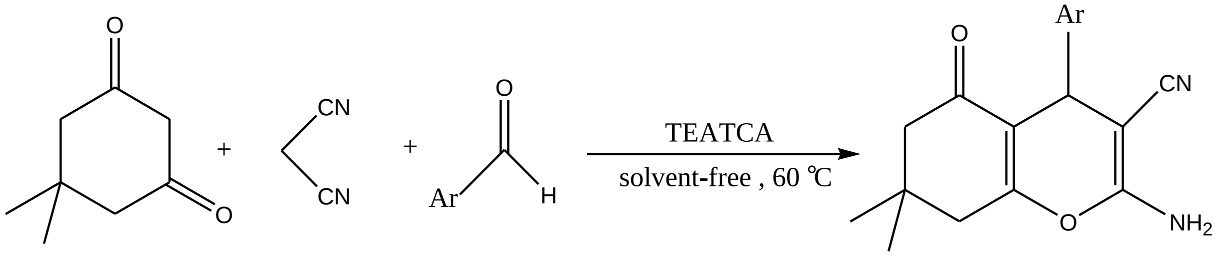
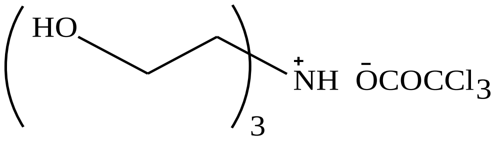
Tetrahydrobenzo[*b*]pyrans are an important class of heterocyclic scaffolds in the field of pharmaceuticals. These compounds are widely used as anti-coagulant, diuretic, spasmolytic, anticancer and anti-anaphylactic agents (1-3).Numerous methods have been reported for the synthesis of tetrahydrobenzo[*b*]pyrans.Nano triethanolammonium trichloroacetate [TEATCA] was used as new catalyst for the synthesis of tetrahydrobenzo[*b*]pyran derivatives under solvent- free conditions at 60 °C.In a typical experimental procedure, a mixture of aromatic aldehyde, malononitrile,dimedone under solvent-free conditions at 60°C, was stirred in the presence of a catalytic amount of TEATCA to afford the tetrahydrobenzo[*b*]pyranin high yields (Figure 1). Use of nontoxic reaction components, short reaction times,easy work-up and high yields are some important advantages of this method.





TEATCA

Figure1. Synthesis of tetrahydrobenzo[*b*]pyran under solvent-free conditions at 60°C.

References

[1] L. L. Andreani, E. Lapi, Boll. Chim. Farm. 1960, 99, 583-586.
[2] K. Singh, J. Singh, H. Singh,Tetrahedron1996, 52, 14273-15280.
[3] L. Bonsignore, G. Loy, D. Secci, A. Calignano, Eur. J. Med. Chem. 1983, 28, 517-520.

Synthesis and characterization some 3,4-dihydropyrimidin-2(1*H*)ones using diimide as a novel organocatalyst under free solvent condition

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Dihydropyrimidinones attract growing interest dueto their therapeutical and pharmacological activity [1]. 4-aryldihydropyrimidinones are powerfulblockators of calcium channels and antihypertonic,drenergicand neuropeptide antagonists [2]. The simplest and direct route to dihydropyrimidinones,suggested for the first time by Biginelliandinvolving ternary condensation of an aldehyde, aketo ester, and urea, often gives the desired productin a low yield, especially with aliphatic aldehydes [3].Therefore,theBiginelli reaction continues to attract the attentionof researchers looking for facile and efficient proceduresfor preparing dihydropyrimidinones. Here we report on a new procedure for preparing3,4-dihydropyrimidin-2(1*H*)-ones in thepresence of *N*,*N*-diimide as organocatalyst. We obtained 3,4-dihydropyrimidinonesin high yield by thereaction of various aldehydes with ethyl acetoacetateand urea in the presence of *N*,*N*-diimideascatalyst under solvent free for 3 h at 120 ^{O}C(Figure 1).

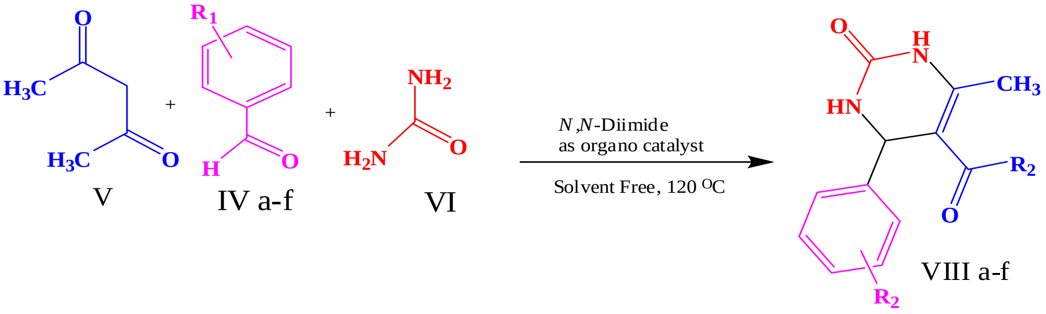

Figure 1.Scheme of the reaction

References

[1] Kappe, C.O., Tetrahedron, 1993, vol. 49, pp. 6937_6963.
[2] Big, F., Carloni, S., Frullanti, B., et al., TetrahedronLett., 1999, vol. 40, pp. 3465_3473.
[3] T.N. Akhaja, J.P. Raval, Design. Chin. Chem. Lett. 23, 446 (2012)

Multi-component reactions in natural deep eutectic solvent

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Room temperature Ionic liquids represent a class of alternative green solvents receiving currently serious consideration is not only important on the laboratory scale but also for industrial applications with the promise of benefits both environmental and technological. By virtue of their nonflammable, chemical and thermal stability, and outstanding solvation ability and negligible vapour pressure ionic liquids have been proposed as new solvents [1]. Unfortunately, cost, toxicity for some aquatic species and high purity are the main disadvantage of these green solvents that limited for chemist and industry. On the other hands, deep eutectic solvent (DES) consisting of an ammonium salt and hydrogen-bond donor compounds such as urea, acid, amine, and carbohydrates are alternatives to ionic liquids for organic transformations [2]. These green and stable eutectic based solvents are cheaper, easier to make; it is necessary to take the two or three solids, mix them together and heat until melt. Furthermore, choline chloride ChCl and urea is both the naturally occurring biocompatible compound as they are easily biodegradable and are not hazardous if they are released back into nature, so processes that use this deep eutectic solvent is economically green [3].

As a part of our research aimed at developing green chemistry by using water and deep eutectic solvent such as urea-choline chloride as a reaction medium. Herein, we describe a simple, highly efficient One-Pot multicomponent reaction (Ugi, Passerini and other important MCR) in deep eutectic solvent under mild reaction condition and excellent yields.

References

[1] N. Azizi, E. Batebi, S. Bagherpour, H. Ghafuri. RSC Advances 2 (2012) 2289.
[2] N. Azizi, E. Gholibeglo. RSC Advances 2 (2012) 7413.
[3] N. Azizi, E. Batebi. Catalysis Science Technology2 (2012) 2445.

Preparation of ionic liquid/graphene oxide composite and application for ring opening of epoxide

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Graphene or grapheneoxide (GO) has many advantages, such as large specific surface area, excellent thermal conductivity, high electrical mobility and great mechanical strength, which has been widely used in synthesizing nanocomposites and fabricating microelectrical devices[1,2]. Ionic liquid/graphene oxide composite was prepared by treating commercially available expandable graphite powder using a modified Hummers method. The structure of catalyst was characterized by various techniques such as Fourier transform infrared spectroscopy (FTIR), and TG-DTA, and the spectral data confirmed were the structures of the title catalyst [3]. As part of our continuing efforts to develop green and sustainable chemistry for useful organic transformations, herein we have used ionic liquid/graphene oxide as a convenient, clean and highly efficient catalyst for ring opening of epoxides at room temperature. The most important features of this procedure are an environmentally benign catalyst and solvent, effective recovering and reusability of the catalyst, operational simplicity and short reaction times (Figure 1).

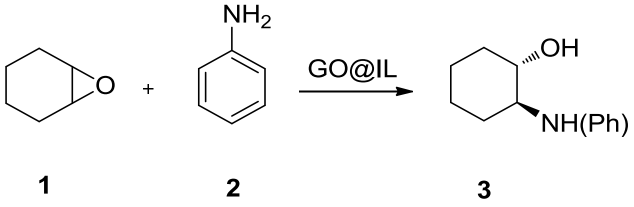

Figure 1. Scheme of the reaction

References

[1] K. Geim, K. S. Novoselov, Nature Materials 6 (2007) 183.
[2] A. Karamania, A. P. Douvalisb, C.D. Stalikas, Journal of Chromatograohy A 1271 (2013) 1.
[3] Chakraborti, Asit K.; Kondaskar, Atul Tetrahedron Letters 44 (2003) 8315.

Synthesis and characterization of imidazolium based poly ionic liquidsas electrolytesin dye-sensitized solar cells

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In the past few years, poly (ionic liquids)(PILs), which combined the unique properties of ionicliquids (ILs) and polymer architecture, have attracted a lot ofattention [1]. Recently, the polymerized ILs have been received growingattentions as alternatives to the organic liquid electrolytes andTraditional ILs electrolytes in dye sensitized solar cell (DSSCs) [2].The electrolyte is one of the most crucial components in it is responsible for the inner charge carrier transport between electrodes and continuously regenerates the dye and itself during DSSC operation. Additionally, the electrolyte has great influence on the light-to-electric conversion efficiency and long-term stability of the devices [3]. PILs usually possess various functions such as transportation of target ions, providing specific polarenvironment, and giving good mechanical strength; these functions depend on both IL structure and polymer main chain. In this work, we report a new type of imidazolium based poly(ionic liquids) (a) prepared usingimidazolium ionic liquid monomer (NVImBr) and methylmethacrylate (MMA)in different molar ratios via free radical polymerization method.For the improvement of mechanical properties of theses ion conductive polymers,addition of small amount of cross-linker is quite effective before polymerization. Therefore, the network copolymers (b) were synthesized by NVImBr and MMA in the presenceof poly (ethylene glycol) dimethacrylate as cross linker (1and 3 mol %). From our study, very small amount of cross-linker did not affect the ionic conductivity but considerably improved the thermal stability and mechanical properties.The obtained PILs and networks were characterized and examined using FT-IR, ^{1}H NMR, DSC, XRD and EIS.

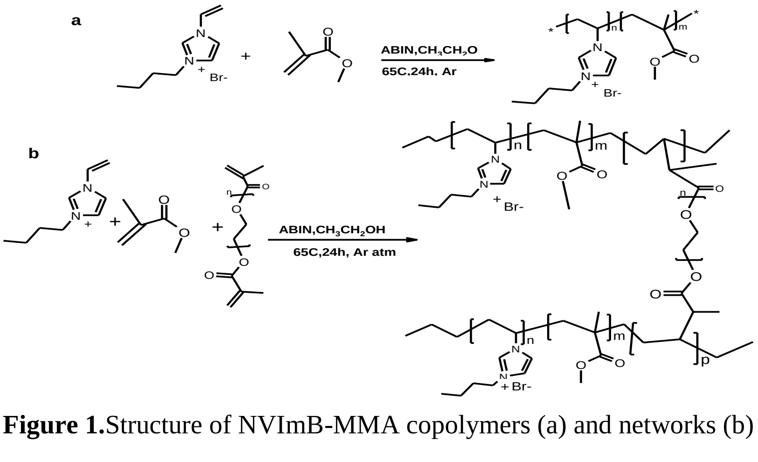

Figure 1. Structure of NVImB-MMA copolymers (a) and networks (b)

References

[1] Y.Ye, Y. A. Elabd, Polymer, 52 (2011) 1309–1317.
[2] K. Lv, W.Zhang, L. Zhang, Z.S. Wang, Appl. Mater. Interfaces 8, (2016) 5343−5350.
[3] H. Nakajima, H. Ohno , Polymer 46 (2005) 11499–11504.

The Production of $CoFe_2O_4$/Graphene Nanocomposite by Hydrothermal Method and Its Catalytic Application in the Reduction of 4-Nitrophenol

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P-aminophenol (4-AP) is an important organic compound, which is widely used as key intermediate in dyes, pharmaceutical industry, etc [1]. At present, 4-AP is synthesized by catalytichydrogenation of *p*-nitrophenol (4-NP), iron powder reduction and the electro-reduction technology, etc [2-3]. However, the process of catalytic hydrogenation of 4-NP is complicated, which requires corrosive acids and produces large amount of by-products. The reduction reaction by iron powder is difficult for product isolation and accompanied by serious waste pollution. Production of 4-NP is thus obstructed because of these limitations as mentioned above.

In this work, $CoFe_2O_4$/graphene nanocomposite was synthesized through hydrothermal process and then identified with different analysis such as FT-IR, XRD, SEM, EDAX, VSM. It was found that the$CoFe_2O_4$/graphene nanocomposite exhibited high catalytic activities on the reduction of *p*-nitrophenol to *p*-aminophenol in the presence of $NaBH_4$. Furthermore, the composite catalyst can be easily recovered due to its magnetic reparability and high stability.

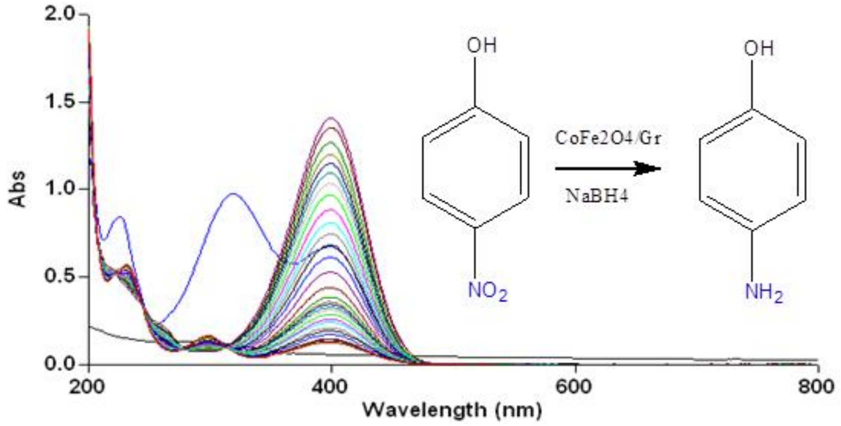

Figure 1. Scheme of the reaction

References

[1] Y. Du, H.L. Chen, R.Z. Chen, N.P. Xu, Applied Catalysis A, 277 (2004), pp. 259-264.
[2] A. Deshpande, F. Figueras, M.L. Kantam, K.J. Ratnamb, R.S. Reddy, N.S. Sekhar, Journal of Catalysis, 275 (2010), pp. 250-256.
[3] S.F. Wang, B.B. He, Y.J. Wang, X.Q. Zhao. Catalysis Communications, 24 (2012), pp. 109-113

Synthesis and characterization novel chemically cross-liked shape memory polymers based on polycaprolactone and hydroxyprpoyl cellulose

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Shape-memory polymers (SMPs) have the ability to recover their original shape from a temporary shape when they are exposed to an appropriate stimulus such as heat, light, electric field, magnetic field, or moisture. In recent years, SMPs have gained an increasing amount of attention for their medical applications, such as smart sutures, vascular stents, esophageal stents,and tissue engineering scaffolds,and in drug delivery[1].Poly (caprolactone) (PCL)as a semicrystalline biodegradable polymeris one of the mostimportant polymer with relatively low melting temperatureand good mechanical properties. For biomedical applications,the biodegradability nature of the polymers and adjustment oftheir Tm around the human body temperature (37–39 °C) arethe essential key factors and a challenging field for researchers[2]. Hydroxypropyl cellulose (HPC) has been widely studied as biomedical or intelligent materials due to its nontoxicity, biocompatibility and high mechanical strength [3].

In this study, the chemically cross linked SMP films of PCL wereprepared in four steps. In the first step bulk polymerization ofPCL, was initiatedby ring-opening polymerization of ε-CL in the present of butandiol and using stannous octoate as catalyst. In the second step,after removing the moisture under nitrogen atmosphere, hexamethylene diisocyanate (HDI) was added on the obtainedpurifiedPCLdiols.The third stepwas performed by addingHPCsolution in$CHCl_3$ to the reaction mixture (Figure1).In the fourth and final step, after obtaining a homogenized solution, the mixture was poured into a Teflon dish andleft atthe room temperature for 24 h. In order to more curing, dried film was placed in an oven at 80 °C for another 24h.The obtained SMP polymers were characterized and examinedusingFT-IR, ^{1}H NMR, DSC, XRD,and tensile and SMP tests.

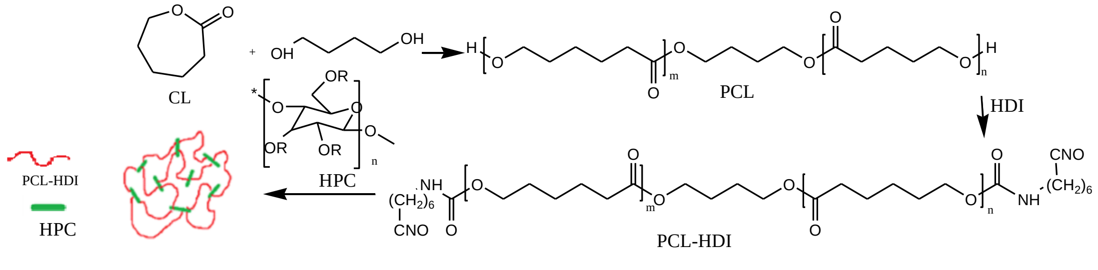

Figure1. Synthetic route of PCL and HPC-g-PCL

References

[1] Y. Liu, Y.Li, G. Yang,X. Zheng, S. Zhou. ACS applied materials interfaces 7(7) (2015) 4118-4126.
[2] M. Jahangiri, M.Bagheri, F.Farshi, F. Abbasi. Journal ofPolymer Research22(10) (2015)1-13.
[3] M. Bagheri, S.Shateri, H.Niknejad, A. Entezami, Journal of Polymer Research 21(10)(2014) 1-15.

Preparation of pyrazole-based compounds in ChCl-urea DES as green solvent

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Within the framework of green chemistry, solvents occupy a strategic place. Green Chemistry aims to replace the hazardous and/or harmful solvents with more environmentally friendly alternatives.A new family of ionic fluids, so-called Deep Eutectic Solvents (DES), exhibit similar physico-chemical properties to the traditionally used ionic liquids, while being much cheaper and environmentally friendlier [1]. DESs contain large, non-symmetric ions that have low lattice energy and hence low melting points [2]. Pyrazoles are one of the most important classes of bioactive heterocycles gaining increased interest from pharmaceutical, chemical, and agricultural industries over the past decade [3]. For example 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 [1]. Hence, in this work we have synthsized pyrazole based compounds 3 in ChCl-urea DES in different conditions. For this purpose, the reactions were performed in two steps. In the first step, pyrazolonewas prepared from condensation of hydrazine hydrate and ethyl acetoacetate under solvent free condition. At the second step, Knovenagel condensation of pyrazolone 1 with aromatic aldehyde derivatives 2followed by Michael addition gave compounds 3(Figure1).Finally, the obtained products were purified and characterizedby x-ray crystallography and spectroscopic methods such as IR, ^{1}H NMR, and ^{13}C NMR.

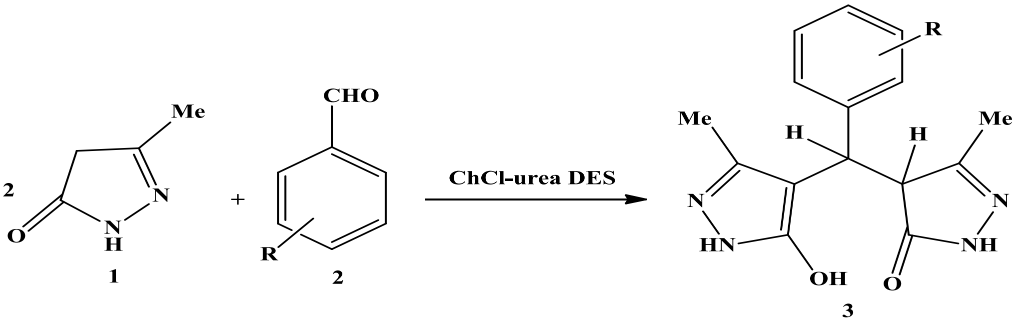

Figure 1. Reaction of Pyrazolone 1, aromatic aldehyde derivatives 2 in DES.

References

[1] A. Moshtaghi Zonouz, D. Moghani, Synth. Commu.46(2016) 220.
[2] E. L. Smith, A. P. Abbott, K. S. Ryder, Chem.Rev. 114(21)(2014) 11060.
[3] D. Enders, A. Grossmann, B. Gieraths, M. Düzdemir, C. Merkens,Org.Lett.14(16) (2012) 4254.

$NiFe_2O_4$@Cu: An Efficient Heterogeneous Catalyst for Reductive-Acetylation of Nitroarenes to Acetanilides

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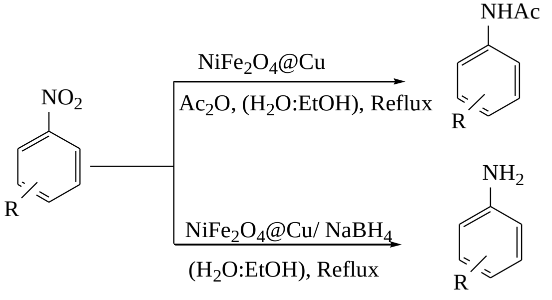
Nanosized spinel ferrite particles, a kind of soft magnetic materials with a structural formula of MFe_2O_4 (M=divalent metal ion, e.g. Mn, Mg, Zn, Ni, Co, Cu, etc.), are one of the most attracting class of materials. The spinel ferrites have many technical applications, such as photoelectric devices, catalysis, sensors,nano devices, and magnetic pigments.

Arylamides are major building blocks and key intermediates of many biologically important compounds as well as a number of drug candidates [1]. Usually, the amides are gottenfrom the corresponding nitro intermediates in two separate steps: the reduction of the nitro group to the corresponding amine, then amidation with an acylating agent. A large number of methods have been applied for One-Pot reductive amidation of nitroarenes [2, 3]. Many of the existing methodologies, however, suffer from the problem of either longer reaction times or low yields and sometimes entail the use of highly expensive reagents. In this work, we have used the core-shell $NiFe_2O_4$@Cu nanoparticles as a heterogeneous catalyst for reduction and also One-Pot reductive-acetylationof nitroarenes (Figure 1).



R = Me, NH_2, OH, OCH_3, CH_2OH, CHO

Figure 1. Scheme of the reaction.

References

[1] S. Budavari, Merck Index14th,pp. 3673.

[2] M.K. Lakshmi, R.S. Reddy, K. Srinivas, R. Chakravarti, B. Sreedhar, F. Figueras, C. V. Reddy, J. Mol. Catal. A: Chem.2012, 355, 96.

[3] A.E. Wahba, J. Peng, M.T. Hamann, Tetrahedron Lett.2009, 50,3901.

A green approach for One-Pot synthesis of cyclicacetals using various aldehydes and diols in the presence of nano-γ-alumina supported BF_3 as a newheterogeneous solid acid catalyst

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Functional group interconversion (protection/deprotection) is an unavoidable protocol in the synthesis of many designed target molecules such as drugs and multifunctional natural products [1]. In this regard, acetals have widely used as protecting agents in organic synthesis and are an important class of compounds that have found their direct applications in diverse areas in the chemical industry such as perfumes, flavours, pharmaceuticals, solvents and polymer chemistry [2,3]. Due to the toxic nature of many organic solvents, it is suggested to design processes that are rooted in green chemistry.In this work, nano-γ-alumina supported $BF_3$was prepared and characterized by FT-IR, XRD, SEM, TEM and TGA. This new type of solid acid used for synthesis of some cyclicacetals using various aldehydes and diols(Figure 1).The structure of products have been characterized by spectroscopic techniques such as IR and ^{1}HNMR.

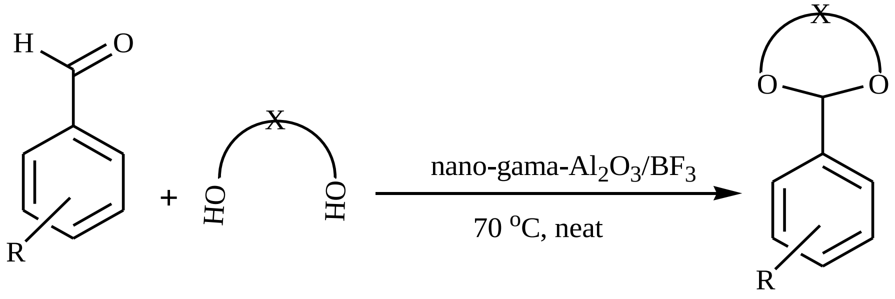

Figure 1. Scheme of the reaction.

References

[1] B.M. Smith, A.E. Graham.Tetrahedron Letters, 52 (2011) 6281.

[2] M. Hong, G. Xiao.Journal of Fluorine Chemistry, 140 (2012) 121.

[3] Y. Guan, D. Zhang, Y. Wang.CatalysisLetters, 142 (2012)1225.

Nano-γ-Alumina supported $SnCl_4$: A novel nitrosating agent for the chemoselective *N*-nitrosation of secondary amines under grinding andsolvent-free conditions

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N-Nitrosamine compounds are present in water, soil and air [1]. Due to the variety applications of these compounds in the various industries as insecticides, pesticides, cosmetics, antioxidants, lubricant additives and N=O agents transmitter [2]. In recent years, the researchers focused on the biological terms of N-nitrosamines.

To date, number of variety reagents such as nitrous acid (HNO_2), dinitrogentrioxide (N_2O_3), nitrosonioum salts and alkyl nitrites (RNO_2) have been used for the nitrosation reactions. The most common of these reagents is nitrous acid [3].

Nano-γ-Alumina supported $SnCl_4$ as a new reusable and green heterogeneous nanocatalyst was prepared and characterized by FT-IR, XRD, SEM, TEM and TGA. Nano-γ-Alumina supported $SnCl_4$ was used for the synthesis of *N*-Nitrosamines by condensation of sodium nitrite, secondryamine and wet-SiO_2 50% (Figure 1).The reaction is proceeded in a short time, simple work-up, easy purification, high yield, solvent-free condition and above all environmental-friendly and further approaches to green chemistry.

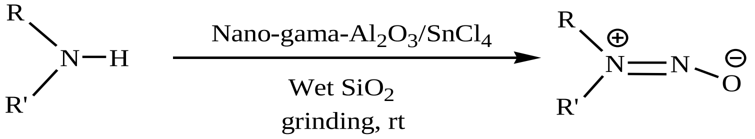

Figure 1. Scheme of the reaction

References

[1] H. Goudarziafshar, A. Ghorbani-Choghamarani, L. Hadian. Journal of the Chinese Chemical Society60 (2013) 1272.
[2] A. Bamoniri, B.F. Mirjalili, R. Tarazian. Journal of Chemical Sciences 127 (2015) 885.
[3] M.A. Zolfigol, D. Habibi, B.F. Mirjalili, A. Bamoniri. Tetrahedron Letters 44 (2003) 3345.

Synthesis of substituted spiropyrano [2,3c]pyrazoles using silica-bonded imidazolium-sulfonic acid chloride (SBISAC)as an efficient nanocatalyst

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The design, synthesis and use of high efficiency nano catalysts in synthetic organic procedures have possessed an important amount of affection from the scientific association so as to improve gradually noteworthy approaches for the synthesis of more target molecules.On the other hand, the spiropyrano[2,3-c]pyrazolesare one of the most important compounds in pharmacecutical field[1] which utlize as antimicrobial[2], anticancer[3], biodegradable agrochemicals[4], and etc.In this paper,preparaion of thespairo heterocycle rings using(SBISAC)as an efficient nano catalyst in water as a green solvent,was studied (Figure 1).

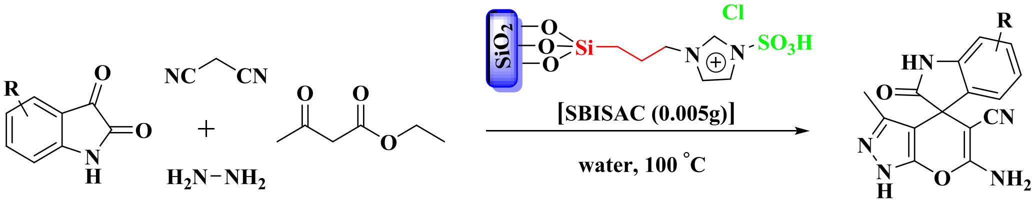

Figure 1. Four component synthesis of substitutedspiropyrano[2,3-c]pyrazoles

References

[1] S. R. Mandha, S.I. Siliveri, M. Alla, V. R. Bommena, M. R. Bommineni, S. Balasubramanian. Bioorg. Med. Chem. Lett. 22 (2012)5272.
[2] (a) W. P. Smith, L. S. Sollis, D. P. Howes, C. P. Cherry, D. I. Starkey, N.K. Cobley, J. Med. Chem. 41(1998)787, (b) K .Mazaahir, S. Shilpi, R. K. Khalilur, S. T. Sharanjit, Bioorg. Med. Chem. Lett. 15 (2005) 4295.
[3] J. L. Wang, D. Liu, Z. J. Zheng, S. Shan, X. Han, S. M. Srinivasula, C. M. Croce, E. S. Alnemri, Z. Huang, Proc. Natl. Acad. Sci. U.S.A. 97 (2009) 7124.
[4] (a) H. Junek, H. Aigner, Chem. Ber. 106 (1973) 914, (b) H. Wamhoff, E. Kroth, K. Strauch, Synthesis , 11 (1993) 1129.

Cyclohexane-1,4-diyl bis(hydrogen sulfate)for the catalytic synthesis of 3, 4-dihydropyrimidones *via* biginelli reaction

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The most simple and straightforward produce, reported by Biginelli more than 100 years ago, and involves the One-Pot three component condensation of an aldehyde, *α, β*-ketoester and urea [1].In recent years, 3,4-dihydropyrimidinone/thiones (DHPMs) have occupied an important place in organic and medicinal chemistry, mainly due to their diverse therapeutic and pharmacological properties [2].This has led to the development of new improved methodologies for the Biginelli reaction, involving the use of a number of catalysts [3].Cyclohexane-1,4-diyl bis(hydrogen sulfate) [CBDH]was prepared by the reaction between cyclohexane-1,4-diol and chlorosulfonic acid (Figure 1). The polarity of the [CBDH]might associate it to interact with starting materials for the smooth conversion to the desired product.

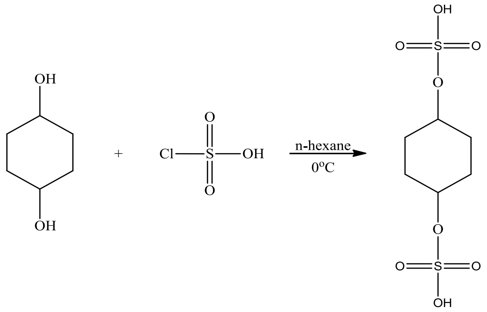

Figure 1. Preparation of cyclohexane-1,4-diyl bis(hydrogen sulfate)

Herein, we report [CBDH] as an efficient and eco-friendly catalyst for the One-Pot synthesis of 3, 4-dihydropyrimidinonesthrough the Biginelli three component condensation by using an aromatic aldehyde, dimedone, and urea (Figure 2).

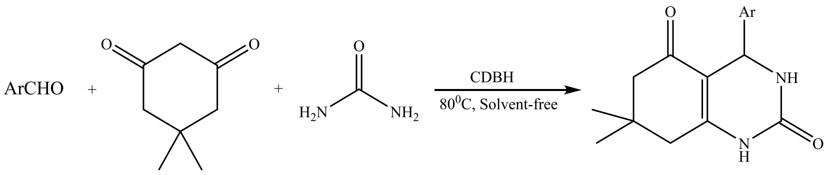

Figure 2. Preparation of dihydropyrimidinones through the Biginelli condensation by using CDBH under solvent-free conditions

References

[1] P. Biginelli, GazzettaChimicaItaliana.,*23* (1893) 360.
[2] S.D. Bajaj, O.A. Mahodaya, P.V. Tekada, Pharmaceutical Chemistry Journal *48* (2015) 681.
[3] K. Kouachi, G. Lafaye, S. Pronier, L. Bennini, S. Menad, Journal of Molecular Catalysis A: Chemical *395*, (2014) 210.

Synthesis of pyranopyrazole compounds using heterogeneous base catalyst based on 1,3,5-triazine-2,4,6-triamine modified nano rice husk silica

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Many researchers have reported that rice husk is an excellent source of high-grade amorphous silica.Silica from rice husk offers a cheap alternative to commercial silica and at the same time help to solve rice husk disposal problem faced by rice milling industry [25]. A reaction between a carbon-halogen functional group and oneof the base organic compounds or ligands is anucleophilic substitution reaction.1,3,5-triazine-2,4,6-triamine (melamine), is a primary amine with three NH_2 groups.These groups can be utilized for catalysis. We thought that the grafting of melamine onto the silica surface could afford a catalyst having a unique catalytic activity and selectivity due to the three NH_2 groups. Pyranopyrazoles are important class of fused heterocyclic compounds, that are known for their wide range of biological activities such as fungicidal, bactericidal, vasodilatory activities [32] and they act as anticancer agents.

There were few studies about the preparation of silica supported basic catalyst and its application for multi-component reactions (MCRs). herein, amorphous nanosilica was successfully extracted from rice husk (RH-SiO_2), functionalized with melamine and used as a basic catalyst for the synthesis of pyranopyrazole compounds.Figure 1 shows the schematic representation of the synthetic pathway for RHA@Melamine solid base catalyst.

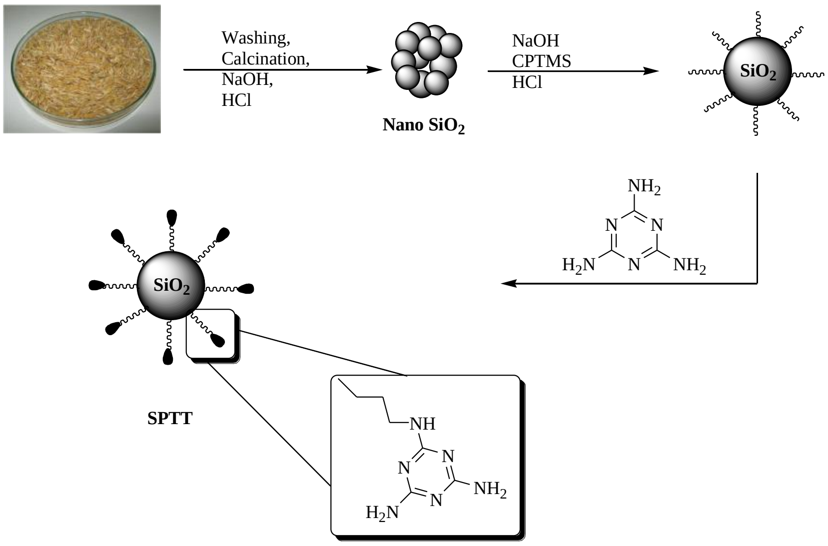

Figure 1.Scheme of the reaction

References

[1] F. Adam, A. Iqbal, Microporous Mesoporous Mater. 141 (2011) 119.
[2] M. N. Nasr, M. M. Gineinah, Arch. Pharm. Med. Chem. 335 (2002) 289.
[3] V. K. Ahluwalia, A. Dahiya, V. Garg, Indian J. Biochem., Biophys. 36 (1997) 88.

Porous acidic catalyst, functionalized with imidazole ionic liquid ([SBA-Im]HSO_4) as a novel phase transfer catalyst for the aqueous synthesis of benzyl thiocyanates and azides

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There were few studies about the preparation of silica supported acidic ionic liquid catalyst and its application for organic transformation. Recently, we focused on developing novel PTC systems for organic transformations and also successfully performed the One-Pot synthesis of phthalazinedione and phthalazinetrione heterocyclic compounds with [SBAIm]HSO_4 composite on SBA-15 mesoporous silica as support [1]. For [SBAIm]HSO_4, the surface of the mesoporous silica was modified by reaction with the ionic liquid 1-(triethoxysilylpropyl)-3-methylimidazolium hydrogen sulfate (IL-HSO_4). Even though some anticancer natural products, drug candidates, synthetic intermediates, antiasthmatic drugs, biocidal compounds and insecticides possess thiocyanate or azide functional groups, there are few reported practical synthetic routes in the literature for this class of compounds [2]. By having this goal in minds and in continuation of our research on using water as a reaction medium [3], in this research, we report the synthetic applicability of porous acidic catalyst functioned with an imidazole ionic liquid ([SBA-Im]HSO_4) as a phase transfer catalyst for the facile preparation of benzyl thiocyanates and azides in water by nucleophilic substitution reaction (Figure 1).

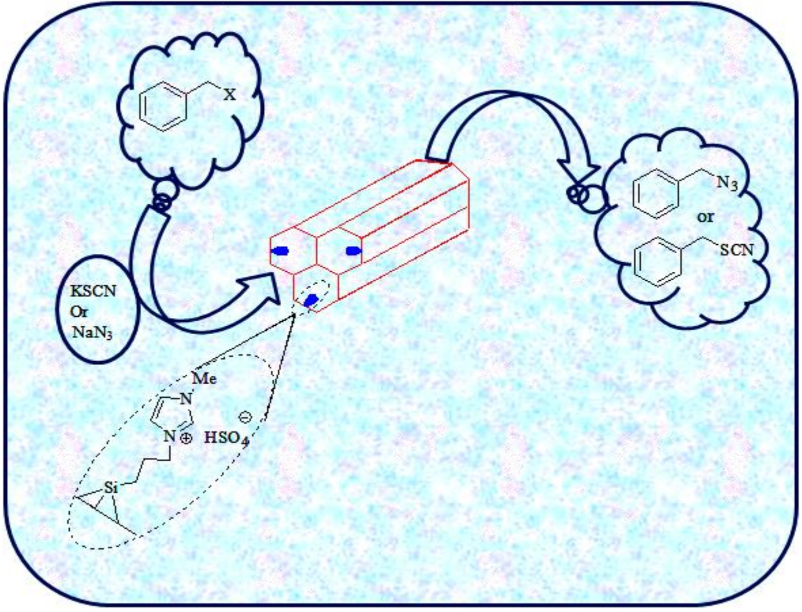

Figure 1. Application of [SBA-Im]HSO_4 as a phase transfer catalyst for the facile preparation of benzyl thiocyanates and azides in water

References

[1] J. Davarpanah, P. Rezaee, S, Elahi, Res. Chem. Intermed. DOI 10.1007/s11164-015-1997-2.
[2] A. R. Kiasat, S. Nazari, Catal.Commun.18 (2012) 102.
[3] J. Davarpanah, A. R. Kiasat, S. Noorizadeh, M. Ghahremani, J. Mol. Catal. A 376 (2013) 78.

Synthesis of new derivatives of symmetric bisarylidene of cyclic ketones based on triazole ring

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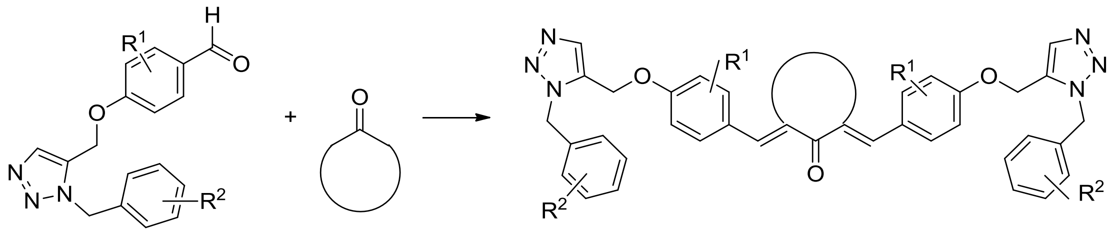
Aldol condensation is an important reaction for the C-C bond formation in most of carbonyl compounds. Among this kind of reactions, Claisen-Schmidt condensation of aryl halides with cycloalkanones is a major procedure for the synthesis of α,α'-bis(arylmethylidene) cycloalkanones [1]. Bisarylidenes of cyclic ketones have diverse synthetic applications in preparation of different compounds such as precursors of pharmaceuticals, pesticides, anti-fungal, anti-bacterial and anti-inflammatory agents, as well as polymeric units (synthons) of liquid crystals [2].

On the other hand, click chemistry is an efficient and selective method for the synthesis of triazoles through a 1,3-dipolar cycloaddition of azide and alkyne. Triazol derivatives have several biological and pharmaceutical properties, such as anti-cancer and anti-HIV effects[3].

Due to the importance of bisarylidenes and triazoles, in this project has been attempted to synthesize new derivatives of symmetric bisarylidenes of cyclic ketones based on triazol ring. For this purpose, at first triazol-based aldehydes (1) were prepared via click reaction between propargyloxybenzaldehydes and benzyl azides. Then, aldol condensation of these compounds with different cylic ketones (2) led to the synthesis of corresponding triazol-based bisarylidenes (3).



1 2 3

R^1= H, OMe
R^2= H, 4-Cl, 2-Cl, 3,4-diCl,...

Figure 1. Scheme of the reaction

References

[1] N.Iranpor,F.Kazemi, Tetrahedron 54 (1998)9475.
[2] I.Kosiova,S.KovackovaP.Koi,Tetrahedron 63 (2007)312.
[3] K. Kacprzak, Synlett6 (2005) 943.

Synthesis of amino silane derivatives by the reaction of imines in the presence of lithium

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Silylmethylamines are defined as compounds in which one silicon and one nitrogen atom are directly linked to a sp^3-carbon atom [1]. Many silylamine derivatives prepared by the reaction of imines and silylation reagents such as trimethylchlorosilane [2]. This compounds have many bilogical activity specialy antioxidant, anticancer, antibacterial and anti-tumor activity [1]. Silylamine reversible ionic liquids were designed to achieve specific physical properties in order to address effective CO_2 capture. The current-and the only implemented-technology that enables the capture of CO_2 is the use of aqueous amine solutions. In particular, 30% monoethanolamin (MEA) in water is most often used because MEA exhibits high CO_2 capacity and high reactivity (chemisorption). Silylamines (molecular liquids) reversibly react with CO_2 to form ammonium carbamates (reversible ionic liquids). Two moles of molecular liquid react with one mole of CO_2 [3], this properties prompted us to synthesize the new derivatives of them. In this work a new α-silylamine derivative was prepared by the reaction of imine 1 with the trimethylsilylchloride in the present of lithium in THF (Scheme 1). The product was extracted from reaction mixture by distillation. The structure of this compound was charactrized from FT-IR and ^{1}HNMR sppctra.

Figure 1: Synthesis of α-silylamine

References
[1] Xiao-Jun Han, Yao, and chong-Dao Lu. Efficient synthesis of α tertiary- α Silylamines from aryl sulfonylimidates 11 (2012) 2906-2909.
[2] Houben-Weyl. Science of synthesis, Methods of molecular transformation compounds with two carbon-Heteroatom bonds, ebook (2007) 455.
[3] Amy L. Rohan, Jackson R. Switzer. The Synthesis and the Chemical and Physical Properties of Non-Aqueous Silylamine Solvents for Carbon Dioxide Capture (2012).

Synthesis of iodobenzamide derivatives as potential dopamine receptor ligands

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IBZM is used frequently for the *in vivo* imaging of D_2 receptors in the brain of human and nonhuman primates [1]. The dopamine D_2 receptor is implicated in the pathogenesis of Parkinson’s disease and in psychiatric disorders including schizophrenia and mania. Measurements of occupancy of this receptor in vivo help to better understand the pathophysiology and pharmacology or such disorders as well as to monitor illness progression and effects of treatment [2]. We first synthesized 2,6-dimethoxybenzoyl chloride using $SOCl_2$ and respective benzoic acid then added((S)-1-ethylpyrrolidin-2-yl)methanamine to prepare of compound **1**[3], that could be converted tocompound **2** with boron tribromide. Finally, both compoundsiodinated with NaI, $Tl(OTf)_3$ intrifluoroacetic acid (TFA) as solvent. All analytical data including IR, ^1H NMR and mass spectroscopy of products were in agreement with the proposed structures.

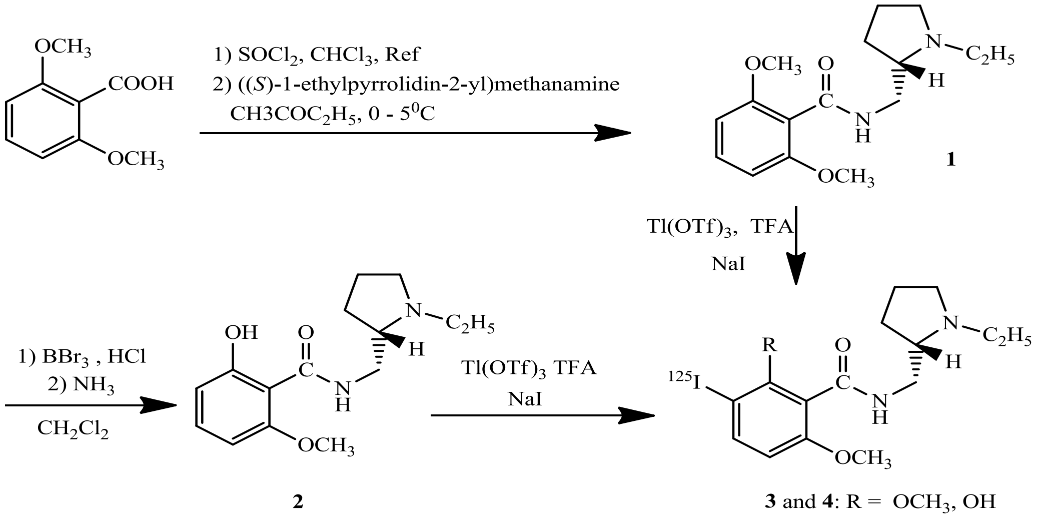

Figure 1.Scheme of the reaction

In conclusion, we synthesized IBZM derivatives with high yield and chemical purity which are highly selective ligands todopamine receptors. Pharmaceutically it is a dopamine antagonist and it can be used by nuclear medicine physicians as a radioactive tracer for SPECT where the radioactive isotope is iodine-123 or iodine-125. The main purpose of a brain study with IBZM is the differentiation of Parkinson's disease from other neurodegenerative diseases such asLewy Body dementia and multiple system atrophy.

References

[1] Y. Zea-Ponce and M. Laruelle, Nucl.Med. Biol.1999, 26, 661–665.
[2] R. M. Baldwin, X. Fu, N. S. Kula, et al., Bioorg. Med. Chem. Lett.2003, 13, 4015–4017.
[3] H. F. Kung, R. Kasliwal, S. Pan, M. Ping Kung, R. H. Mach, Y. Zhi Guo,J. Med. Chem.1988, 31, 1039–1043

Application of biological-based nano catalysts in the preparation of arylbispyranylmethanes

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The catalytic active species with small metal-free organic molecules entitled “organocatalysts” found their key roles as promoter and established highly dynamic area in the academic and also industrial sectors in the past few years and the organocatalysis has grown dramatically [1]. A striking advantage of organocatalysts is their high surface to volume ratio which can intensifythe possibility of the interaction between reactants and catalyst and lead to multiplying the catalytic performance of the applied organocatalysts [2,3].

Herein, the utilization of 2-carbamoylhydrazine-1-sulfonic acid and carbamoylsulfamic acid were described as biological-based nanoorganocatalystswith urea moiety for the synthesis of arylbispyranylmethane derivatives under mild and eco-friendly conditions. A good range of aromatic aldehydes were treated with 4-hydroxy-6-methyl-2-pyrone to give arylbispyranylmethane derivatives through a tandem Knoevenagel condensation and Michael addition procedure in relatively short reaction times with high yields. The presented protocols have merits like the eco-friendly nature, high efficiency, simple operational procedures and benign reaction conditions(Figure 1).

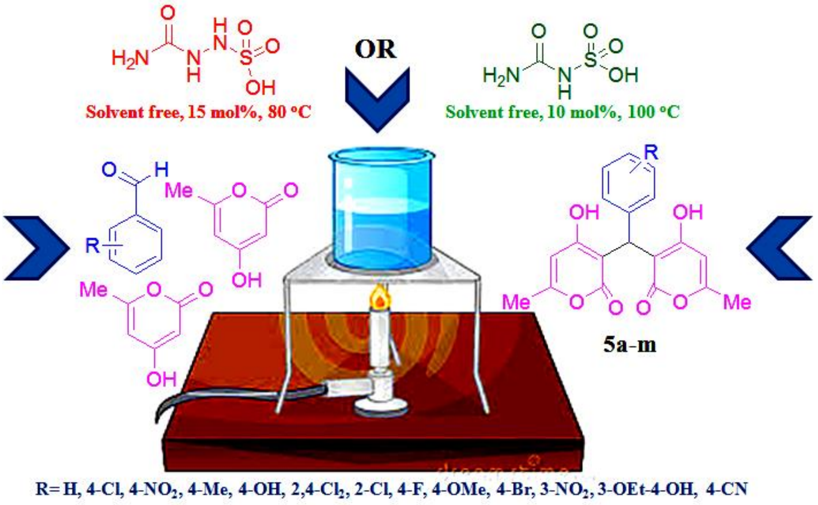

Figure 1: Synthesis of arylbispyranylmethane derivatives in the presence of biological-based nano catalysts

References

[1] Benjamin List, Chem. Rev., 107 (2007) 5413.
[2] M. A. Zolfigol,R. Ayazi-Nasrabadi, S BagheryRSC Adv.,5 (2015) 71942
[3] V. Polshettiwar, R. S. Varma, Green Chem., 12 (2010) 743.

Promoter catalytic application of $\{Fe_3O_4@SiO_2@(CH_2)_3\text{-Urea-}SO_3H/HCl\}$ at the synthesis of 2-aminobenzothiazolomethyl naphthols

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Solid acid catalytic systems have been employed for various chemical processes because of their eco-friendly nature of them and play a key role in preventing pollution in our environment and in past few years, a wide range of solid acids and their supported forms have been developed and extensively reviewed for various chemical catalytic processes [1]. 2'-Aminobenzothiazolomethyl naphthol derivatives are renowned as they show wide variety of biological and pharmaceutical applications in medical chemistry [2, 3]. In this study, we have introduced an efficient procedure for the synthesis of these interesting heterocyclic scaffold in in the presence of$\{Fe_3O_4@SiO_2@(CH_2)_3\text{-Urea-}SO_3H/HCl\}$ as a urea-based ionic liquid stabilized on silica-coated Fe_3O_4 magnetic nanoparticles catalyst under solvent free and benign reaction conditions as depicted in Figure 1.

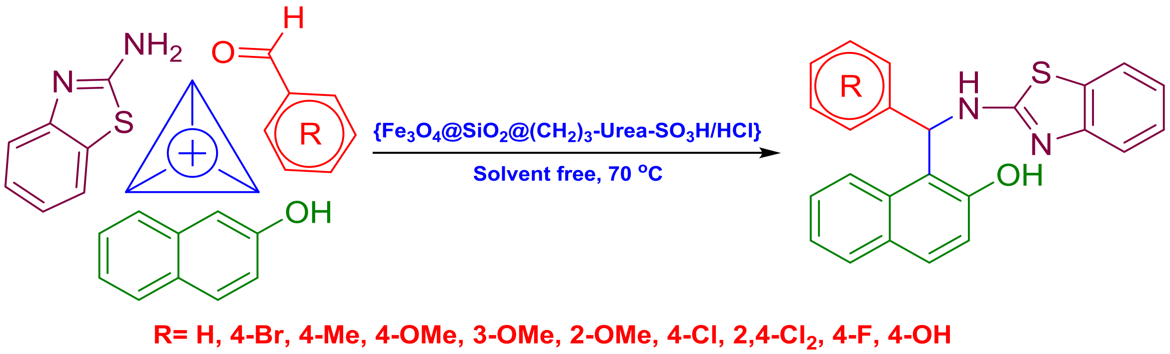

Figure 1: Catalytic application of $\{Fe_3O_4@SiO_2@(CH_2)_3\text{-Urea-}SO_3H/HCl\}$ at the synthesis of 2'-aminobenzothiazolomethyl naphthol derivatives

References

[1] M. A. Zolfigol, R.Ayazi-Nasrabadi and S. Baghery, Appl. Organometal. Chem. 30 (2016) 273.
[2] A. Shaabani, A. Rahmati and E. Farhangi, Tetrahedron Lett.48 (2007) 7291.
[3] C. J. Paget, K. Kisner, R. L. Stone, D. C. Delong, J. Med. Chem. 12 (1969) 1010.

Synthesis of novel phenylalaninol-based benzamidesas dopamine receptor ligands

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The formation of amides has attracted considerable interest due to their importance in organic and bioorganic chemistry, their value as intermediates in organic synthesis and a wide range of applications in the chemical industry. The amide bond is an important structural component of peptides, polymers and many natural products and pharmaceuticals.Numerous amides are biologically active and show antifungal, antihistamine, anthelmintic, and antibacterial properties.[1] Amides show biological activity in a variety of ways when they are conjugated to aliphatic, aromatic rings, and heterocyclic rings [2]. In First, we began this study by preparing L-phenylalaninol in one step from the reduction of corresponding amino acid namely L-phenylalanine1under standard conditions using NaBH$_4$-I$_2$ in dry THF [3].The conversions of phenylalaninolinto the corresponding *N*-alkyl, allyl or propargyl amino alcohol derivatives were carried out through its reaction with N-tert-butyloxycarbonyl-2-bromo-l-aminoethane and Intermediate 2was synthesized by Boc-deprotection with HCl gas in ethyl ether. Finally compound 2 coupled with 2,6- dimethoxy benzoyl chloride for synthesis of new phenylalaninol-based benzamides. All characterization data including IR,^{1}H and ^{13}C NMR of products were in agreement with the proposed structures.

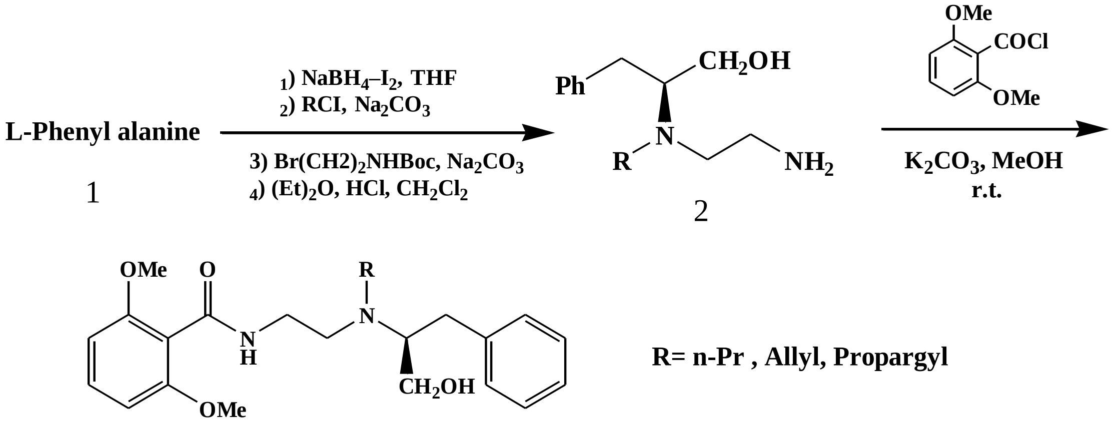

Figure 1.Scheme of the reaction

Given the similarities between these compounds and known selective dopamine receptor ligands include benzamide functional group and at least one stereocenter, we hope new synthesized compounds can be used as dopamine receptor ligands.

References

[1] M. Ghaffarzadeh , S. Shahrivari Joghan, F. Faraji, Tetrahedron Letters 53 (2012) 203
[2] N. Kushwaha, R.K. Saini, S.K.S. Kushwaha, Int. J. Chem. Tech. Res. 3 (2011)203
[3] M.J.McKennon,A.I.Meyers,K.Drauz,M.Schwarm,J.Org.Chem.58(1993)3568

Application of a biological-based nano magnetic catalyst in the synthesis of bis-pyrazols and pyrano[3,2-*c*] pyrazoles

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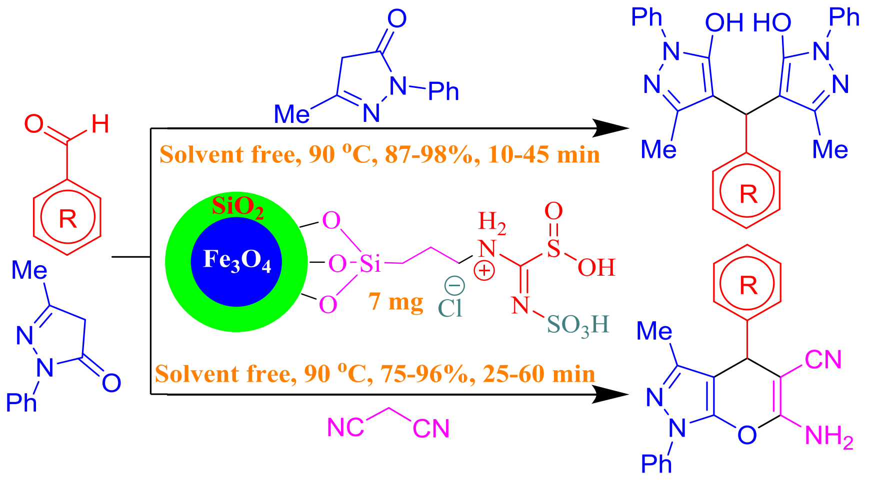
Nowadays, the knowledge-based designing, synthesis and applications of nano magnetic particles (NMPs) are of great demand, and a wide variety of nanostructured magnetic catalysts have been used because of their recycle and reusability, high activity and selectivity in chemical processes. Application of recycle and reusable catalysts or catalytic systems in the chemical processes is in close agreement with the green chemistry disciplines because of their using will be decreased the activation energy, waste of reactions, and energy consumption. The development of nano magnetic catalysts and their roles in the pollutionprevention in our environment at the past, present and future have been extensively reviewed [1-3]. {Fe_3O_4@SiO_2@$(CH_2)_3$-thiourea dioxide-SO_3H/HCl} a newly reported nano magnetic core-shell supported solid acid catalyst was successfully employed at the preparation of 4,4'-(arylmethylene)bis(1*H*-pyrazol-5-ol) and pyrano[3,2-*c*] pyrazole derivatives. The presented methods are very efficient and high-yielding. Also, the catalyst exhibited powerful potent of reusability in both cases of the reactions (Figure1).



R= H, 4-Cl, 2,4-Cl_2, 4-Br, 4F, 3-NO_2, 4-NO_2, 3-Br, 4-OH, 4-Me, 3-OMe, 4-OMe

Figure 1 : Synthesis of of 4,4'-(arylmethylene)bis(1*H*-pyrazol-5-ol) and pyrano[3,2-*c*] pyrazole derivatives

References

[1] B. Karimi, F. Mansouri, H.M. Mirzaei, Chem. Cat. Chem. 7 (2015) 1736.
[2] S. Ganesh Babu, R. Karvembu, Catal.Surv.Asia, 17 (2013) 156.
[3] R. Hudson, Y. Feng, R. S. Varma, A. Moores, Green Chem., 16 (2014) 4493.

[Fe_3O_4@SiO_2@$(CH_2)_3$-Imidazole-SO_3H]Cl acts as a powerful and efficient solid acid catalyst for the preparation of arylbispyranylmethane derivatives under solvent free conditions

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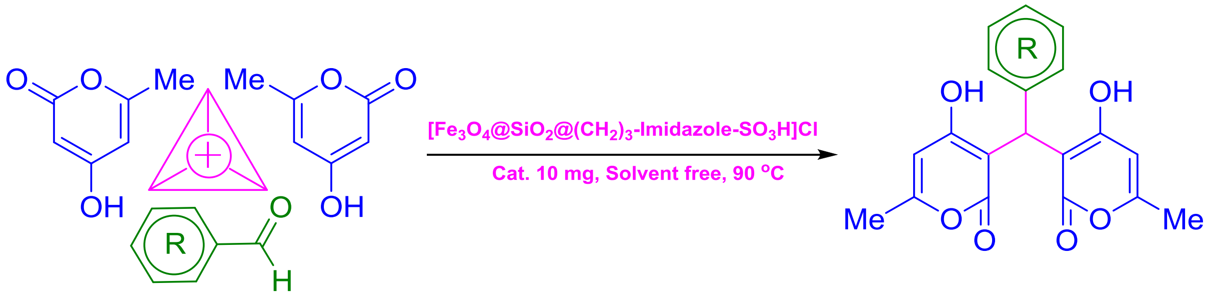
Magnetic nano particles with acidic tags have advantaged due to the merits including many active acidic sites, high thermal stability with good selectivity, easy recyclability and reusability potential, high TON and TOF and also the eco-friendly nature of them. Therefore, due to the mentioned merits, great deal of chemist's attention has focused on the synthesis and applications of these versatile catalytic systems [1-2]. In this present, we would like to explore the application of imidazole-based ionic liquid-stabilized on silica coated Fe_3O_4 magnetic nano particles namely [nano-Fe_3O_4@SiO_2@$(CH_2)_3$-Imidazole-SO_3H]Cl as a heterogeneous core-shell catalystfor the preparation of arylbispyranylmethane derivatives under mild and eco-friendly conditions. The target molecules obtained with good to high yields in relatively short reaction times (Figure1).



R= H, 4-Me, 4-Br, 4-CN, 4-F, 2,4-Cl_2, 4-OMe, 4-OH

Figure 1: Synthesis of arylbispyranylmethane derivatives under mild and eco-friendly conditions

References

[1] M. A. Zolfigol, R. Ayazi-Nasrabadi, S. Baghery, V. Khakyzadeh, S. AzizianJ. Mol. Catal. A: Chem.,418 (2016) 54.
[2] Y.C. Sharma, B. Singh, Biofuels Bioprod. Biore.5 (2011) 69.

Catalytic application of $Fe_3O_4@TiO_2@O_2PO_2(CH_2)NHSO_3H$ at the preparation of triarylpyridines via an anomeric based oxidation

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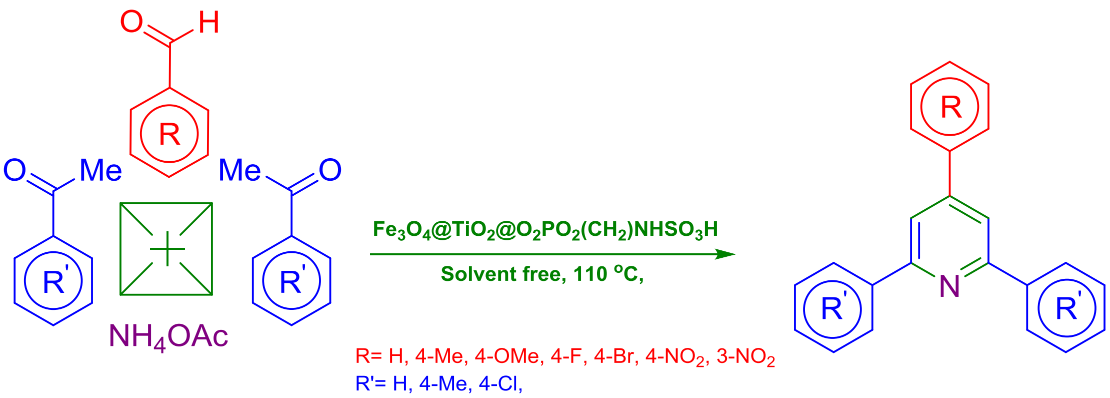
Among the pyridine ring system,2,4,6-triarylpyridine derivatives have emerged as potent biologically active heterocyclic compounds due to theirunique applications as therapeutic agents in the field of medicinal chemistry [1,2]. Some of the medical applications of 2,4,6-triarylpyridines are anesthetic, vasodilator, anti-covulsant, antimalarial, antiepileptic and agrochemicals for example pesticidial, fungicidal and herbicidal [3]. Herein, we have developed a green, efficient and powerful protocol for the synthesis of 2,4,6-triarylpyridine derivatives by the reaction of arylaldehydes, acetophenonederivatives and ammonium acetate as nitrogen source. The reaction was performed in the presence of $Fe_3O_4@TiO_2@O_2PO_2(CH_2)NHSO_3H$as a nanomagnetic core-shell catalyst under mild and solvent free conditions (Figure 1). It is worthy to mention that the final step of the mechanistic pathway for the synthesis of target molecules has proceeded*via* an anomeric based oxidation mechanism.



R= H, 4-Me, 4-OMe, 4-F, 4-Br, 4-NO_2, 3-NO_2
R'= H, 4-Me, 4-Cl,

Figure1 : Synthesis of 2,4,6-triarylpyridine derivatives *via*an anomeric based oxidation mechanism

References

[1] V. Klimesova, M. Svoboda, K. Waisser, M. Pour and J. Kaustova, IL Farmac.4 (1999) 666.
[2] B.Y. Kim, J.B. Ahn, H.W. Lee, S.K. Kang, J.H. Lee, J.S. Shin, S.K. Ahn, C.I. Hong and S.S. Yoon, Eur. J. Med. Chem., 39 (2004) 433.
[3] M. A Zolfigol, M. Safaiee, F. Afsharnadery, N. Bahrami-Nejad, S. Baghery, S. Salehzadeh and F. Maleki, RSC Adv.,5 (2015) 100546.

One-Pot synthesis of 1*H*-pyrazolo[1,2-b] phthalazine-5,10-diones catalyzed by Fe_3O_4/Caffeine under solvent-free conditions

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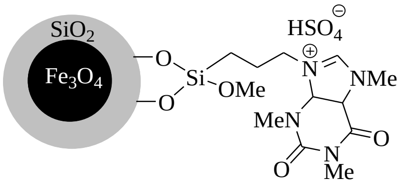
Multi-component reactions (MCRs) are considered to be important concepts of organic chemistry[1]. Heterocyclic compounds containing phthalazine moiety are important in medicinal field due to their pharmacological and biological activities. Pyrazolo[1,2]. Phthalazine-dione derivatives were reported as anti-inflammatory, analgesic, antihypoxic, and antipyretic agents [2]. Fe_3O_4 magnetite nanoparticles are well known as the most promising nanomaterials for biomedical and catalyst purposes. Easy separation, high thermal stability, high surface area and low toxicity for biological systems make these nanoparticles as an excellent catalyst in organic synthesis even in large scales [3]. Herein, we have reported an eco-friendly multicomponent reaction for the synthesis of Pyrazolo[1,2] phthalazine-dione derivatives using a recyclable Fe_3O_4/Caffeine hydrogen sulfate as a catalyst. The reaction proceeds by mixing the pthalhydrazide, malononitrile, aldehydes and the catalyst in 80 ^oC under solvent-free condition to afford the desired products in excellent yield.



catalyst

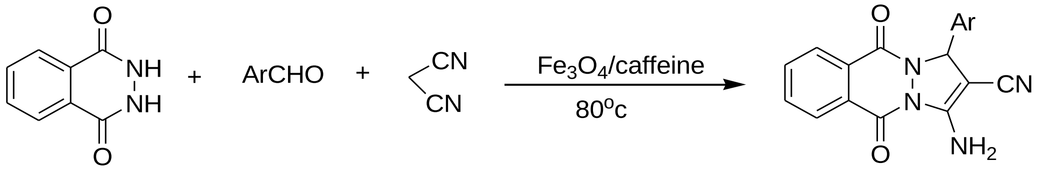


Figure 1. Scheme of the reaction

References
[1] C. O. Kappe, Curr. Opin. Chem. Biol., 2002, 6, 314.
[2] F.A. Assar, K.N. Zelenin, E.E. Lesiovskaya,. Chem. J,2002. 36,598.
[3] F. M. Moghaddam, S. E. Ayati, RSC Adv, 2015,5,3894.

A Computing Model for Gap Energy of Graphene Molecules

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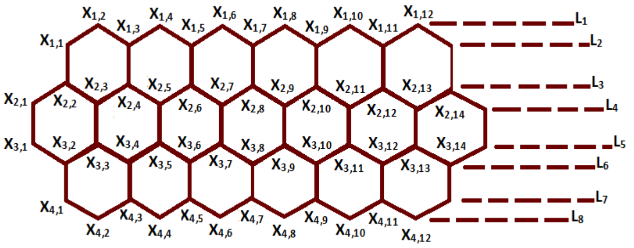
Topological indices are real numbers that are presented as graph parameters (e.g., the degree of vertices, distances, etc.) during studies conducted on the molecular graphs in chemistry and can describe some physical and chemical properties of molecules [1].In this article, the ISI index was calculated in the family Circumacenes and a suitable model was provided to predict the Gap Energy property through ISI index while considering some elements of this family [2]. Therefore, we first provided the ISI index for the family of Circumacenes (Figure 1) given by:

$$ISI(G) = \frac{61n + 53}{15} \qquad (1)$$

Where n is number of rings. Gap Energy of the Circumacenes family ($C_{8n}H_{2n+6}$), were calculated using Gaussian 09 software and the experimental data of references were compared with those mentioned in valid papers [3]. Figure 2 shows the changes in Gap Energy of Circumacenes family according to the ISI index. Therefore, Gap Energy (E_{gap}) of molecules $C_{8n}H_{2n+6}$ could be well predicted by the following relations:

$$E_{gap} = 0.0004(ISI)^2 - 0.0954(ISI) + 6.0339 \qquad (2)$$



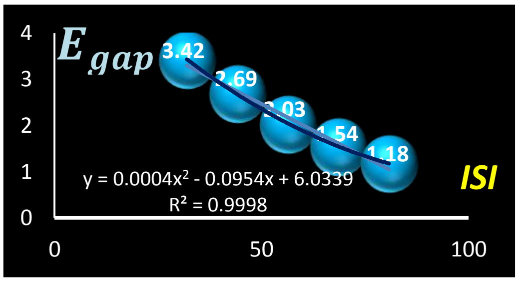


Figure1. Simple molecular graph of Circumacenes.

Figure2. E_{gap} of Circumacenes according to ISI index.

References

[1] N. Trinajstic, Chemical Graph Theory. 2nd Edition, CRC Press, Boca Raton (1992).
[2] Vukičević, D. and Gašperov, M. Croat. Chem. Acta., 83, 3, 243-260 (2010).
[3] G. Malloci, G. M ulas, G. Cappellini and C. Joblin, Chem. Phys. 340 (2007).

Reductive Cleavage of C=N Double Bond Using Transfer Hydrogenation Catalyzed by Ni Nanoparticles (NiNPs)

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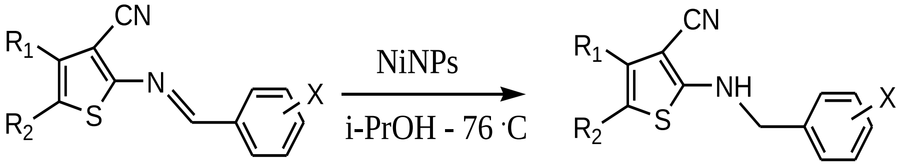
Hydrogen-transfer reactions are advantageous with respect to other reduction methods because of several reasons:(a) the hydrogen donor is easy to handle (no gas containmentor pressure vessels are necessary), cheap and environmentallyfriendly (e.g., isopropanol), (b) possible hazards are minimised,(c) the mild reaction conditions applied can afford enhanced selectivity, (d) catalytic asymmetric transfer hydrogenation can be applied in the presence of chiral ligands [1]. Recently, Alonso et al. have reported the hydrogen-transfer reduction of carbonyl compounds and olefins by nickel nanoparticles(NiNPs) as a catalyst [2]. They have also demonstrated that NiNPs catalyze the Wittig-type olefination of alcohols [3]. Herein, we wish to present a methodology for the reductive cleavage of C=N double bond in some imine molecules based on the catalytic transfer hydrogenation by NiNPs and 2-propanol as hydrogen donor.



References

[1] S. Gladiali, G. Mestroni.Transition Metals for Organic Synthesis, Eds.; Wiley-VCH:Weinheim2 (2004) Chapter 1-3.
[2] F. Alonso, P. Riente, M. Yus, Acc. Chem. Res 44 (2011) 379.
[3] F. Alonso, P. Riente, M. Yus.Eur. J. Org. Chem34 (2009) 6034.

2-Aminothiophen-3-carboxamide as Starting Materials in Synthesis of Thieno[2,3-d]pyrimidine derivatives

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Variety of substituted 2-aminothiophenes has been developed by Gewald and co-workers[1]. Application of 2-cyanoacetamide in Gewald reaction leads to formation of 2-aminothiophene-3-carboxamides (Gewald's amide) which are 1,5-dinucleophiles applied for synthesis of diverse thieno[2,3-d]pyrimidine derivatives. Previously, pharmacological studies of the thienopyrimidine derivatives extensively showed variety of activities such as antibacterial, antimicrobial, anxiolytic, and psychotropic[2]. The synthesis of the target compounds 2-amino-thiophene-3-carboxamides were prepared from cyclic ketones and sulfur with either ethyl cyanoacetate or cyanoacetamide, in the presence of morpholine via the Gewald thiophene synthesis. Treatment 2-aminothiophene-3-carboxamides with aromatic aldehydes and molecular iodine gave products 4[3].

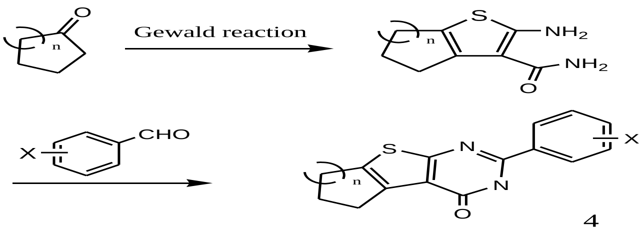

Figure 1. Scheme of the reaction

References

[1] K. Gewald, E. Schinke, H. Boettcher. Chem. Ber. 99 (1966) 94.
[2] S.G. Dzhavakhishivili, N.Y. Gorobets, B.V. Paponov, V.I. Musatov, S.M. Desenko. J. Heterocyclic Chem 45 (2008) 573.
[3] S.B. Kanawade, S.P. Patil, P.S. Nikam, S.A. Gangurde, M.N. Jachak. J. Heterocyclic Chem 49 (2012) 363.

Base and Catalyst-free preparation of Silyl ethers in Deep Eutectic Solvents (DESs)

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Alcohol and phenol moieties represent one of the most ubiquitous functional groups in nature. The formation of siliyl ether from a hydroxyl function can be utilized either to provide a volatile derivative for GC and GC-MS, or as a means of protection in synthesis. The popularity and extensive use of silyl ethers as protecting groups for alcohols come from their ease of formation, resistance to oxidation, good stability toward most non-acidic reagents, and easy deprotection to provide free alcohols [1,2]. Recently, deep eutectic solvents (DESs) have been emerged as new alternative renewable reaction media or catalyst for the development of environmentally benign organic transformations [3,4]. The properties of DESs are similar to that of conventional ionic liquids in terms of low vapour pressure and flammability. They often show low volatility, water-compatibility, non-toxicity, biocompatibility, bio-degradability and recyclability [5].

In conclusion we have described a simple and efficient method for the synthesis of silylethers using deep eutectic solvent as a dual catalyst and environmentally benign reaction medium.

$$ROH + R'_3SiCl \xrightarrow[rt]{DES} ROSiR'_3$$

R= alkyl and aryl

R'= Me, Et, t-BuMe$_2$

Figure 1. Scheme of the reaction

References

[1] Langer, S. H; Connell S; Wender I. J. Org. Chem, 1958, 23, 50.
[2] (a) Olah, G.A; Gupa, B.G.B; Narang, S.C; Malhotra, R. J. Org. Chem. 1979, 44, 4272.
[3] C. Rub, B. König, Green Chem. 2012, 14, 2969.
[4] Q.H. Zhang, K. De Oliveira Vigier, S. Royer, F. Jérôme, Chem. Soc. Rev. 2012, 41, 7108.
[5] Wang, P; Ma, F; Zang, Z; J. Mol Liq. 2014, 198, 259.

Experimental and MBO theoretical method studies of HBF_4 catalyst for 2-amino-4,6-diphenylnicotinonitrile preparation *via* an anomeric based oxidation

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After revealation and declaration of the anomeric effect (The Edward-Lemieux effect) by J.T. Edward in 1955 for the first time, much consideration was focused on the topic of anomeric effect for a generation of chemists and a great deal of research has been done in this area [1]. An experimental and computational studies in the synthesis of 2-amino-4,6-diphenylnicotinonitrile using HBF_4 as oxidizing promoter catalyst under mild and solvent free conditions were occurred. The suggested anomeric based oxidation mechanism was supported by experimental and theoretical evidences. The theoretical study shows that R- and S- isomers of intermediate have suitable structures for the aromatization through an anomeric based oxidation (ABO) in the final step of the mechanistic pathway (Figure 1).

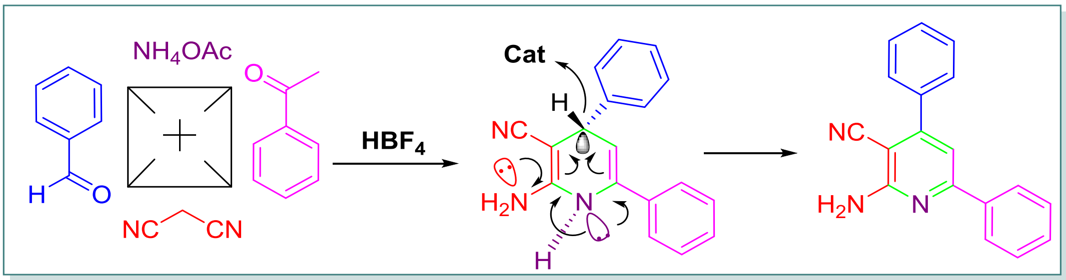

Figure 1: Synthesis of 2-amino-4,6-diphenylnicotinonitrile using HBF_4 as oxidizing promoter catalyst

References

[1] E. Juaristi, G. Cuevas, Tetrahedron.48 (1992) 5019.

Solvent-free reaction as green chemistry for the synthesis of substituted tetrahydrocarbazoles by oxalic acid catalyst.

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Thrust in the preparation of new heterocyclic molecules is increasing due to their proven significant biological activities[1]. The paramount importance of heterocycles such as indoles and their derivatives in natural product chemistry and pharmacology constantly drives the search for the new procedures for their construction and also for the preparation of variety of their derivatives to exploit their useful biological activities. Substituted tetrahydrocarbazoles belongs to the class of indole alkaloids that have been reported to possess an array of biological properties[2].In general the carbazoles synthesis is carried out by multistep Fisher reaction[3] which requires the usage of organic solvents with very meager product yields. Hence a simple and efficient method for the synthesis of these pharmaceutically important class of compounds is highly desirable precluding the usage of organic solvents. Initially Substituted phenyl Hydrazine's were used to optimize the reaction conditions such as different acids, solvents, and reaction temperature. Among, several Acids were tested, finally we found that oxalic acid catalyst and solvent-free conditions given excellent yields. Various substituted phenyl hydrazine have been reacted with cyclohexanone in the presence of oxalic acid catalyst at 60°C to obtain the final product in high yields,mild reaction condition and green synthesis in solvent-free condition.(Scheme1)

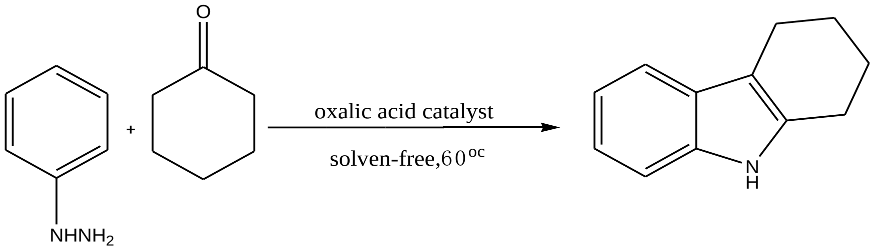

Figure1.synthesis substituted tetrahydrocarbazoles using oxalic acid catalyst.

References

[1] I.A.Danish,K.J.R.Prasad,Indian.J.Chem45B(2006)540.
[2] M.Akazome,T.Kondo,Y.Watanabe.J.Org.Chem59(1994)3372.
[3] S.W.Dantale,B.C.G.Soderberg.Tetrahedron59(2003)5507

An efficient, novel method for the synthesis of substituted tetrahydrocarbazoles using catalyzed sulfanilic acid in methanol solvent.

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The synthesis of substituted and condensed indoles has attracted considerable attention due to their importance as building blocks for many therapeutically useful materials and the wide ranging biological activity of both synthetic and naturally occurring derivatives[1]. Tetrahydrocarbazoles condensed with indole, furan, pyrimidine, pyrazoline, and thiophene,moieties have been known to processes wide spectrum biological activities.There has been many methods of synthesis which includes cyclization of diphenylhydrazone of cyclohexane-1,2-dione or 2-phenylhydrazono cyclohexanone via Fischer indole synthesis[2]. However the Bischler synthesis served as one of the simplest and attractive method to obtain tetra hydrocarbazoles and carbazoles by the condensation of α-halocyclohexanones with aromatic amines[3]. Improved method for the synthesis of tetrahydrocarbazoles by the Bischler reaction was also reported. Hence in this work, we report the application of sulfanilic acid as a catalyst for efficient One-Pot Fischer phenyl hydrazine whith cyclohexanone synthesis of tetrahydrocarbazoles and by using methanol solvent in summary, involving rapid mild and high yielding product with good purity and excellent yields and also for the simple synthesis of new hetrocycles via modifications of existing methodologies and their biological activities.(Figure1)

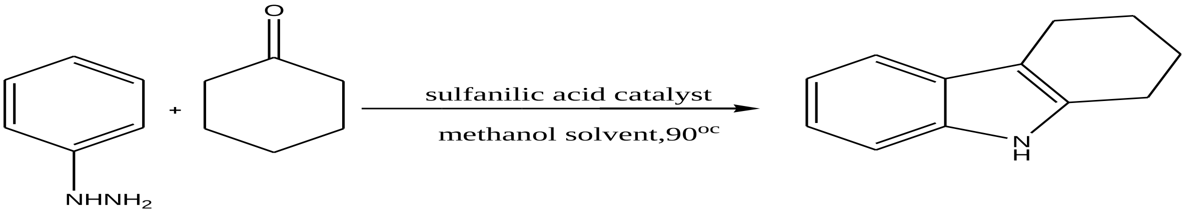

Figure1.synthesis substituted tetrahydrocarbazoles using sulfanilic acid catalyst.

Reference

[1] S.Neogi,A.Roy,D.Naskar,One-Pot Synthesis of New Substituted 1,2,3,4-Tetrahydrocarbazles Via Petasis Reaction.J.Comb. Chem12(2010)617-625.

[2] X.N.Li,R.Vince,Conformationally Restrained Carbazolone-Containing Diketo Acid as Inhibitors of Hiv Integrase,Bioorg.Med.Chem14(2006)2942-2955.

[3] F.Maertens,S.Toppet,G.J.Hoornaerrt,F.Comper Nolle,Incorporation of an Indole-Containing Diarylbutylamine Pharmacophore Into Furo[2,3-a]Carbazole Ring Systems,*Tetrahedron61(*2005) 1715-1722.

Synthesis of Calixarene-Polyglycerol Conjugates and their Self-Assembly toward Nano and Microtubes

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Calixarenes as macrocyclic oligomers with 4-20 phenol units represent two defined rims and a hydrophobic core. Since they show extensive host properties for small guest molecules, calixarenes are of high interest in supramolecularscience[1-2]. Due to the many unique properties, calixarenes are interesting candidates for the preparation of supramolecular polymers and nanostructures.In this work, new type of hyperbranched polymers and copolymers with calixarene core (HPCs) have been synthesized and characterized by different methods. Depend on the time and also composition of polymer, conjugated to calixareneself-assembly of HPCs in aqueous solutions lead to nano- and microtubes (Figure 1). Those supramolecular tubes are able to encapsulate anticancer drugs such as curcumin and therefore show a potential application for future cancer therapy.

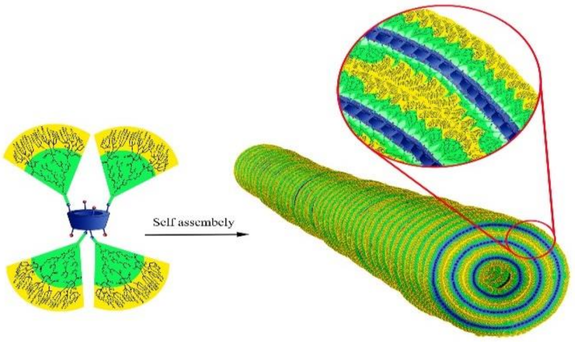

Figure 1. Self-assembly ofCalix-PG-PCA copolymer to produce vesicles and microtubes.

References

[1] C. D. Gutsche, D. R. Stewart, J. Am. Chem. Soc121(1999) 4136–4146.
[2] N. Basilio, V. Francisco, L. Garcia-Rio, J. Mol. Sci14(2013) 3140-3157.
[3] V. Villari, G. Gattuso, A. Notti, A. Pappalardo, N. Micali,J. Phys. Chem. B 116(2012)5537–5541.
[4] Y. Liu, H. Wang, H.-Y. Zhang , P. Liang,Chem Commun(2004) 2266–2267.

A One-Pot multicomponent reaction for facile synthesis of novel 2-((1H-Benzo[d]imidazol-2-ylamino) (Aryl) methylthio) Acetic acid by $La(NO_3)_3.6H_2O$ as an efficient catalyst

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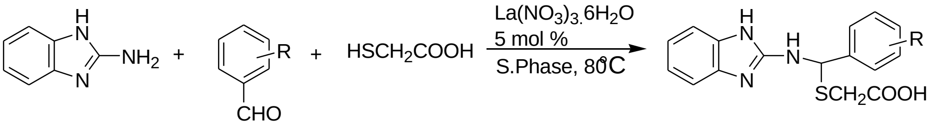
Heterocycles containing 2-aminobenzimidazole moiety exhibit a large variety of biological activities including inhibitors of HIV-1 reverse transcriptase, antitumor, anticancer, antihepatitis C virus (HCV), antiviral, antibacterial and antifungal activities [1]. Multicomponent reactions (MCRs) are known as one pot reaction in which three or more easily accessible compounds are combined in a single reaction vessel. MCRs also increase the efficiency by combining several operational steps without isolation of intermediates or changing the reaction conditions. Speed and short reaction time, diversity, efficiency and environmental amiability, easy work up, good to excellent yields are some of the major advantages of these reactions [2-3]. The conventional methods for the synthesis of Schiff's bases require long reaction times and use of organic solvents [4]. We report an eco-friendly One-Pot multicomponent reaction permitting the ''green synthesis'' of 2-(1H-Benzo-[d]imidazole-2-ylamino)(aryl)methylthio acetic acid analogs by stirring 2-aminobenzimidazole and thioglycolic acid with various aromatic aldehydes in solid state at 80˚C and in the presence of $La(NO_3)_3.6H_2O$ as an efficient homogeneous catalyst. This method is experimentally simple, clean, high yielding, green, and with reduced reaction times. The reaction followed by adding water and filtering the solid product at room temperature and drying them in vacuum condition.



R : H, 4-NO_2, 3-NO_2, 2-OH, 2-0H-5-Br, 4-Cl, 4-Br, 2-OMe, 4-OMe, 3,4-di OMe

Figure 1.Scheme of the reaction

All of the compounds were characterized by FT-IR and ^{1}H-NMR, ^{13}C-NMR and GC- Mass spectroscopy method.

References

[1] A. Mobinikhaledi, N. Foroughifar, M. Kalhor, Synthesis and Reactivity in Inorganic, Metal-Organic, and Nano-Metal Chemistry, 2009, 39, 509–511.

[2] A. Mobinikhaledi, N. Foroughifar, M. Kalhor,M. Mirabolfathy, J. Heterocyclic Chem., 2010, 47, 77-80.

[3] M. Kalhor, Org. Chem. Res., Vol. 1, No. 1, 59-65, September 2015.

[4] L.F. Tietze, A. Modi, Med. Res. Rev. 2000, 20, 304-322.

Zirconium tetrachloride as a highly efficient catalyst for the synthesis of xanthendione derivatives

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Xanthene and its derivatives are known as an important class of heterocyclic compounds, and widely used as lecodyes, pH-sensitive fluorescent materials for visualization of biomoleculesand are utilized in laser technologiesdue to their photochemical and photophysical properties.They possess diverse biological and therapeutic propertiessuch as anti-inflammatory, anti-viraland anti-bacterial activities. These compounds are being utilized antagonists for paralyzing action of zoxazolamineandphotodynamic therapy[1,2]. Xanthendiones are important builing blocks in a number of natural products and have been used as versatile synthons because of the inherent reactivity of the inbuilt pyranring. For the synthesis of xanthendionederivatives, zirconium tetrachloridewas added to dimedone and different aromatic aldehydes in at 60 °C under solvent freecondition (Figure1).

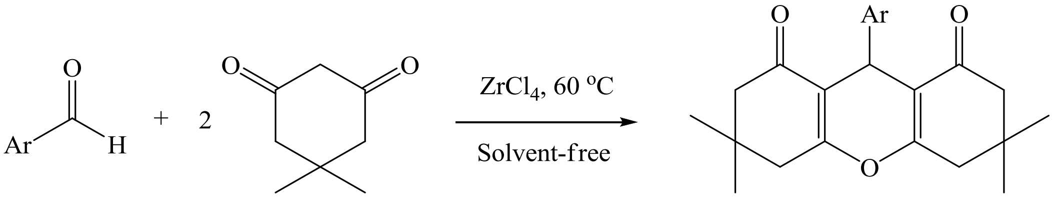

Figure 1. Synthesis of different xanthenediones by the $ZrCl_4$ catalyst

References

[1] A. Khazaei, M.A. Zolfigol, A.R. Moosavi-Zare, A. Zare, M. Khojasteh, Z. Asgari, V. Khakyzadeh, A. Khalafi-Nezhad, Organocatalyst tritylchloride efficiently promoted the solvent-free synthesis of 12-aryl-8,9,10,12 tetrahydrobenzo[*a*]-xanthen-11-ones by in situ formation of carbocationic system in neutral media, *Catal. Commun.*, 20, 2012, 54–57.

[2] M. Kidwai, A. Jahan, N.K. Mishra, A novel method for the synthesis of tetrahydrobenzo[a]-xanthen-11-one derivatives using cerium(III) chloride as a highly efficient catalyst, *C. R. Chimie*, 15, 2012, 324–330.

Computational Insights into the Structure and Electronic Characteristics of Guanabenz: An Antihypertensive Drug

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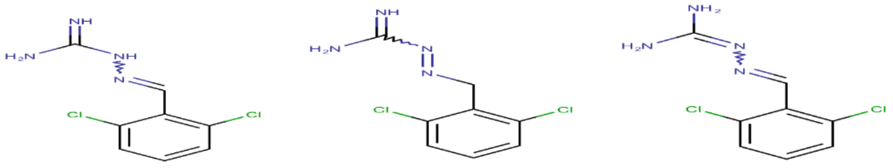
All of the tautomer structures of antihypertensive drug, Guanabenz, have been investigated using computational and molecular modeling methods. The conformational preferences of these tautomers also have been evaluated in order to see theise dominant form in both *vacuo* and aqueous solution. Furthermore, electronic analysis of this tautomers have been calculated to acquire significant insights into the nucleophilicity and electrophilicity, which plays an important role in drug-receptor interactions. The *Beck-3-Lee-Yang-Parr* (B3LYP) functional has been used with 6-31+G(d) basis set to acquire an initial orientation (approximated structure) of the drug. Subsequently, for the sake of accuracy the structures obtained have been re-optimized with the high-level 6-311+G(2d,p) basis set. The acquired results demonstrated that the first tautomer (depicted in figure 1) has the lowest energy, so it is the most stable form of this drug. Since the drug-receptor interactions relate with the structures and conformers of the drugs, so finding the right conformer and understanding its electronic analysis is crucial. In this study, the structures of Guanabenz, antihypertensive drug, has been sought to find its dominant structure.



1 2 3

Figure 1. Guanabenz tautomers

References

[1] Gadre, S. R.; Shirsat, R. N. Electrostatics of Atoms and Molecules; Universities Press: Hyderabad, India, (2000).

[2] Murray, J. S.; Politzer, P. The Use of Molecular Electrostatic Potential in Medicinal Chemistry. In Quantum Medicinal Chemistry.Wiley-VCH: New York, 2002; Vol. 17, pp 233-254.

[3] Becke, A. D. Density-Functional Thermochemistry. III. The Role of Exact Exchange. J. Chem. Phys. (1993), 98, 5648-5652.

Silver chloride as an efficient heterogeneous catalyst for the synthesis of different xanthenedione derivatives

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Xanthenediones are an important class of organic compounds that have been used as dyes, fluorescent material for visualization of biomolecules and in laser technologies due to their useful spectroscopic properties [1]. In the recent past, there is a renewed interest in the synthesis of this class of compounds as number of its applications increased, both in the field of medicinal chemistry and material science [2].

We have demonstrated the method to study an efficiency of silver chloride catalyst to synthesize xanthenedione derivatives from the reaction of dimedone and different aromatic aldehydes at 80 °C in solvent free conditions (Figure 1).

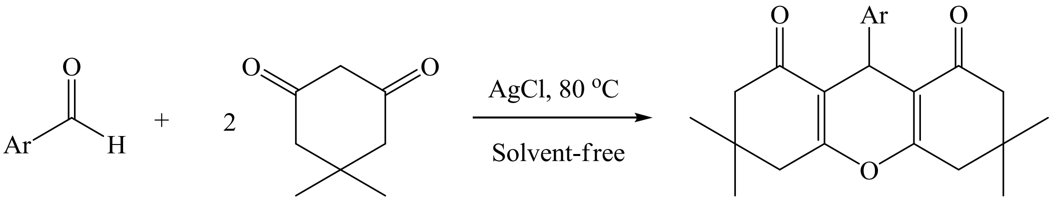

Figure 1. Synthesis of different xanthenediones by the AgCl catalyst

References

[1] J. Amaraj, J. P.Y. Palamari, P. Srinivasan, J. Mol. Catal. A. Chem. 2006, 248, 121.
[2] S. Hatakeyma, N. Ochi, H. Numata, S. Takano, J. Chem. Soc. Chem. Commun. 1988, 1202.

One-Pot three-component synthesis of pyrano [2,3-d] pyrimidines derivatives using silica-bonded ionic liquid as recyclable catalyst

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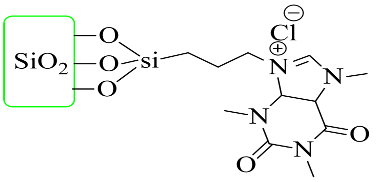
Multi-component reactions (MCRs) achieve significant role in combinatorial chemistry due to the ability to prepare target compounds with more efficiency and atomic economy by the reaction of three or more compounds together in a single step [1]. In the recent years, ionic liquids (ILs) have become powerful alternatives to the conventional molecular organic solvents due to their particular properties such as the ability to dissolve many organic and inorganic substances [2]. Among them, basic ILs have attracted unparalleled attention because, compared to the combination of an inorganic base and an IL, they have represented more advantages such as high catalytic efficiency and simple catalyst recycling for some base-catalyzed processes [3]. Pyrano[2,3- *d*]pyrimidines have received considerable attention owing to their wide range of diverse pharmacological activity. They are nicotinic acid receptor (NAR) agonists and show antitumor, hepatoprotective, antibronchitic, and anti-AIDS activity, among others [4]. Here in, we have reported that the synthesis of pyrano[2,3-*d*]pyrimidines derivatives in the presence of silicapropyl-caffeine chloride ([SP-Caff]Cl) as a recyclable solid basic catalyst from the reaction of an aldehyde, malononitrile, and *N*, *N′*-dimethyl barbituric acid in water at 60 ºC.



[Sipcaf]Cl

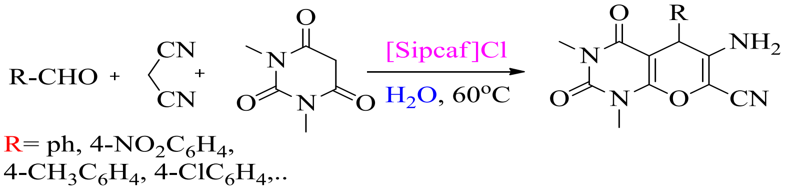


Figure 1.Scheme of the reaction

References

[1] M. A. Zolfigol, A. Khazaei, A. R. Moosavi-Zare, A. Zare, Z. Asgari, V. Khakyzadeh, A. Hasaninejad. Journal of Industrial and Engineering Chemistry 19 (2013) 721.
[2] P. Wasserscheid, T. Welton. Ionic Liquids in Synthesis, 2nd ed., Wiley-VCH, Weinheim 2007.
[3] H. Chen, D.R. Justes, R.G. Organic Letters 7 (2005) 3949.
[4] J. A. Valderrama, P. Colonelli, D. Vasquez, M. F. Gonzalez, J. A. Rodriguez, C. Theoduloz. Bioorganic & Medicinal Chemistry Letters 16 (2008) 10172.

A Novel Task-Specific Ionic liquid Supported on Magnetic Nanoparticles as a Highly Water-Dispersible Catalyst for Aqueous Phase Suzuki Reaction

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Palladium-catalyzed Suzuki cross-coupling reaction is one of the most important and versatile transformations in biaryl synthesis from both academic and industrial viewpoints [1]. Despite the considerable success achieved in the field of magnetically separable nanocatalysts [2], the application of these systems in water as a green solvent has still remained a great challenge in the Suzuki reaction in which water-soluble boronic acids fall off to the homocoupling reaction or hydrolytic deboronation as side reactions. Therefore, it seems that there is still much room to make novel magnetically recyclable catalysts displaying improved catalytic performance in pure water. Here, a novel ionic liquid functionalized magnetic nanoparticle was prepared by anchoring an imidazolium ionic liquid bearing triethylene glycol moieties on the surface of silica-coated iron oxide nanoparticles. The material proved to be an effective host for the immobilization of a Pd catalyst through a subsequent simple ion-exchange process giving a highly water dispersible, active and yet magnetically recoverable Pd catalyst in the Suzuki coupling reaction of challenging substrates such as heteroaryl halides and ortho-substituted aryl halides as well as aryl chlorides in water. Since the catalyst exhibited extremely low solubility in organic solvent, the recovered aqueous phase containing the catalyst can be simply and efficiently used in ten consecutive runs without significant decrease in activity and at the end of the process can be easily separated from the aqueous phase by applying an external magnetic field. This novel double-separation strategy with negligible leaching makes the material an eco-friendly and economical catalyst to perform this transformation.

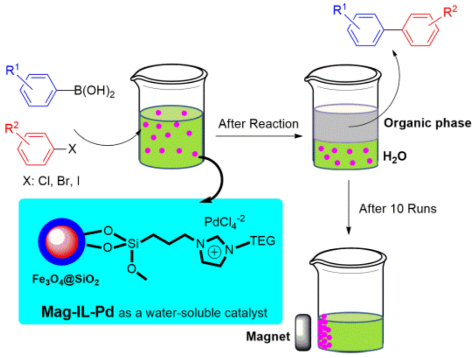

Figure 1. Scheme of the reaction

References

[1] A. Suzuki, Angew. Chem., Int. Ed. 50 (2011) 6723.
[2] B. Karimi, F. Mansouri, H.M. Mirzaei, ChemCatChem 7 (2015) 1736.

The use of Cu-Y Zeolite as efficient catalyst for the synthesis of Schiff bases containing benzimidazole moiety and facile conversion to some novel related oxaziridines

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Oxaziridine is interest because of an inherently weak N–O bond due to the strained ring that makes the molecule unusually highly reactive. These heterocycles have been shown to be promising reagents with potent anti-tumour, anti-malarial, and antifungal activities, and as effective analogues for penicillin. They are also widely used as reagents and intermediates in the preparation of biologically active molecules[1,2].Thecompoundscontaining a benzimidazole moiety attached to a heterocyclic system are important chemical classes as a result of their significant biological activities against several viruses such as HIV,herpes(HSV-1), influenza, and Epstein-Barr. Moreover, benzimidazole derivatives have been studied as anticancer and antiproliferativechemicals[3,4].Schiff bases derived from aromatic amines and aromatic aldehydes are also a very important class oforganic compounds because of their applications in many fields including biological,inorganic, andanalytical chemistry. Several synthetic methods have beenreported for thesynthesis of Schiff bases. However, most of them have limitations including longreactiontimes, need for a special catalyst, low yields, and extensive recrystallization.Cu-Y Zeoliteis easily prepared, stable for months, conveniently recovered by filtration and recyclable. It can be used in safe solvents and even without solvent, and thus fully comply with the Green Chemistry. In view of this report and also due to our attention in the synthesis of Schiff bases, we studied a simple and efficient synthetic method for the preparation of Schiff bases containing benzimidazolemoiety in the presence of Cu-Y zeolite as heterogeneous catalyst.In continuation,a novel series of 2-(1*H*-benzo[*d*]imidazol-2-yl)-3-aryl-1,2-oxaziridines were synthesized from the related Schiff basesby a simple method at room temperature and with good to excellent yields (Figure 1).

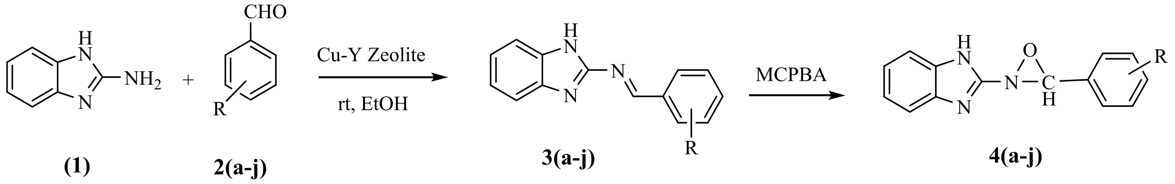

Figure1. Synthetic pathway of oxaziridines

References

[1] F. A. Davis, A. C. Sheppard, Tetrahedron, 45 (1989) 5703.

[2] Aubé, J. Chem. Soc. Rev. 26 (1997) 269.

[3] Z. Kazimierzcuk; D.Shugar, Nucleosides, 8(1989) 1379.

Diazotization and diazo coupling reactions using the triethyl ammonium acetate as a ionic liquid

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Aromatic diazonium salts have drawn increased attention as important intermediates in many organic reactions, especially for carbon-carbon bond formation via cross-coupling reactions[1,2]. Azo dyes are very important synthetic dyes which are used extensively in industry, So the topics of diazonium salts are interested to researchers. Since the coupling reactions are often carried out in strong acid conditions which are adverse to protection the environment. [3] Herein, we wish to report the diazo coupling reactions in ionic liquids wich don't have the disadvantages of using strong acid,[4] recently using of ionic liquids as solvents has been developed. Triethyl ammonium acetate is known as an ionic liquid wich has biological applications, so has been chosen as the reaction substrate to elimination the disadvantages of the old methods.[5,6]

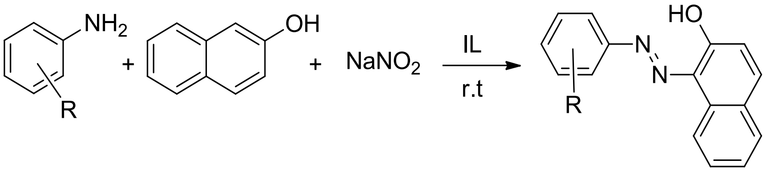

Figure 1.Scheme of the reaction

References

[1] T. I. Godovikova, O. A. Rakitin, L. I. Khmelnitskii, Russian Chemical Reviews 52 (1983) 440.
[2] S. Kotha, K. Lahiri, D. Kashinath, Tetrahedron 58 (2002) 9633.
[3] H. Zollinger, Color chemistry-syntheses, properties and applications of organic dyes and pigments. New York: VCH Publishers; 1987. pp. 92e102.
[4] A. Zarei, A. R. Hajipour, L. Khazdooz, B. F. Mirjalili, A. Najafi Chermahini, Dyes and Pigments, 81 (2009) 240.
[5] J. Hanusek, V. Machacek, A. Lycka, Dyes and Pigments, 73 (2007) 326.
[6] H. Valizadeh, A. Shomali, Dyes and Pigments, 92 (2012) 1138.

Synthesis of the new heterocyclic compounds based on xanthene

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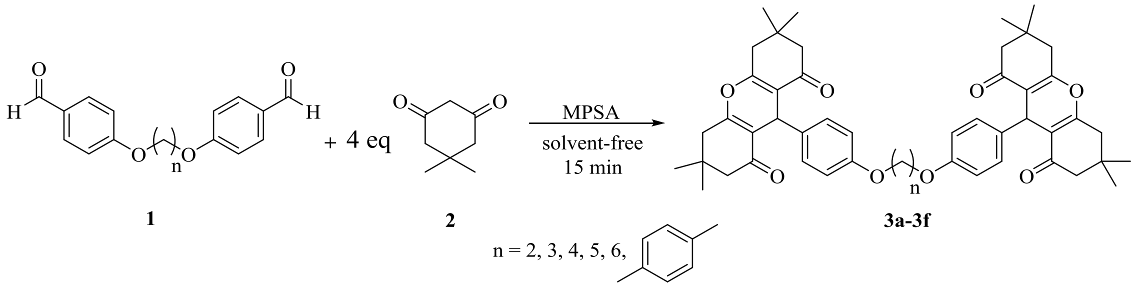
Xanthenes and benzoxanthenes are important classes of compounds that find use as dyes, fluorescent materials for visualization of biomolecules and in laser technologies due to their useful spectroscopic properties (1). Upon oxidation these compounds can be converted to corresponding xanthylium salts which are also useful as dyes and fluorescent materials (2). Xanthene based compounds have also been investigated for agricultural bactericide activity, photodynamic therapy, anti-inflammatory effects, antiviral activity and for antagonism of the paralyzing action of zoxazolamine (3). In our research, we introduce a novel catalytic route for preparation of new *bis*-xanthene derivatives (9,9'-((hexane-1,6-diylbis(oxy))bis(1,4-phenylene))bis(3,3,6,6-tetramethyl-3,4,5,6,7,9-hexahydro-1*H*-xanthene-1,8(2*H*)-dione)) by using from One-Pot five-compounds reaction between *bis*-aldehydes and dimedone under solvent-free conditions at 100 °C.



References

[1] A. Banerjee, A. K. Mukherjee. Stain technology 56 (1981) 83-85.
[2] M. Kamel, H. Shoeb. Tetrahedron 20 (1964) 491-495.
[3] G. Saint-Ruf, J-P. Poupelin. Naturwissenschaften 62 (1975) 584-585.

Fluoroalcohol-water two-phase systems: A new green solvent for organic synthesis

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A solvent is the common medium for running organic reactions due to, easy control over mass and heat transference, stabilization of transition states, and fast modification of reactivity (rate,selectivity, etc.). To avoid the drawbacks of conventional organic solvents, new media have been investigated, all of them having a certain number of advantages, as well as disadvantages [1]. Green solvents can be considered the ideal solvents, because they are verynontoxic, non flammable, biorenewable, and safe for humans and the environment. Various solvents have been proposed as a green solvents such as a water, fluoro alcohol,supercritical fluids, biomass-derived solvents, ionic liquids, and deep eutectic solvent [2]. In this work,fluoroalcohol-water system (two-phase) as a new green solvent has been described. The addition of organic reactants to aqueous solutions of fluoroalcohol (FA) leads to the formation of a two-phase system with one phase enriched in FAand the organic reactant and another largely aqueous phase. These systems were used as a reaction medium for isocyanide-based multicomponent reactions. Excellent yields were achieved in the presence of large amounts of water (10–20 % FA v/v). Surprisingly, the reactions performed in the two-phase systems outperformed those in pure (100%) FA or water. The presence of the aqueous phase offers advantages over single-phase reaction media in terms of driving the reaction and product recovery.

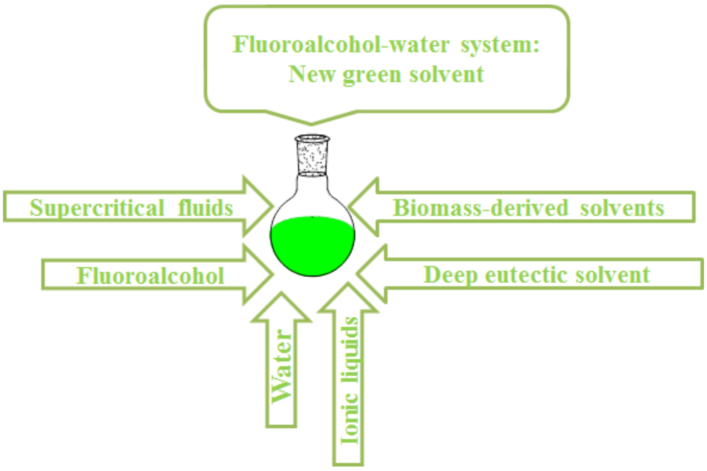

Figure 1. Green solvents

References

[1] N.Weisner, M.G. Khaledi, Green Chem. 18 (2016), 681.
[2] D.A. Alonso, A.Baeza, R. Chinchilla, G.Guillena, I.M. Pastor, D.J. Ramon,Eur. J. Org. Chem. 2016(2016), 612.

A Novel Double-Separation Strategy for Aqueous Phase Catalysis

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Development of efficient methods to complete recovery of supported catalysts is one of the important goals of "Green Catalysis". In this context, magnetic nanoparticles (MNPs) have gained a great deal of attention because of their easy separation from the reaction mixture [1]. Despite the substantial success achieved in the field of magnetically separable nanocatalysts, the application of these systems in pure water as reaction solvent remained a major challenge. Although MNPs display good dispersion in many solvents, in the case of using pure water as the reaction medium, the organic substrates often cannot favorably react at the catalytically active sites. Therefore, it seems that there is still much room to make novel magnetically recyclable catalysts displaying improved catalytic performance in pure water.

In this study, a novel imidazolium ionic liquid bearing triethylene glycol moiety was prepared and immobilized on the surface of silica-coated iron oxide nanoparticles. After introduction of Pd species through a subsequent ion-exchange process the material was found as a highly water dispersible, active and yet magnetically recoverable catalyst in some important organic transformations such as aerobic oxidation of alcohols, Ullmann homocoupling of chlorobenzene, transfer hydrogenation and direct reductive *N*-formylation of nitroarenes in water. Owing to the presence of hydrophilic ionic liquid on the surface, the catalyst showed highly stable dispersion in water and an extremely low affinity to the organic phase; thus providing the possibility of recovering the catalyst from the reaction mixture by using a simple and efficient double separation strategy (successive extraction/final magnetic separation) This novel double-separation strategy with negligible leaching makes the material an eco-friendly and economical catalyst to perform the organic transformation in pure water as a green solvent.

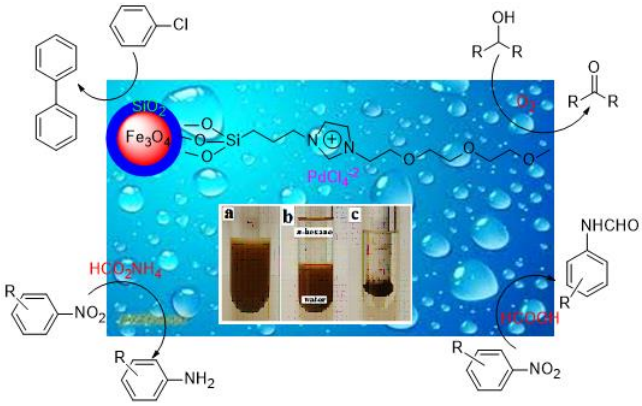

Figure 1.scheme of the reaction

References

[1] B. Karimi, F. Mansouri, H.M. Mirzaei, ChemCatChem 7 (2015) 1736.

Biosynthesis of Silver Nanoparticles by *Umbilicaria Americana*

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The synthesis of nanoparticles from biological processes is evolving a new era of research interests in nanotechnology (1-2). In this project, we aimed to develop a rapid ecofriendly method for the synthesis of silver nanoparticles using aqueous extract of *Umbilicaria Americana*. The synthesized nanoparticles were characterized using UV-Vis spectroscopy, FT-IR, x-ray diffraction (XRD), scanning electron microscopy (SEM). UV-vis spectroscopy derived spectrum demonstrated a peak of 420 nm which corresponds to the absorbance of silver nanoparticles. The results revealed that the aqueous extract of *U. Americana* is a clean, nontoxic and ecologically sound manner and very good bioreductant for the synthesis of silver nanoparticles.

References

[1] Rajendran Kumar, et al., SpectrochimicaActa Part A 90 (2012) 173–176

[2] Amit Kumar Mittal, et al., Biotechnology Advances 31 (2013) 346–356

The One-Pot synthesis of 14-aryl-14*H*-dibenzo[a,j]xanthenederivatives using nanoparticles of hydrogen sulfate ionic liquid immobilized on nanosilica

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The synthesis of xanthenes, especially benzoxanthenes has attracted interest due to their biological and pharmaceutical properties such as antiviral, antibacterial, and antiflammatory. Various methods are available for the construction of xanthenes and benzoxanthenes.A novel and efficient procedure for the synthesis of 14-aryl-14H-dibenzo[a,j] xanthenes1 through One-Pot condensation of β-naphtol with benzaldehyde derivatives in aqueous media catalyzed by nanoparticles of hydrogen sulfate ionic liquid immobilized on nanosilica is described. An important advantage of this catalyst is the ease of separating it from the reaction mixture, as well as the fact that it could be recycled a number of times; mild conditions, excellent yield and short reaction time are other advantages of this catalyst as efficient and novel method.All reactions were monitored by TLC, and spectroscopic techniques such as 1HNMR and FT-IR, have been used to identify the products.

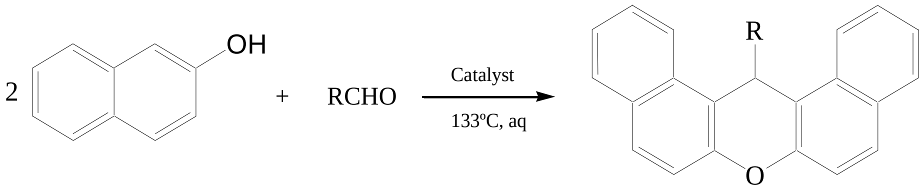

Figure1. Synthesis ofDibenzoxanthenes.

References

[1] Bacci, J.P.; Kearney, A.M.; van Vranken, D.L. Efficient two-step synthesis of 9-aryl-6-hydroxy-3H-xanthen-3-one fluorophores. *J. Org. Chem*. 2005, *70*, 9051–9053.

Biocompatible Catalysis of the Biginelli Reaction by Hybrid Magnetic Fe_3O_4-λ-carrageenan Nanoparticles

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A simple and efficient protocol has been developed for the synthesis of 3,4-dihydropyrimidin-2-ones using Fe_3O_4-λ-carrageenan Nanoparticles as magnetically recyclable, heterogeneous, environmentally benign catalysts under mild reaction conditions.[1] The yields of dihydropyrimidin-2 (1H)-ones (DHPMs) obtained via this novel protocol are significantly higher than those utilizing the conventional ethanol/HCl method.[2,3]

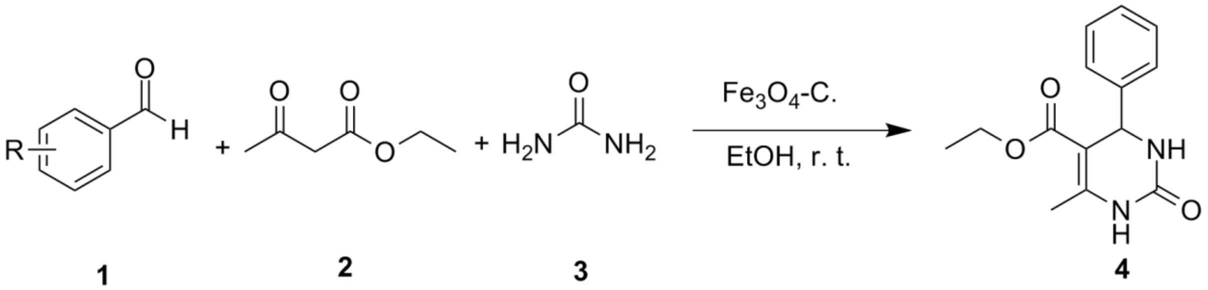

Figure 1. The Biginelli Reaction catalyzed by Fe_3O_4-λ-carrageenan nanoparticles.

References

[1] C. O. Kappe, Tetrahedron 1993, 49, 6937-6963.
[2] K. Oya, T. Tsuru, Y. Teramoto, Y. Nishio, Polymer Journal 45 (2013) 824.
[3] J. Necas, L. Bartosikova, Veterinarni Medicina 58 (2013) 187.

Chemical Composition of the Methanolic Extract From the Aerial Parts and Leaves oil of *Convolvulus schirazianus Boiss.* From Iran

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The genus *Convolvulus* comprises about 250 species, 45 are described in the flora of Iran, among which 19 are endemic [1]. Various species of this genus are used as food, food flavoring, natural medicine and also, decorative flowers. Some of the species showed diuretic, tranquillizing, hyploglycemic, antihemorrhagic, antioxidant, antitumor, antibacterial and antifungal activities [2].

The aerial parts of *Convolvulus schirazianus*, which is endemic to Iran, was collected from Bushehr, in May 2015. The methanolic extract of the air-dried aerial parts of *C.schirazianus* was obtained by percolation method. The leaf oil obtained by solvent free microwave extraction (SFME) method. Both oils were analyzed by GC and GC/MS.

17 Components were identified in the extract of *C. schirazianus* representing (86.3%) of the total components detected. The major component of methanolic extract was phenol, 2, 4-bis (1.1- dimethyl ethyl) (43.7%) followed by hexadecane (8.2%), tetradecane (6.1%) and tridecane (5.2 %).

Twenty- seven compounds in the leaf oil of *C. schirazianus*, which represented about 90.0% of the total oil were identified. The main compounds of the oil were occidentalol (17.2%), bicyclogermacrene (12.9%), elemol (10.2%) and germacrene B (10.0%). Other notable constituents were germacrene D (6.7%) and β- caryophyllene (6.3%). The oil of the plant was characterized by high amounts of sesquiterpenes (79.4%).The monoterpenes fraction was relatively small, representing (3.1%) of the total oil.

In the flower oil of *C. althaeides*, germacrene D (12.5%), T- cadinol (11.8%) and verbenone (6.9%) were the major components [3].

References

[1] V. Mozaffarian, A Dictionary of Iranian Plant Names, Farhang Moaser Publisher, Tehran, Iran (1996)144.

[2] H. Sadeghi- aliabadi, N. Ghasemi, M. Kohi, Research in Pharmaceutical Sciences 3 (2008) 31.

[3] M. Hassine, A. Zardi – Berguaoui, M. Znati, G. Flamini, Natural Product Research 28 (2014) 769.

Intrinsic Catalytic Activity of $ZnFe_2O_4$ Nanoparticles for Nucleation and Growth of Carbon Nanotubes and Nanofibers

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The simultaneous in situ growth of carbon nanofibers (CNFs) and nanotubes (CNTs) are accomplished in a single step by thermal gradient chemical vapor deposition using $ZnFe_2O_4$ as the catalyst and vaporized acetylene under atmospheric pressure at 750 ºC.The morphology of the grown product is analyzed by scanning electron microscopy (SEM). The length of CNFs can reach several micrometers and the diameters are about 20 nm.[1,2,3]

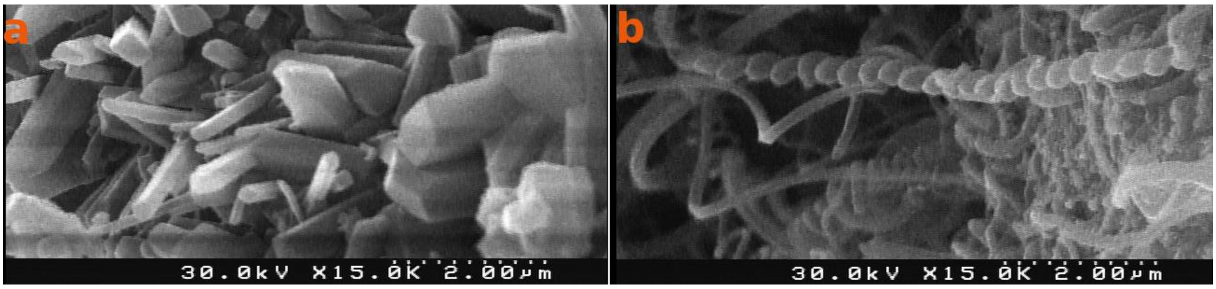

Figure 2.SEM images of (a) $ZnFe_2O_4$, (b) carbon nanotubes and nanofibers grown on $ZnFe_2O_4$ NPs

References

[1] K. P. De Jong, J. W. Geus, Catalysis Reviews 42 (2000) 481.
[2] E. Hammel, X. Tang, Carbon 42 (2004) 1153.
[3] M. L. Toebes, M. K. van der Lee, Journal of Physical Chemistry B 108 (2004) 11611.

Highly Thermo-Sensitive Biodegradable Shape Memory Polymers with Drug-Releasing Capabilities

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Smart materials can undergo conformational orphase changes in response to environmental signals.Shape-memory polymers (SMPs) are an emerging class ofsmart materialswhich have the ability to change shape on demand in response toan environmental stimulus.The development of these materials isoften motivated by the requirement of specific applicationssuch as smart textiles, aerospace industry and medicaldevices[1].Hydroxypropyl cellulose (HPC) is one of the most important nontoxic, biodegradable, and biocompatible cellulose derivatives, which was used in producing the smart materials.On the other hand, PCL isof particular interest in biomedical applications due to the biocompatibility, biodegradability, elasticity, sharp and tunable T*m*, and good mechanical properties. Thus, PCL-based SMPs have been widely studied and prepared[2]. In this study, we have developed novel biodegradable drug loaded SMPs with strongly temperature-sensitive shape recovery based on HPC and PCL.Drug loaded PCL filmswith shape memory properties were prepared by performing a reaction involving HPC-g-PCL graft copolymers with hexamethylenediissicyanate (HDI) as a cross-link agent in the presence of naproxen (as a model drug). A series of HPC-g-PCL having different chain lengths of graft PCL were prepared by ring opening polymerization of CL with HPCas initiator and$Sn(Oct)_2$ as catalyst in bulk condition.Subsequently, in order to obtain cross-linked drug loaded films, appropriate amount of naproxen (as a model drug) andHDI were added into the solution of purified prepolymer at the same time. After casting and drying the films, final products were characterized by FTIR, ^{1}H NMR DSC and XRD. The swelling ratio and gel content were determined to evaluate the cross-linking degree of grafted polymer networks. The shape-memory properties of the samples were investigated by cyclic thermomechanical tensile tests.The results of SMP behavior along with the degradation tests and in-vitro drug release studies on the drug loaded films approved that these polymers have great potential to be successfully used as biodegradable SMPs with good mechanical properties in controlled drug release.

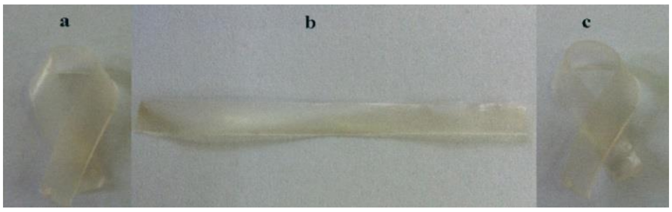

Figure 1. Thermally induced shape-memory behavior of HPC-g-PCL SMP films (a) Permanent shape (b) temporary shape fixed at25 °C (c) the recovered shape after 10 s immersion in waterat 42 °C.

References

[1] Q. Zhao, W. Zou, Y. Luo, and T. Xie. Science advances,2(2016)e1501297.
[2] M. Jahangiri, M.Bagheri, F. Farshi,andF. Abbasi.Journal of Polymer Research, 22(2015) 1.

Growth of Phosphore Doped Nanotubes by Chemical Vapor Deposition

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We wish to report the growth of P-doped carbon nanotubes (PCNT) using chemical vapor deposition (CVD). The nano-sized Fe/$CaCO_3$ was employed as catalyst, acetylene gas was introduced in CVD furnace as carbon resource and the solid triphenylephosphine powder was applied as phosphor resource. The structures, sizes and specifications of prepared PCNTs were determined and confirmed by field emission scanning electron microscopy. The presented method could be employed as an efficient, fast and low cost technique for preparation of PCNT.

Figure 3. FESEM image of PCNT by CVD

References

[1] S. Some, J. Kim, K. Lee, A. Kulkarni, Y. Yoon, S. Lee, T. Kim, H. Lee, Advanced. Material 24 (2012) 5481.
[2] A. L. M. Reddy, A. Srivastava, S. R. Gowda, H. Gullapalli, M. Dubey,P. M. Ajayan, ACS Nano 4 (2010) 6337.
[3] Z.-H. Sheng, H.-L. Gao, W.-J. Bao, F.-B. Wang, X.-H. Xia, Journal of Materials Chemistry 12 (2012) 390.

Eggshell-supported-Cu(I) metphormine complex: An efficient and green catalystfor synthesis of 1,2,3-triazolesin water

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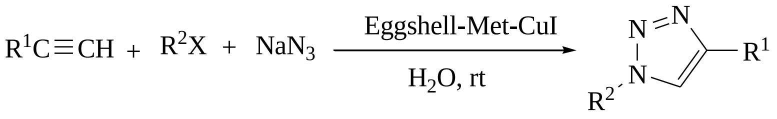
1,2,3-Triazoles are important nitrogen heterocyles which display many interesting properties including antibacterial, antiallergic, anti-HIV, GSK-3 inhibiting, and antineoplastic activities[1-3].

Copper-catalyzed azide-alkyne cycloaddition (CuAAC), also known as the “click reaction,” has become one of the most important reactions for the preparation of 1,2,3-triazoles. This important reaction is widely applied in organic synthesis, biochemistry, medicinal chemistry, and material science[4].

In this letter we wish to report an efficient, safe, and green One-Pot synthesis of 1,4-disubstituted 1,2,3-triazoles from benzyl chloride/alkyl halides, sodium azide, and alkynes catalyzed by eggshell-supported-Cu(I)Metphormine complex in water at room temperature.



R^1: Ph, CH_2, n-C_4H_9, n-C_7H_{15}

R^2: Bn, n-Bu, n-Pr

X: Cl, Br

Figure 1. Scheme of the reaction.

References

[1] Holla, B. S.; Mahalinga, M.; Karthikeyan, M. S.; Poojary, B.; Akberali, P. M.; Kumari, N. S. European Journal of Medicinal Chemistry*40* (2005) 1173.
[2] Buckle, D. R.; Rockell, C. J. M.; Smith, H.; Spicer, B. A. European Journal of Medicinal Chemistry. *29* (1986) 2262.
[3] Alvarez, R.; Velazquez, S.; San-Felix, A.; Aquaro, S.; De Clercq, E.; Perno, C. F.; Karlsson, A.; Balzarini, J.; Camarasa, M. JEuropean Journal of Medicinal Chemistry*37* (1994**)** 4194.
[4] Tornoe, C. W.; Christensen, C.; Meldal, M. The journal of organic chemistry.*67*(2002) 3057.

Extraction and isolationof chrysophanol from *Rheum ribes* roots and synthesis of its the silicon derivatives

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Rheum ribes, a perennial plant of polygonaceae family, is native to asia. It has been growing in Europe since the 16th century chrysophanol and other anthraqinone derivative were isolated from the root and areal parts of *Rheum ribes*. Chrysophanol and its derivatives are active compounds as anti-inflammatory, anti-bacterial and anti-viral. In this study triethylsilyl and tert-buthyldimethylsilyl derivative of chrysophanol were synthesized [1-2].

Alcohol readily reacts with compounds such as trimethylchlorosilane and base to turnedmethylsilylether, and in contact with water become primary alcohol andsilanol.

Silicon derivatives synthesis was carried out as follows, Dry Tetrahydrofuran (THF) was the solvent used in the synthesis and tri-ethyl amine (ET_3N) as a bases. The reaction mixture was refluxed for 24hours under argon gas at room temperature.The solvent was filtered and evaporated under reduced pressure.

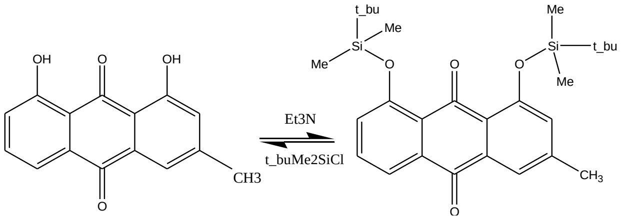

Figure1. Synthesis of tert butyl dimethyl silylchrysophanol.

The products were isolated by TLC and column chromatography techniques. The synthesised structures were confirmed by FT-IR, ^{1}HNMR.

References

[1] Mehmet zturk, FatmaAydogmus, Mehmet EminDuru, Antioxidant activity of stem and root extracts of Rhubarb (Rheum ribes) : An edible medicinal plant, food chemistry, 2007, 103. 623.

[2] Bazzas, B. S. F., Khajehkaramadin, M., &Shokooheizadeh, H. R., In vitrovantimicrobial activity of Rheum ribes extract obtained from various plant parts against clinical isolates of gram-negative patho gens. Iranian Jurnal of pharmaceutical Research, 2005, 2, 87.

Rheum ribes Extract Mediated, Synthesis of Metal Nanoparticals

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The plant mediated synthesis of metal nanoparticles has been studing since last two decates. The plant mediated nanoparticles show great biological activites in comparison with chemicaling synthesised particles. So, in this work, the *Rheum ribes*extract mediated synthesis of Silver nanoparticle was investigated [1-2]. By sampling the *Rheum ribes*extract its properties in isolation in a variety of combinations of metals for nanotechnology, tested and evaluated.In this research, silver nanoparticle with green synthesis without the use of any harmful chemicalsToxicsolvent was synthesized.The beginning aqueous extract of *Rheum ribes* to boiling method developed by smoothing filter paper was then 1 mM solution of silver nitrate at a ratio of 9: 1 water: silver nitrate was added to it at room temperature.After a few minutes the color change of the solution began to change color, which is indicative of the silver recovery.Biosynthesis of silver nanoparticles using UV-VIS spectrophotometer that absorption peak at a wavelength of about 420 nm is indicative of this.At first the solution was centrifuged at 15000 rpm then precipitate product that includenano particles was isolated. The synthesised nanoparticles were isolated by ultracentrifuge. Their size were identified by UV-Vis, SEM and Xray analysis.

References

[1] T.U. Santhoshkumar, A.A. Rahuman, G. rajakumar, S. Marimuthu, A. Bagavan, C. jayaseelan, A.A. Zahir, G. Elango, C. Kamaraj.Parasitol Res, 2001, 108, 693.
[2] BC Ardogan, H Baydar, S Kaya, M Demirci, D Ozbasar and UE Mum, Archives of Pharmacal Research, 2002, 25, 860.

Preparetion and use of *O*-(trimethylsilyl)hydroxylamine for N-Hydroxy-α-amino phosphonates Synthesis in Eutectic Solvent

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N-Hydroxyphthalimide derivatives are readily obtained in good yields by the reaction of phthalic anhydrides with hydroxylamine hydrochloride in the presence of triethylamine.

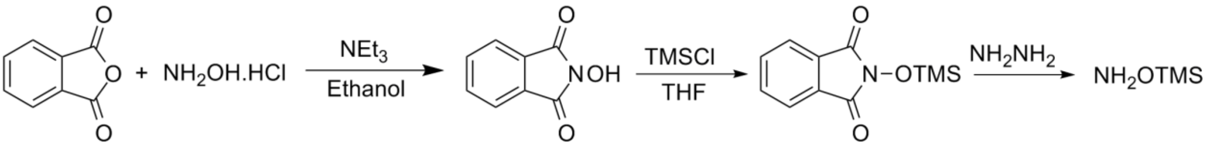

Figure 4. The *O*-(trimethylsilyl)hydroxylaminePreparation**.**

Benzaldehyde, *O*-(trimethylsilyl)hydroxylamine, dimethylphosphite were added. The same procedure is successfully applied to remaining compounds.

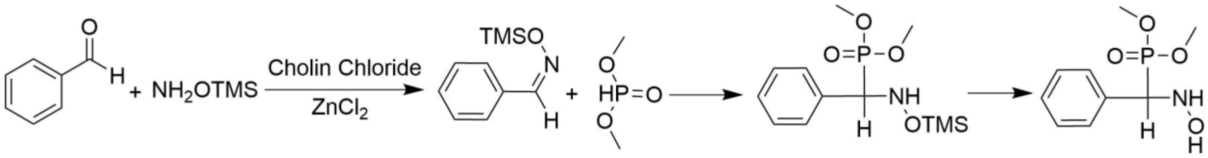

Figure 5.α-AminoPhosphonates Synthesis

References

[1] K. Sugamoto, Y. Matsushita, Y. Kameda, M. Suzuki, T. Matsui, Synthetic Communications 35 (2005) 67.

Chemical Composition of the Essentiol Oil from Leaves of *Ferula haussknechtiiWolff ex Rech.f.* Grown Wild in Iran

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The genus *Ferula* comprises perennial herbs distributed from the Mediterranian region to central Asia. Thirty species of genus *Ferula* are found in Iran among which 15 are endemic [1].Several species of the genus *Ferula* are used in traditional medicine, e. g. the roots of*F. persica* have been used in folk medicine to treat diabetes [2].There have been several studies of the genus *Ferula*. The reported compounds were mainly coumarins and sesquiterpene esters. Conversely only a few studies have reported the chemical composition of *Ferula* essential oils. Theaim of our studyisto identify the constituents of the essential oil of leaves of*F.haussknechtii*(syn:*Ferula physokoleo*Rech.f.) collected from Ilam, Iran, in July 2015. The oil was obtained by solvent free microwave extraction method and analyzed by GC and GC/MS.Forty-two components in the leaf oil of *F. haussknechtii*, which represented about (90.1%) of the total oil were identified.The leaf oil of the plant consisted of one monoterpene hydrocarbon (0.5%), three oxygenated monoterpenes (2.4%),fourteensesquiterpene hydrocarbons (26.4%), twelve oxygenated sesquiterpenes (32.8%), two diterpenoides (8.9%) and ten nonterpenoides compounds (19.1%). The major components of this oil were caryophyllene oxide (17.7%) and tetracosane (12.7%).Other notable constituents were neophytadiene (8.6%) and β- caryophyllene (12.7 %). As can be seen from the above information the leaf oil of *F. haussknechtii* was characterized by high amounts of sesquiterpenes (59.2%).

References

[1] V. Mozaffarian, A Dictionary of Iranian Plant Names, FarhangMoaser Publisher, Tehran, Iran (1996) 228.

[2] Y. Diab, R. Doimazon, J.M. Bessiere, Flavour and Fragrance Journal 16 (2001) 120.

An Afficient Approach To Catalyst-Free, One-Pot SynthesisOf New Fused Heterocyclic Compounds

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Heterocyclic compounds especially, nitrogen containing heterocycles are important natural and synthetic materials. Among them, the benzo[g]quinoline-5,10-dione derivatives exhibits excellent biological activities in pharmaceuticals. Some structures of naturally occurring benzo[g]quinoline-5,10-dione skeletonsare Cleistopholine(antimicrobial and anticancer), Phomazarin(cytotoxic), Jadomycins(antibacterial, anti-tumor, antiviral, cytotoxic, and Aurora-B kinase inhibitory activities)[1,2]. This work represents a successful synthesis of a new class of benzo[g]Imidazo[1,2-a]quinolinedione derivatives via four components reaction between 1,1- bis(methylthio)-2-nitroethylene, ethylene diamine, 2-hydroxy-1,4-naphthoquinone and aromatic aldehydes (Figure 1). This reaction proceeded without any catalyst. The ready availability of the startingmaterials, good yields of the products and the reaction's simplicity of the process are theother advantages of this method. All structures were confirmed by IR, MS, ^{1}H- and ^{13}C-NMR Spectra.

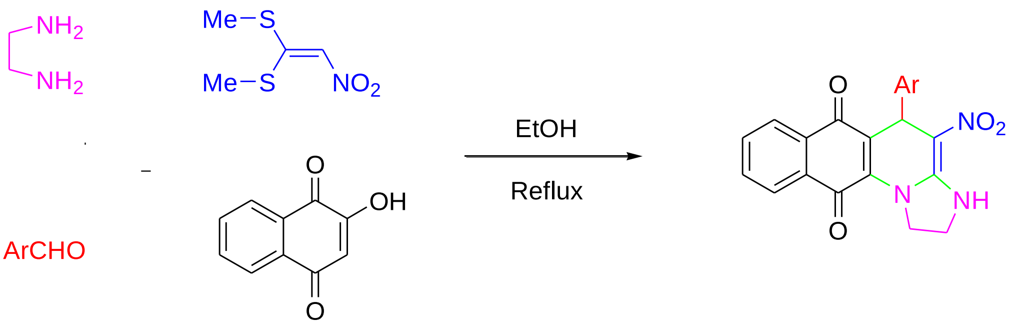

Figure 1. Preparazion of benzo[g]imidazo[1,2-a]quinolinedione derivatives

References

[1] L. R. Wen, Q. C. Sun, L. H. Zhang, M. Li.Organic &Biomolecular Chemistry 11 (2013)781-786.
[2] A. Alizadeh, R. Ghanbaripoura, S. W. Ng.HelveticaChimicaActa98 (2015).

A Novel Procedure For The Rapid and Stereoselective Synthesis of Fused Pyrimidines

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The chemistry of heterocyclic compounds is the most important in the discovery of new drugs. Among all heterocyclic compounds, pyrimidines areone of the most important heterocycles.various fused pyrimidines like purines, quinazolines, pyridopyrimidines, triazolopyrimidines, pyrazolopyrimidines, pyrimidoazepines, furopyrimidines and pyrrolopyrimidines were studied in the past decade and were found to possess remarkable biological andpharmacological activities including anticonvulsant, antibacterial, antifungal, antiviral andanticancer properties.[1,2]

In this paper we report a new, rapid procedure involving the addition reaction of ninhydrine and 4-amino-1,3-dimethyluracil, which leads to dihydroxyindenopyrrolo-pyrimidinesunder Reflux conditions in ethanol (Figure 1). This reaction proceeded without any catalyst in excellent yields and the other advantages of this work are simple work-up, no toxic byproducts and milder reaction conditions. All structures were confirmed by IR, MS, ^{1}H- and ^{13}C-NMR Spectra.

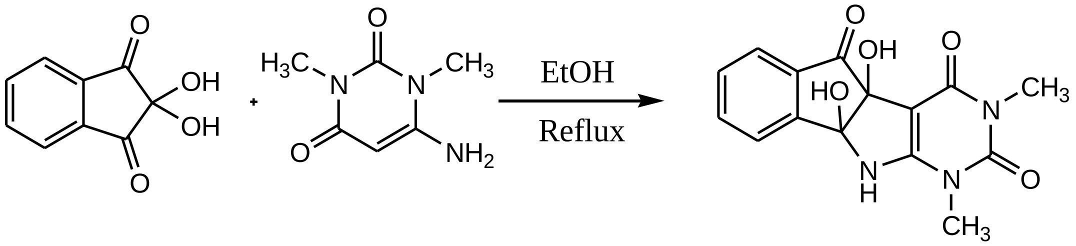

Figure 1. Generation of dihydroxyindenopyrrolopyrimidine.

References

[1] B. A. Mousa1, A. H. Bayoumi, M. M. Korraa1, M. G. Assy,S. A. El-Kalyoubi. International Journal of Organic Chemistry 5 (2015) 37-47.
[2] R. Singh, A. World Journal of Pharmacy and Pharmaceutical Sciences 3 (2014) 574-597.

Magnetic catalyst oxidative coupling of carboxylic acids with N,N,Dialkylformamides: an approach to the synthesis of amides

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Amides linkages (-CONH-) are widely found in nature and play significant role in biological systems and in the fields of pharmaceuticals,natural products and polymers[١].Although several attractive approaches involving a non-carboxylic acids rout have been reported over the last few decades[2].In recent years ,cross dehydrogenative couplings or oxidative cross-couplings have becameapowerful synthetic strategy in organic chemistry[3].Formamides are known to be useful as solvents and oxygen in metal-catalyzed organic reactions.In this most methods use for this purpose,homogeneous catalysts have been employed.Due to their improved efficacy,homogeneous catalysis has received more attention and consideration than heterogeneous approaches.In this study we examinedamid synthesis by oxidative coupling of carboxylic acids with N,N-dialkylformamides in the presence of cu(II)acetate complex immobilized on the surface of magnetic nanoparticles as an efficient and magnetically seperablecatalyst.The magnetic catalyst was charactrized by FT-IR, SEM, VSM, XRD, EDX.

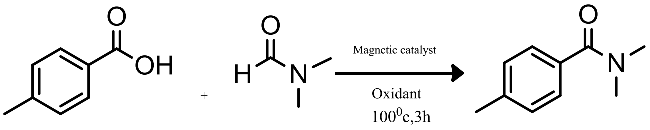

Figure 1. Scheme of the reaction.

References

[1] a)V.R.Pattabiraman,J.W.Bode,nature2011,480,471-479;b)T.Cupido,J.Spengeler,F.Albericio, Cure. Opin.Dru Discovery Dev. 2007, 10, 768-783.

[2] a) J.Zhang, M. Senthikkumar, S. C. Ghosh, S. H. Hong, An-gew.Chem.2010, 122, 6535; Angew. Chem. Int. Ed.2010, 49,6391-6395;b) L.Cao,J. Ding, M. ,Gao,Z. Wang, J. Li, A. Wu, Org. Lett. 2009, 11, 3813.

Acetic acid functionalized ionic liquid as an environmentally friendly catalyst for the synthesis of spiro[indeno[1,2-b]quinoxaline-11,4-pyran]-2′-amines

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Recently, ionic liquids have attracted significant attention as an alternative reaction medium for homogeneous catalysis. Acidic ionic liquids are of special importance because they possess simultaneously proton acidity and the characteristic properties of an ionic liquid [1-2].

The tetrahydrobenzo[b]pyrans are an important calss of the hetrocyclic compunds. these ring systems have long been the subject of numerous studies and successfuly applied as anti-coagulant, diuretic, spasmolytic, anti-cancer, and anti-anaphylactic [3]. Also, these compunds posess the Physical properties and they can be widely applied as photoactive materials [4]. On the other hand, indenoquinoxalines exhibit different pharmacological activity such as anti metabolism and anti tubercular [5].Herein, we have utilized acetic acid functionalized pyridinium salt (1- (carboxymethyl) pyridinium chloride {[cmpy]Cl}) as an efficient catalyst for the preparation of spiro[indeno[1,2-b]quinoxaline-11,4-pyran]-2′-amines(Figure 1).

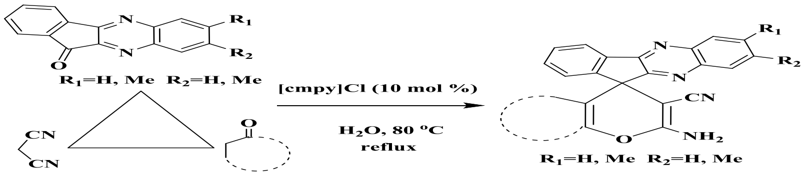

Figure 1: The Synthesis of spiro[indeno[1,2-b]quinoxaline-11,4-pyran]-2′-amine derivatives.

References

[1] Hallett, J. P., Welton T. Chem. Rev 111(2011) 3508.
[2] Wilkes, J. S. J. Mol. Catal. A: Chem 214(2004) 11.
[3] L. Bonsignore, G. Loy, D. Secci and A. Calignano, Eur. J. Med. Chem 28 (1993) 517.

Synthesis of 4,4´-(arylmethylene)-bis(3-methyl-1-phenyl-1*H*-pyrazol-5-ol) derivatives using Zirconium Dioxid

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Bis(pyrazolyl)methanes (BPMs) such as 4,4´-(arylmethylene)-bis(3-methyl-1-phenyl-1H-pyrazol-5-ol)s have a broad spectrum of approved biological activities[1], being used as anti-inflammatory[2], antipyretic [3], gastric secretion stimulatory[4], antidepressant[5], antibacterial[6], and anti-filarial agents. In this work, we have reported the synthesis of 4,4'-(arylmethylene)-bis(3-methyl-1-phenylpyrazol-5-ols) using ZrO_2 as reusable catalyst (**Figure1**). The promising points for the presented methodology are efficiency, generality, high yields, very short reaction times, cleaner reaction profile and simplicity.

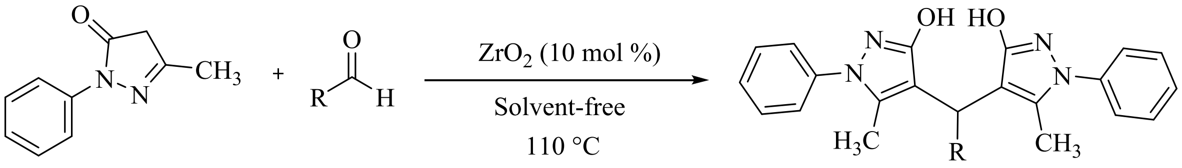

Figure 1. The Synthesis of 4,4´-(arylmethylene)-bis(3-methyl-1-phenyl-1H-pyrazol-5-ol) derivatives from of 1-phenyl-3-methyl-5-pyrazolone and aldehydes.

References

[1] S. Sugiura, S. Ohno, O. Ohtani, K. Izumi, T. Kitamikado, H. Asai, K. Kato, J. Med. Chem. 20 (1977) 80.
[2] L. C. Behr, R. Fusco, C. H. Jarboe, The Chemistry of Heterocyclic Compounds, Pyrazoles, Pyrazolines, Pyrazolidines, Indazoles and Condensed Rings, A. Weissberger (Ed.), Interscience Publishers, New York, 1967.
[3] C. E. Rosiere, M. I. Grossman, Science 113 (1951) 651.

Synthesis of novel hydrazone derivatives based on 4-methylcoumarin-7-yloxyacetohydrazide using catalytic amounts of zinc oxide nanoparticles

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Some novel hydrazone derivatives of the 4-methylcoumarin-7-yloxyacetohydrazide was synthesized. Different acetophenone and benzaldehyde derivatives and 4-methylcoumarin-7-yloxyacetohydrazide were used as starting materials. The reaction was performed under reflux condition using zinc oxide nanoparticles as catalyst and ethanol as solvent. The reactions were monitored by tlc technique. Purification of the products afford the desired hydrazones in good to excellent yield.IR and NMR techniques were used for characterizing the products.

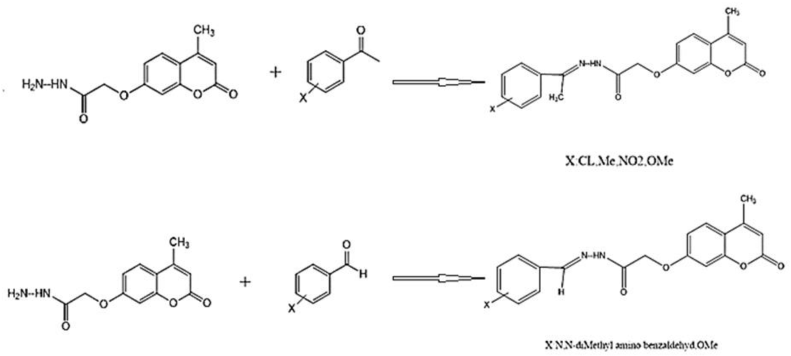

Figure 1. Scheme of the reaction.

Refernces

[1] Singh, H, Kapoor VK, Paul D. Progress in Medicinal Chemistry, 1979, 16, 35-149.
[2] Mohammed, A. E.; Mamdouh, S.; Taha, A. M.; Sharshira, E. M. Advances in Heterocyclic Chemistry, 1991, 52, 1-153.
[3] Petra , K. P.; Klimeš, Z. M. J. of Pharm. and Biomed. Anal. 2008, 47, 360-370.
[4] Mohareb, R. M.; Ho, J. Z.; Alfarouk, F. O. J of the Chin. Chem. Soc. 2007, 54, 10531066.

Di-Sulfonic Acid Imidazolium Chloroaluminate [Dsim]$AlCl_4$ as an efficient catalyst for the preparation of hexahydroquinoline derivatives

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Quinoline derivatives with a 1,4-dihydropyridine scaffold are promising structures because of their pharmacological properties.Hexahydroquinolines (HHQs) have used as anti-bacterial, anti-hypertensive, antimalarial, anti-inflammatory, antiasthamatic, and tyrosine kinase inhibiting agents [1,2]. Some methods and catalysts have been reported for the preparation of HHQs [3,4]. In this work, we have used di-Sulfonic acid imidazolium chloroaluminate[Dsim]$AlCl_4$as an efficient, heterogeneous, and reusable catalyst for the synthesis of hexahydroquinolines by the One-Pot multi-component condensation reaction of dimedone aryl aldehydes, (5,5-dimethylcyclohexane-1,3-dione), *β*-ketoesters and ammonium acetate under solvent-free conditions (Figure).

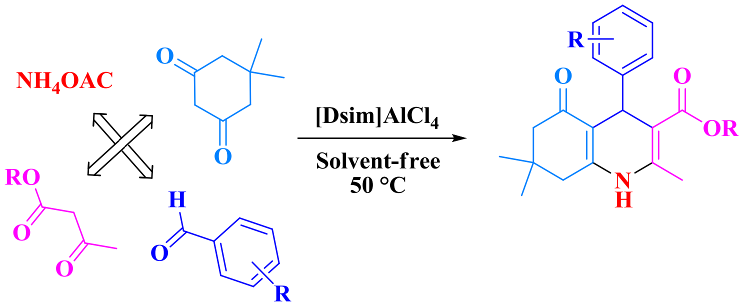

Figure 1. The One-Pot multi-component preparation of hexahydroquinoline derivatives catalyzed by [Dsim]$AlCl_4$.

References

[1] Y. L. Chen, K. C. Fang, J. Y. Sheu, S. L. Hsu, C. C. Tzeng, Journal of Medicinal Chemistry 44 (2001) 2374.
[2] G. Roma, M. D. Braccio, G. Grossi, M. Chia, European Journal of Medicinal Chemistry 35 (2000) 1021.
[3] X.-L. Zhang, S.-R. Sheng, X.-L.Liu, *ARKIVOC*, 13 (2007) 79.

Synthesis and characterization of new keto stabilized phosphorus ylide and its complexes with mercury(II) and study their antibacterial properties

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Phosphorus ylides are important reagents in organic chemistry, especially in the synthesis of naturally occurring products with biological and pharmacological activities.[1] Since its development the Wittig reaction has remained one of the primary routes utilized in synthetic organic chemistry for the construction of carbon-carbon double bonds.[2] The preparation and characterization of stabilized phosphorus ylides, and metal complexes incorporating in this type of ylides, has attracted much attention in recent years.[3] This work reports on thesynthesis and characterization of a new phosphonium salt and related phosphorus ylide of the type $R\text{-}COCH=PAr_3$ and also The reactions of phosphorus ylide $(PPh_3)_3PCHC(O)C_5H_4CN$ (Y1) with HgX_2 (X = I, Br and Cl) in equimolar ratios using methanol as a solvent. These reactions led to binuclear complexes. The IR, ^1H, ^{13}C and ^{31}P NMR technique have been useful for characterization of this complexes. The synthesized ligand and its mercury complexes were screened for their antibacterial activity with using agar disc diffusion method against bacterial species, six Gram negative and positive bacteria. The data showed that have metal complexes much antibacterial activity against bacteria tested.

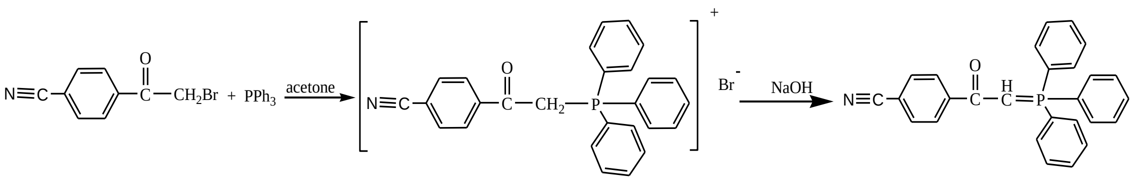

Figure 1. Synthesis of salt and ylide

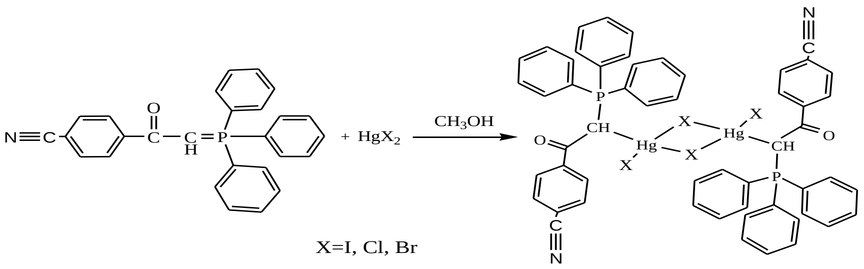

Figure 2. Synthesis of Hg(II) complexes

References

[1] Wittig, G. Science 1980, 210, 600.
[2] Maryanoff, B. E.; Reitz, A. B. Chem Rew. 1989, 89, 863
[3] O.I. Kolodiazhnyi, Tetrahedron 52 (1996) 1855;

New Palladium (II) complex containing α-keto Phosphonium ylide; Synthesis, characterization and highly efficient Suzuki-Miyaura cross-coupling reactions

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Palladium-catalyzed reactions, such as carbon-carbon bond formation, have attracted considerable interest [1]. Specifically, the Suzuki cross-coupling reaction of aryl halides with organoboron reagents is one of the most important and reliable methods for the construction of biaryls, which are present in a wide range of natural products, pharmaceuticals, agrochemicals and functional polymer materials [2]. In this abstract it is reported the synthesis of the complexes of the type $\{[(PPh_3)_3PCHC(O)C_5H_4CN]PdCl2\}$ derived from the reactions of the dichloro(1,5cyclooctadiene) palladium(II) with related phosphorus ylide $\{(PPh_3)_3PCHC(O)C_5H_4CN\}$ in dichloromethane. These compound have been characterized by, spectroscopic methods. Their structures consist of the ylidic carbon atom coordinated to the metal center. The coordination geometry around the Pd atoms in this complex can be defined as square planar[3]. The potential of this complex in catalyzing Suzuki-Miyaura cross-coupling of phenylboronic acid with several aryl halides has been done. Excellent yields of the desired products are obtained in competitive reaction time and under relatively mild conditions.

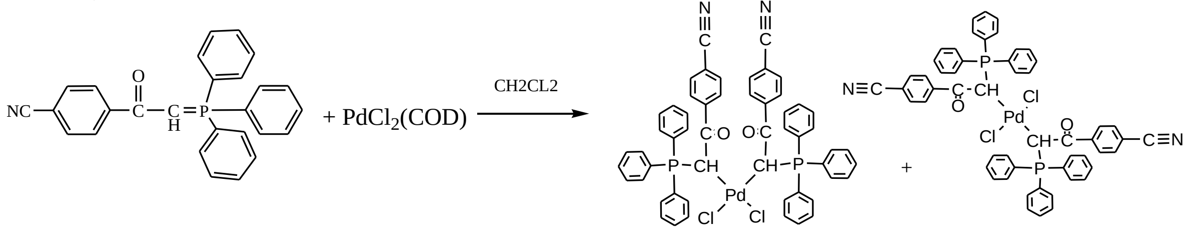

Figure 1. Synthesis of Pd(II) complexes

$$R^1\text{-}X + R^2\text{-}B(OR)_2 \text{ or } R^2\text{-}BR_2 \xrightarrow{\text{catalyst}} R^1\text{-}R^2$$

Figure 2. Suzuki-Miyaura cross-coupling

References

[1] F. Diederich de Meijer, Metal-Catalyzed Cross-Coupling Reactions, 2nd Edn., WileyVCH, Weinheim, Germany, Vols. 1 and 2 (2004).
[2] N. Miyaura, A. Suzuki. Chem. Rev., 95, 2457 (1995).
[3] S. Sabounchei . S. Samiee. D. Nematollahi. A. Naghipour. D. Morales-Morales. Inorganica Chimica Acta., 3973,3980 (2010).

LiOH.H_2O/Ultrasonic-Assisted Synthesis of Bisarylmethylidene Derivatives of 2,2-Dimethyl-1,3-Dioxan-5-one System

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There is a great current interest in ultrasound assisted organic synthesis because these environmentally benign chemical methodologies are strongly required in light of the paradigm shift to “Green Chemistry”. In continuation of our studies to develop environmentally friendly processes[1,2] here we report the synthesis of bis(arylmethylidene)dioxan-5-one derivativesunder environmentally clean LiOH.H_2O/ultrasonic conditions.Synthesis of these compounds could provide a pathway to access vicinal tricarbonyl derivatives[3] which are important as coupling reagents for biopolymer conjugates, antibiotic drugs, contact allergen, and photoconductive agents.The α,β diketoester and amide derivatives of these compounds have found synthetic applications in the preparation of various natural products or their precursors such as fusedring β-lactams, indole alkaloids, marine metabolites, enzyme inhibitors, and bioactive depsipeptides[4].The present approach has been carried out by the reaction of 2,2-dimethyl-1,3-dioxan-5-one and aromatic aldehydes in the presence of LiOH. H_2O and by using ultrasonic irradiation.A broad scope of aromatic aldehydes was successfully assessed in this work.We believe that the method surpasses limitations that other methodsmay encounter.

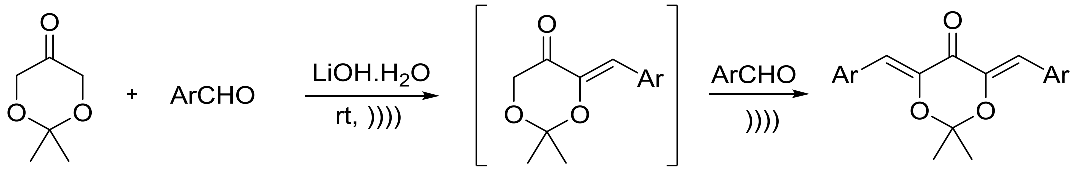

Figure 1. Scheme of the reaction.

References

[1] Mojtahedi, M. M.; Pourabdi, L.; Abaee, M. S.; Jami, H.; Dini, M.; Halvagar, M. R. Tetrahedron2016, 72, 1699.
[2] Mojtahedi, M. M.; Abaee, M. S.; Samianifard, M.; Shamloo, A.; Padyab, M.; Mesbah, A. W.; Harms, K. Ultrason. Sonochem.2013, 20, 924.
[3] Abaee, M. S.; Mojtahedi, M. M.; Hamidi, V.; Mesbah, A. W.; Massa, W.Synthesis2008, 2122.
[4] Wasserman, H. H.; Parr, J. Acc. Chem. Res. 2004, 37, 687.

Synthesis of 2,4,5-trisubstituted imidazolesover reusable $CoFe_2O_4$ nanoparticles: an efficient and green sonochemical process

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Magnetic nanocatalysts are the most interesting owing to their easy and efficient isolation and recovery with an external magnetic field, which avoids loss of the catalyst associated with filtration or centrifugation and they have been widely applied in organic reactions.[1,2]Among various magnetic nanoparticle, Cobalt ferrite ($CoFe_2O_4$) nanocrystals with spinel structure have attracted much attention because of their outstanding properties, their catalytic properties depend on the tetrahedral and octahedral sites of the spinel structure of ferrite nanoparticles. The imidazole ring is a fertile source of biologically important molecules. Compounds containing imidazole moiety have many pharmacological properties, and play important roles in biochemical processes. Among these imidazoles, 2,4,5-triarylimidazoles can be used as light-sensitive materials in photography and are known as inhibitors, fungicides and herbicides, plant growth regulators, and therapeutic agents.[3]Here in, we report a simple and high yielding protocol for the synthesis of trisubstituted imidazoles via One-Pot condensation of 1, 2-diketone with aldehyde and NH_4OAc using magnetic $CoFe_2O_4$ nanoparticles as an eco-friendly heterogeneous catalyst (Figure 1). This method is an efficient and rapid ultrasonic assisted route for the synthesis of wide variety of imidazoles.

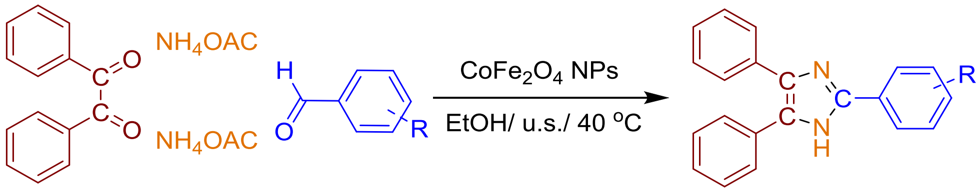

Figure 1. One-Pot synthesis of 2,4,5-trisubstituted imidazoles catalyzed by $CoFe_2O_4$ NPs under ultrasonic irradiation.

References

[1] M. B. Gawande, P. S. Branco and R. S. Varma, Chem. Soc. Rev. 42 (2013) 3371.
[2] H. Lu, E. L. Salabas and F. Schueth, Angew. Chem., Int. Ed. 46 **(**2007**)** 1222**.**
[3] S. Balalaie, A. Arabanian and M. S. Hashtroudi, Monatsh. Chem. 131**(**2000**)** 945**.**

Synthesis of Benzimidazoles from Acetophenone and O-Aryldiamines derivatives in the Presence of Copper Nanoparticles on Charcoal (Cu/C) as a Heterogeneous Catalyst

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Benzimidazoles play a vital role in the synthesis of pharmaceuticals. 2-Substituted benzimidazoles are used as anthelminticsinveterinary medicine and display significant anticancer, antiviral, antiallergic, antiulcer, and anticoagulant properties in human therapeutics[1]. Methods of benzimidazole synthesis include the condensationof *o*-aryldiamines and aldehyde in refluxing nitrobenzene, the condensation of o-aryldiamines with carboxylic acids or theirderivatives in the presence of strong acids such as polyphosphoricacid or mineral acids and the thermal or acid promoted cyclizationof N-(N-arylbenzimidoyl)-1,4-benzoquinoneimines. Directcondensation of o-aryldiamines and aldehydes is not a good syntheticreaction, as it is well known to yield a complex mixture of1,2-disubstituted benzimidazoles, thebisanil and dihydrobenzimidazoles. However, in this reaction, the addition of a transition metal, namely copper(II) acetate, mercury oxide,titanium dioxide,iron(III) nitrate, or leadtetracetate allows a partial selective synthesis of benzimidazoles. Unfortunately, many of these processes suffer some limitations, such as drastic reaction conditions, low yields, tedious work-upprocedures and co-occurrence of several side reactions[2]. On the other handDomino reactions, by virtue of their significant advantages, have emerged as a powerful tool in synthetic organicchemistry. Up to now, many novel domino reactionstrategies have been proposed. More recently, coupleddomino reactions, wherein two or more domino processesare sequentially assembled in the same reaction vessel, haveattracted much attention as a valuable synthetic approach.[3]

Inspired by the above graceful strategy,we herein developed a domino strategy to access benzimidazoles from acetophenone and o-aryldiamines derivatives in the presence of copper nanoparticles on charcoal (Cu/C) as a heterogeneous catalyst.

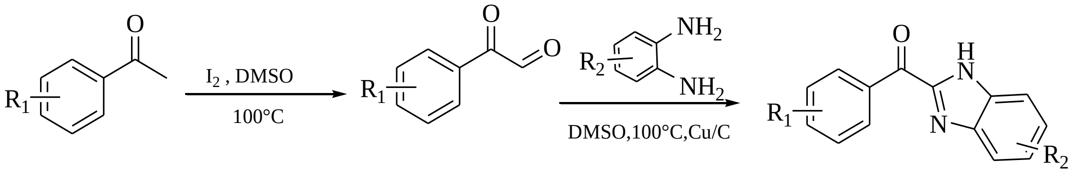

Figure 1. Scheme of the reaction.

References

[1] Bansal, Y.; Silakari, O, "The therapeutic journey of benzimidazolesa review", Bioorg.Med Chem.,20, 6208-6236(2012).
[2] Q. Sun, B. Yan, Bioorg,."Signal bead IR monitoring of a novel benzimidazolesyenthsis"Med. Chem. Lett, 8, 361(1998).
[3] Tietze, L. F.;Brasche, G. Gericke, K. Domino Reactions in Organic Synthesis; Wiley-VCH:Weinheim,Germany, 2006..

Synthesis of 2-(aryl) imidazo[1, 2-a] pyrimidin-3-ol from the reaction of arylglyoxal and 2-aminopyrimidine

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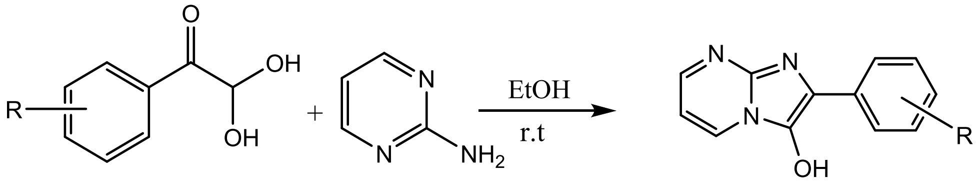
The reaction of some glyoxal derivatives with different2-amino heterocycles in acidic media has been investigatedpreviously by several authors. Thus, Goto et a1 havereported the synthesis of compounds 2-methyl-3,8a-dihydroimidazo[1,2-a]pyridin-3-oland 2,6-dimethylimidazo[1,2-a]pyrazin-3(7H)-one, themodel compounds of *Cypridinaluciferine*by heating2-aminopyridine or aminopyrazines with both phenylglyoxaland pyruvaldehyde in aqueous acid solution[1- 3].

In this work, we reported synthesis of 2-(aryl) imidazo[1, 2-a] pyrimidin-3-ol from arylglyoxal in the presence of 2- amino pyrimidine in ethanol solvent at room temperature. The products was identified by IR, ^{1}H-NMR, ^{13}C-NMR.



R= Cl, Me, naph, H, NO_2

Figure 1. Scheme of the reaction.

Reference

[1] For a preliminary communication see: Alcaide, B.; Pgrez-Ossorio, R.; Plumet, J.; Sierra, M. A. Tetrahedron Lett.1986, 27, 1627.
[2] (A) Inoue, S.; Sugiura, S.; Kakoi, H.; Goto, T. Tetrahedron Lett. 1969, 1609. (b) Sugiura, S.; Kakoi, H.; Inoue, S.; Goto, T. YakugakuZasshi, 1970, 90, 441.
[3] Yamaguchi, I. Biochem. J. 1975, 151, 9.

Application 3-sulfonic acid 1-imidazolopyridinium 2-hydrogen sulfate as an efficient catalyst for the synthesis of4,4′-(arylmethylene)bis(1 *H*-pyrazol-5-ols)

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Pyrazolones and bis-pyrazolones have been paid much attention for their various biological activities such as the selective COX-2 inhibitory, antitumor, and cytokine inhibitory ones [1]. In recent years, ionic liquids (ILs) have become powerful alternatives to the conventional molecular organic solvents due to their particular properties such as the ability to dissolve many organic and inorganic substances [2]. Herein we report the use of the mild, rapid, efficient, and environmentally friendly 3-sulfonic acid imidazolopyridinium hydrogen sulfate [Simp]HSO_4[3] catalyst for the preparation of 4,4'-(arylmethylene)-bis-(3-methyl-1-phenyl-1H-pyrazol-5-ols) from the solvent-free reaction of aromatic aldehydes with two equivalents of 5-methyl-2-phenyl-2,4-dihydro-3H-pyrazol-3-one in EtOH at room temperature.

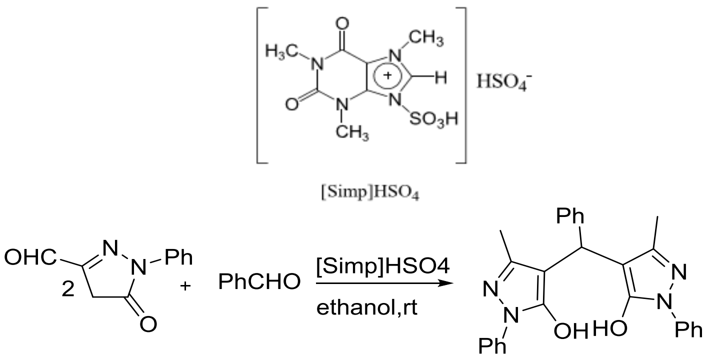

Figure 1. Scheme of the reaction.

References

[1] Mahajan, R. H. Havaldar, F. H.; Fernandes, P. S. J. Indian Chem. Soc. 1991, 68, 245.
[2] Olivier-Bourbigou. H, Magna, D. Morvan. L, Appl. Catal. A Gen.2010. 373. 1.
[3] Tayebee, R. Jomei, M. Maleki, B. Kargar Raz, M. Veisi, H. Bakherad, M. J. Mol. Liq. 2015, 206, 119.

Zirconium dioxide efficiently promoted the synthesis of pyrano[2,3-*c*] pyrazole derivatives under Solvent-free conditions

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Pyranopyrazoles are an important class of heterocyclic compounds. They have some applications such as pharmaceutical ingredients and biodegradable agrochemicals. At first, pyranopyrazole was synthesized by the reaction of 3-methyl-1-phenylpyrazolin-5-one with tetracyanoethylene [1]. Various pyrano[2,3-*c*] pyrazoleswere prepared by the different methods [2-5]. In this work, we have reported an efficient and eco-friendly four-component reaction condensation protocol in solvent less and neutral media using ZrO_2 as catalyst at 80°C (Figure1). Some advantages for the presented methodology are efficiency, generality, high yields, very short reaction times, cleaner reaction profile and simplicity.

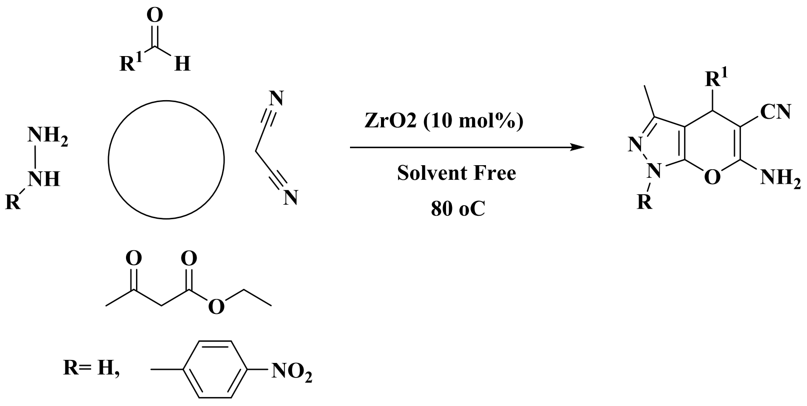

Figure 1. The condensation between aromatic aldehydes, malononitrile, ethyl acetoacetate and hydrazine hydrate or (4-nitrophenyl)hydrazine hydrate using ZrO_2.

References

[1] G. Vasuki, K. Kumaravel, Tetrahedron Lett. 49 (2008) 5636.
[2] Wamhoff, H.; Kroth, E.; Strauch, K. Synthesis. 11 (1993) 1129.
[3] Sharanin Yu, A.; Sharanina, L. G.; Puzanova, V. V. Zh. Org. Khim. 19 (1983) 2609.

Synthesis of 1*H*-Tetrazole Derivatives from Amine Compounds in the Presence of Copper Nanoparticles on Charcoal (Cu/C) as a Heterogeneous Catalyst

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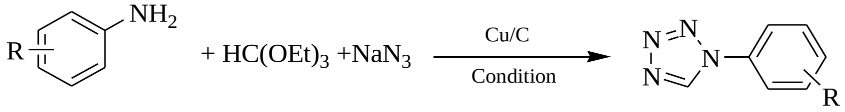
Tetrazoles are a class of nitrogen-rich heterocycles. They have received considerable attention due to their wide range of application such as HIV inhibitors, anti-bacterial, anti-fungal,anti-inflammatoryand explosive agents. They can also be used as isosteric replacements in drug design[1].Due to such interesting properties, improving of known methods for their synthesis is needed.The general method for the synthesis of 1-substituted 1H-tetrazole is via cyclization reaction of primary amine, triethylorthoformate and sodium azide in the presence of a catalyst. Some common catalysts which were used are Ytterbium triflate,Cobalt-Yttrium, $CuFe_2O_4$, acidic ionic liquid and acetic acid[2]. Unfortunately, these methods have one or more drawbacks, for instance, using expensive metal catalysts, utilization of toxic organic solvents and harsh reaction conditions[3].Thus, using an inexpensive, benign catalyst and mild reaction condition is an important challenge that must be solved.For a greener process, it is preferable to choose a catalyst with reusability.

An efficient and straightforward synthesis of 1H-tetrazoles is achieved from primary amines, triethylorthoformate and sodium azide, through consecutive condensation, C–N and N–N bond formations that catalyzed by a novel heterogeneous Cu/C catalyst with reusability. Interestingly, the Cu/C exhibited good catalytic activity for various amines derivatives.



R= X(Hallogen), Alkyl

Figure 1. Scheme of the reaction.

References

[1] Wittenberger s., "Recent developments in tetrazole chemistry", Org. prep. Proced. Int. 26(1994) 499.
[2] Naeimi H., Kiani F., Moradian M., "Facile and mild synthesis of 1-substituted-1H-1,2,3,4-tetrazoles catalyzed by methanesulfonic acid under solvent-free conditions", Iran. J.Catal. 3 (2013) 243.
[3] 3Darvish F., Khazraee S., "FeCl3 Catalyzed One Pot Synthesis of 1-Substituted 1H-1,2,3,4-Tetrazoles under Solvent-Free Conditions", Int. J. Org. Chem. 5 (2015) 75.

Copper Nanoparticles on Charcoal (Cu/C) as a Heterogeneous Catalyst for the One-Pot Synthesis of 2,4,5-Trisubstituted Imidazoles

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Imidazoles have been identified as important biologically active compounds with antibacterial, anti-inflammatory, and antihypertensive properties [1]. Among these, 2,4,5-trisubstituted imidazoles are of great interest because of their chemical and biological activity, making them common structures in numerous synthetic compounds, for example fungicides , herbicides , plant-growth regulators , and therapeutic agents [2].There are several methods reported in the literature for the synthesis of 2,4,5-triaryl-1H-imidazoles from benzil/benzoin, aldehydes and ammonium acetate using different catalyst such as $ZrCl_4$, $NiCl_2.6H_2O$ [3].Nevertheless, many of these approaches suffer from a long reaction time, low yield, acidic media, difficult work-up, expensive catalysts and excessive use of reagents and catalysts. Therefore, introducing a new green catalyst having good recyclability is of prime importance . An efficient and straight forward synthesis of 2,4,5-trisubstitutedimidazoles is achieved from benzil/benzoin, aldehydes and ammonium acetate, in optimized condition that catalyzed by a novel heterogeneous Cu/C catalyst .Interestingly, the Cu/C exhibited good catalytic activity for the 2,4,5-trisubstituted imidazoles. In this study we have reacted a range of aldehydes contain electron-donating and electron-withdrawing group to give desired products.

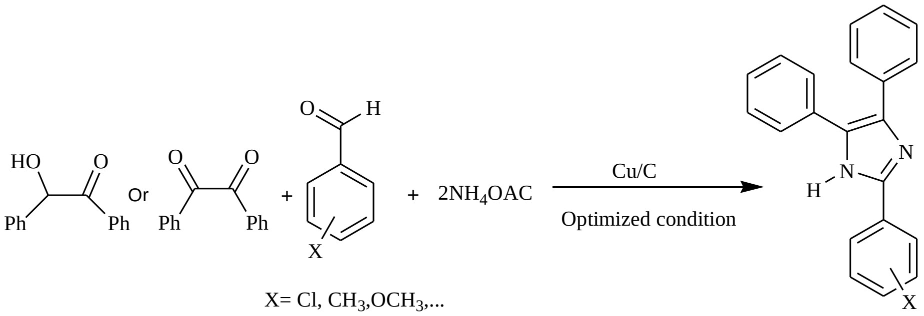

Figure 1. Scheme of the reaction.

References

[1] D. Biswanath, K.Jajula , A.K. Rathod , J. Paramesh.Monatsh Chem 144 (2013) 223–226.
[2] W. Liang , C. Chun.Monatsh Chem 140 (2009) 541–546.
[3] S.J. Ratnadeep, G.M. Priyanka, U.S. Mohammad, P.K. Rajesh, H.G Charansingh. Chinese Chemical Letters 21 (2010) 429–432.

Iron oxide nanoparticles loaded with Deferasirox in cancer therapy

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Two broad strategies in the use of iron chelators in cancer treatment have been explored. The first has been using iron chelators to reduce the iron level in cancer cells. Cancer cells typically require more iron than normal cells to mediate their generally rapid DNA synthesis and growth. Second, more recent strategy has been using chelators that help the redox cycling of iron to generate cytotoxic ROS within tumors. Both methods are currently being pursued. According to these strategies [1- 2], the present study has reported the synthesis of iron oxide-based deferasirox (DFX) loaded nanoparticles (Fe_3O_4@DFX). The surface of magnetic nanoparticles (MNPS) was first coated with (3-aminopropyl) trimethoxysilane (APTMS) and then was linked with deferasirox via the amidation reaction between–NH_2 and –COOH to form a well-dispersed surface functionalized biocompatible MNPs. The obtained nanoparticles were thoroughly characterized by various spectroscopic and microscopic methods such as SEM, FT-IR, TGA, and VSM. The cytotoxicity of Fe_3O_4@DFX was screened for antitumor activity against human breast cancer cells (MCF-7), human cervix epithelial carcinoma (HeLa), human colon cancer cell line (HT-29), human leukemia cell line (K-562), mouse neuroblastoma cell line (Neuro-2a), mouse fibroblast L-929 cell line and cisplatin used as a comparative standard by MTT assay. Obtained results provide experimental evidence that magnetite nanoparticles loaded with deferasirox induce apoptosis in cancer cell lines. Also, flow cytometry results confirm that investigated compound show a high population of apoptotic cell (69.3%) and 1.2-fold higher than cisplatin (58.1%) at the same concentration and could induce apoptosis of human leukemia cell line (K-562).

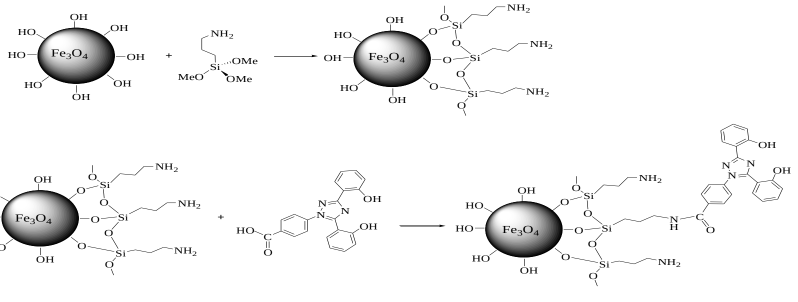

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Figure 1. Scheme of the reaction.

Refrences

[1] Salehi S, Saljooghi AS and Shiri A, (2016) Synthesis, characterization and in vitro anticancer evaluations of two novel derivatives of deferasirox iron chelator, European Journal of Pharmacology 781: 209–217.

[2] Salehi S, Saljooghi AS, Izadyar M, (2016) A theoretical study on the electronic structures and equilibrium constants evaluation of Deferasirox iron complexes, Computational Biology and Chemistry 64: 99–106.

Homopiperazine sulfamic acid functionalized mesoporous silica nanoparticles (MSNs-HPZ-SO_3H) as an efficient catalyst for One-Pot synthesis of 1-amidoalkyl-2-naphthols

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Multicomponent reactions (MCRs) are very elegant and efficient methods for accessing complex structures in a single synthetic operation from the corresponding building blocks. The MCRs are often carried out in One-Pot and designed to go through easy procedures with high atom-economy and great selectivity. This is mostly due to the generation of carbon–carbon and carbon heteroatom bonds.[1]One of these MCRs is the preparation of 1-amidoalkyl-2-naphthols.These compounds and their derivatives which bear 1, 3-amino oxygenated functional groups have attracted intense attention.Therefore, it is still desirable to seek novel catalysts that are recyclable and capable of performing the reaction under mild conditions. On the other hand, recently mesoporous materials have received much attention,particularly those that are designed based on functionalized mesoporous silicas because of their high surface area, tunable nanoscale pores, ease of the grafting of organic scaffolds to balance between the hydrophilic and hydrophobic character of the porous architecture, exciting host−guest chemistry, and supramolecular interaction to different extents with the reactant molecules. [2,3]Here in, we have developed a synthetic strategy for the design of a Homopiperazinesulfamic acid functionalized mesoporous silica (MSNs-HPZ-SO_3H) and its use as an efficient nanocatalyst for the One-Pot synthesis of 1-amidoalkyl-2-naphthols via three-component reaction of β-naphthol, aldehydes, and amides/urea, under solvent-free conditions.

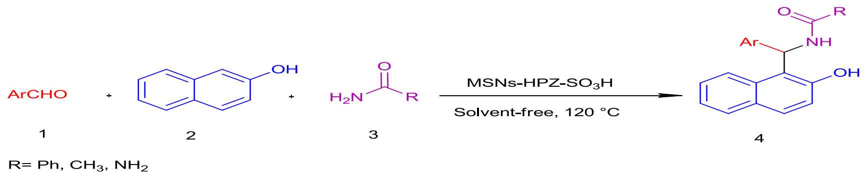

Figure 1.Synthesis of 1-amidoalkyl-2-naphthols in presence nanocatalyst.MSNs-HPZ-SO_3H

References

[1] A. Domling and I. Ugi, Angew. Chem., Int. Ed., 39 (2000) 3168.
[2] B. M. Pereza, J. Roeserb, A. Thomasb and P. Hesemanna, Appl. Organomet. Chem., 27 (2013) 290.
[3] E. Merino, E. V. Sesto, E. M. Maya, M. Iglesias, F. Sanchez and A. Corma, Chem. Mater., 25 (2013) 981.

Facile Route for Preparation of Benzil Derivatives via Oxidation of Alkenes under Metal-Free Conditions

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1,2-Diketones are one of the most important materials in biologically active molecules [1] and are very useful compounds that can easily be transformed into a variety of other chemicals, especially heterocyclic compounds [2]. Among 1, 2- diketones, benzil derivatives also exhibit bioactivities in antitumor applications [3]. Different methods for the synthesis of 1, 2-diketones have been developed, and they mostly involve the oxidation of varioustype of substrates such as olefins, methylene ketones, and alkynes. However, alkenes are cheaper and more easily available than others. Alternatively, the oxidation of stilbenes provides a simple and efficient route to benzil derivatives in both academia and industry.Also, to synthesis of benzil derivatives, a number of catalytic systems have been built in previous years, mainly containing transition metals such as Cu [4], Pd [5], Ru [6] and Mn [7] in combination with oxidants. Here, we report a new green, mild and efficient method for synthesis of benzil derivatives from stilbenes in the presence of TBAI and TBHP as an oxidant system withoutuse of any metal.

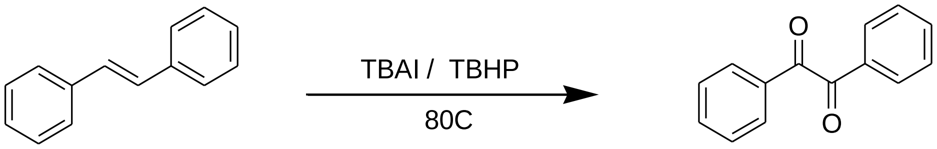

Figure 1. Scheme of the reaction.

References

[1] B. T. Ngadjui, S. F. Kouam, E. Dongo, G. W. F. Kapche, B. M. Abegaz, Phytochemistry 55 (2000) 915.
[2] S. E. Wolkenberg, D. D. Wisnoski, W. H. Leister, Y. Wang, Z. Zhao, C. W. Lindsley, Org. Lett. 6 (2004) 1453.
[3] Y. M. S. A. Al-kahraman, M. Yasinzai, G. S. Singh, Arch. Pharm. Res.35 (2012) 1009.

Synthesis, characterization and spectroscopy study of some transition metals complexes (Ni, Co, Zn, Cu) with 5-hydroxy-2-{[4-(hydroxymethyl)-1,2,3-triazol-1-yl]methyl}-4*H*-pyran-4-one as a new ligand

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Kojic acid is a bioactive γ-pyrone derivative. It is widely used in the pharmaceutical, food and agricultural industries [1]. Kojic acid forms stable complexes of metal kojates via the reaction of kojic acid with metal acetate salts such as tin, zinc, copper, nickel, cobalt, iron, manganese, chromium, gold, palladium, indium and aluminium [2]. In this study,Azidokojic acid was synthesized by the reaction of chlorokojic acid with sodium azide in 70% yield. 5-Hydroxy-2-{[4-(hydroxymethyl)-1,2,3-triazole-1-yl]methyl-4*H*-pyran-4-one as a new ligand was synthesized by the reaction of azidokojic acid with propargyl alcohol. Copper, zinc, cobalt and nickel complexes were synthesized by the reaction of new ligand with metal acetate.The chemical structure of the synthesized complexes was confirmed by FT-IR, UV-Vis and elemental analysis.

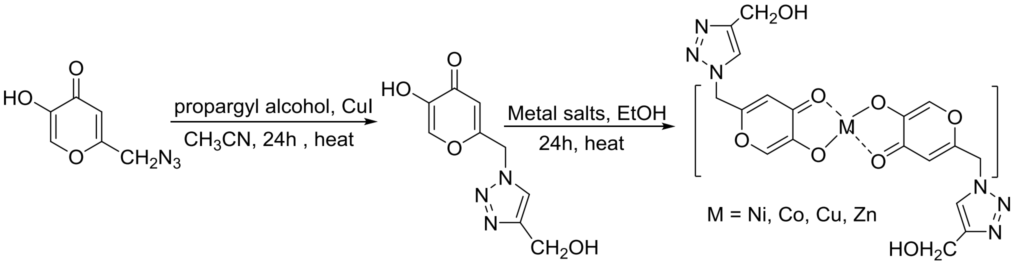

Figure 1. Preparation of metal complexes

References

[1] Hua Chen.Yu., Jung Lu.Pei., Hulme. Ch., Shaw. A.Y. Synthesis of kojic acid-derived copper-chelating apoptosis inducing agents, Medicinal Chemistry Research, 2012,22:995–1003.

[2] Aytemir, M. D., Karakaya, G. Kojic acid derivatives, Medicinal Chemistry and Drug Design2012,1-26.

Synthesis, characterization and catalytic activity of new Pd(II) complex containing∝-keto stabilized phosphonium ylide in green Mizoroki–Heck reaction protocol

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Palladium-catalyzed Heck reaction is one of the most important C-C bond forming reactions for synthesis of drugs, fine chemicals, and natural products in laboratory as well as industrial scales [1].The utility of metalated phosphonium ylides in synthetic chemistry has been well documentedMizoroki-Heck cross-coupling reaction catalyzed by palladium complex containing a ligand (usually a phosphane) is one of the most important and reliable methods for the construction of biaryls, which are present in a wide range of natural products, pharmaceuticals and functional polymer material is the most commonly used catalytic system for the Mizoroki-Heck cross-coupling reaction [2]. In view of the economy and environmental aspects, the use of cheaper ligands such as phosphonium ylides instead of bis-phosphonium ylides as catalyst precursor and water as solvent provides another attractive route. Herein, we report the synthesis, characterization and application of new Pd(ll) complex ((*p*-tolyl)$_3$P=CHCOC$_6$H$_4$(*p*-CN)) toward the Mizoroki-Heck cross-coupling reaction in aqueous media (Figure.1). Reaction of a-keto stabilized phosphonium ylides ((*p*-tolyl)$_3$P=CHCOC$_6$H$_4$(*p*-CN)) with PdCL$_2$ (COD) in 2:1 ratios leads to mono nuclear products of the type Characterization of the complex by IR, ^{31}P, ^{1} H and ^{13}CNMR spectroscopy confirmed coordination of the ylide to the metal through the carbon atom.

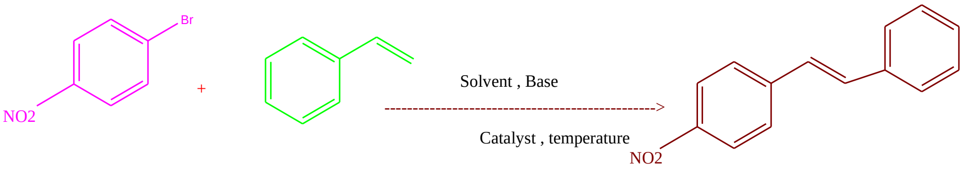

Figure.1.The Mizoroki-Heck Cross-Coupling reaction

References

[1] F. Diederich de Meijer, Metal-Catalyzed Cross-Coupling Reactions, 2nd Edn., WileyVCH, Weinheim, Germany, Vols. 2004.
[2] S.J.Sabounchei, M. Ahmadi, Inorganica Chimica Acta 2013, 405, 15.

Synthesis and in-vitro evaluation of smart nanogel for cisplatin delivery

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Cisplatin, cis-diamminedichloroplatinum(II) (CDDP), is a chemotherapy drug used in the treatment of solid tumours; but it showes significant dose-related sideeffects such as nephrotoxicity, neurotoxicity, nausea and vomiting. In order to maintain the efficacy and reduce the undesired disadvantages of cisplatin, Nanoparticle-based drug delivery systems were designed[1].Among the various drug nanocarriers , synthetic polymer nanoparticles have devoted more attention for reason of their excellent properties including biocompatibility and biodegradability particularly easy chemical modification or surface functionalization. A large number of these nanoparticles can respond to various stimulus such as temperature, magnetic, light, PH, enzymes, glucose and etc.These are termed as ‘smart’or ‘intelligent’. Introducing stimulus-responsive property to synthetic polymer nanoparticles can led to better therapeutic applications[2].In the present study, A dual-responsive nanogel, poly(*N*-isopropylacrylamide-*co*-*N*,*N*-(dimethylamino)ethyl methacrylate) P(NIPAAM-*co*-DMA) containing NIPAAM as thermoresponsive monomer and DMA as PH-responsive monomer and methylene-bis-acrylamide as cross linking agent, was synthesized by emulsion polymerization(Figure1). Cisplatin was loaded into the nanogel, by the swelling method. Properties of this nanogel such as size, swelling ratio, drug loading efficiency, and drug release kinetics were evaluated in vitro for controlled drug delivery in different temperature and PH conditions. Nanogelshowed significantly higher cisplatin release at 42°C compared to 37°C and at PH5.7 compared to PH7.4, demonstrating its temperature and PH sensitivity respectively.

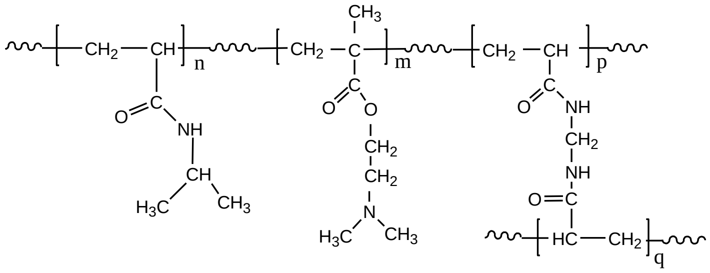

Figure 1. P(NIPAAM-*co*-DMA) nanogel

References

[1] X. Li, R. Li, X. Qian,. Pharm. Biopharm. 70 (2008) 726.
[2] Gao GH, Li Y, Lee DS. J Control Release 4 (2013) 169.

Composite Scaffolds Based on Electrospun Nanofibers of Alginate for Tissue Engineering Application

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Electrospun nanofibers from biomaterials have been widely used in regenerative medicine, including tissue engineering applications. Nanofiber matrices have become attractive due to their large surface area, high porosity, controlled mechanical properties, and their ability to interact with cells in a manner which mimics the natural ECMs [1]. Within this class of biomaterials, alginate, a polysaccharide derived from brown algae, exhibits excellent biocompatibility that bears structural resemblance to glycosaminoglycan, one of the major components of ECMs in human tissue. But the utilization of electrospun scaffolds of alginate is strongly limited by its high solubility in aqueous environments and by the difficulty to adjust its degradation dynamics. To overcome these drawbacks, modification of alginate nanofibers with other biopolymers and inorganic materials were developed [2, 3].

Composite nanofibers scaffolds based on alginate with chitosan, gelatin and poly (vinyl alcohol) incorporated with inorganic materials such as hydroxyapatite and montmorillonite were prepared via electrospinning method with different ratio of polymers and fillers.The scaffolds were characterized by scanning electron microscopy (SEM), X-ray diffraction (XRD), Fourier transform infrared (FTIR), mechanical measurement and cell-scaffold interaction study.The results exhibited improvement in stability, degradation rate, mechanical properties and cell-scaffold behaviors of composite scaffolds compared to pure electrospun alginate which is useful in tissue engineering (TE) applications. This developing field aims to regenerate damaged tissues by combining cells from the body with porous biomaterials, which act as templates, to guide the growth of new tissues.

References

[1] K.Y. Lee, L. Jeong, Y.O. Kang, S.J. Lee, W.H. Park. Advanced Drug Delivery Reviews 61 (2009) 1020.
[2] Y. Luo, A. Lode, C. Wu, J. Chang, M. Gelinsky. Applied Materials & Interfaces 7 (2015) 6541.
[3] W.W. Hu, H.N. Yu. Carbohydrate Polymers 95 (2013) 716.

Extraction of ∝-pinene from brazmyl essence and analysis and determinating it

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Brazmyl is a plant with the scientific name of perovskia abrotanoides, and it is from thefamily labiatae. Eating this plant has analgesic effects. Thus, in recent years these Mint essence is extracted. And in the pharmaceutical industry comes as a liquid formulation. So that it can be better used. Its main properties are anti-malarial and anti-seeker.Volatile essence of the leaves and stems of plants were extracted with water distillation (Clevenger method) and by using GC / MS. Kvats identify the composition of the index and compared with the standard combination has been done in some scientific sources. The result of this work has taken place with careful study and compare all the different components of standard components and the combination. We have found 22 combinations in this plant's essence. In general, the combinations in the essence have been reported by other researchers were extracted by different amounts.Alpha-pinene is much more to be seen in this essence. Monoterpenes hydrocarbons such as alpha-pinene is used for the production of perfumes and pharmaceuticals for shower and air fresheners.

Refrences

[1] Duke JA. CRC Handbook of medicinal herbs. Boca Raton: CRC press, 1989:412-3
[2] British herbal pharmacopoeia: Bournemouth: British herbal medicine Association, 1989:1810
[3] Dent bown. Encylopedia of herbs and other uses. 1996:192
[4] Dictionary of Natural Products, 1994. Vol. 4, pp. 4685. Published by Chapman.

The synthesis of aryl isothiocyanate derivatives by copper(II) catalyst located on the substrate of nano magnetic

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In recent years,the hetrogenizationof homogeneous catalysts has attracted immense attention[1].Recovery and reuse of expensive catalysts after catalytic reactions are important factors for sustainable process management.The surface of themagnetic nanoparticles is usually coated with a layer of silica to prevent aggregation. Because of the importance ofmagnetic catalysts, the synthesis and characterization ofthese types of catalyst are of interest, and there have beenmany reports dealing with this area[2]. In the past decade, transition-metal-catalyzed C−Hfunctionalization has been developed as an attractive andpowerful strategy, because this method permits more-efficient synthesis of functionalized molecules by minimizingthe number of synthetic steps[3].In this paper, to prepare a heterogeneous catalyst , Fe_3O_4 nanoparticles coated by silica ($Fe_3O_4@SiO_2$), then reflux in three stages , with (3-Aminopropyl)trimethoxysilane (APTMS), PhNCO and copper(II) acetate were functionalized nanoparticles.The new magnetic catalyst was charactrized by FT-IR,XRD,TGA,VSM,EDX,SEM,We used new magnetic catalyst for synthesis of aryl isothiocyanate derivatives.

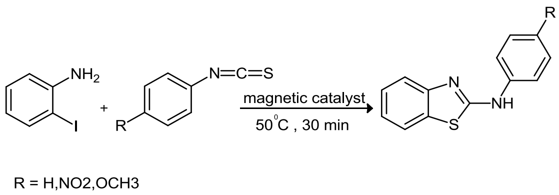

Figure 1. Scheme of the reaction.

References

[1] Minakata,S.; Komatsu,M.Chem.Rev.2009,109,711.
[2] (a) Wang, S.; Zhang, Z.; Liu, B.; Li, J.Catal. Sci. Technol. 2013,3,2104. (b) Stevens, P. D.; Li, G.; Fan, J.; Yen, M.; Gao, Y.Chem.Commun. 2005, 4435.
[3] (a) Yamaguchi, J.; Yamaguchi, A. D.; Itami, K.Angew. Chem. Int.Ed. 2012,51, 8960. (b) Xie, J.; Pan, C.; Abdukader, A.; Zhu, C.Chem. Soc. Rev. 2014,43, 5245.

Synthesis, characterization and antibacterial activity of new Hg(II) complex containing ∝-keto stabilized phosphonium yllide

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Phosphorus ylides are important reagents in organic chemistry, especially in the synthesis of naturally occurring products with biological and pharmacological activities.Due to the high versatility from the applications as pharmaceutical and biological active agents point of view and also wide scope of suitability in industrial and chemical processes, The synthesis and usability of the metalated phosphorus ylides have attracted the synthetic chemist's attention[1,2].Herein, a new stable phosphorus ylide with formula of (*p*-tolyl)$_3$P=CHCOC$_6$H$_4$(*p*-CN) was synthesized (Fig.1) and a series of binuclur complexes based on metalated phosphorus ylides were prepared through the reaction of (*p*-tolyl)$_3$ P=CHCOC$_6$H$_4$(*p*-CN)with mercury(II) halides in equimolar ratios using MeOH as solvent (Fig.2). The structure of the prepared phosphorus ylide and complexes were confirmed by using IR, ^{1}H, ^{31}P and ^{13}C NMR analys. In another study, the antibacterial applicability of the synthesized mercury (II) complexes was successfully explored against both the five Gram-positive and four Gram-negative bacteria.

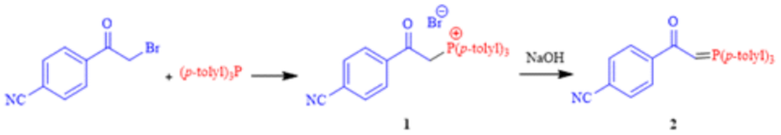

Fig.1.The synthesis of ylide

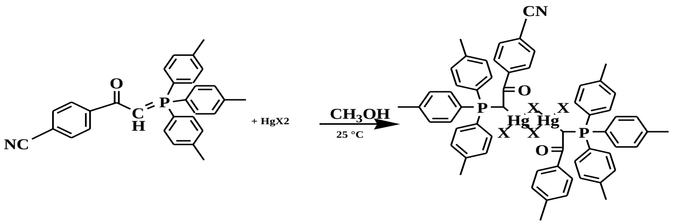

Fig.2. Synthesis of Hg(II) complex

References

[1] Spencer, E. C.; Mariyatra, M. B.; Howard, J. A. K.; Kenwright A. M.; Panchanatheswaran, K.; J. Organomet. Chem., , 692(2007) 1081.
[2] Sabounchei, S. J.; Nemattalab, H.; Salehzadeh, S.; Bayat, M.; Khavasi, H. R.; H. Adams, J. Organomet. Chem. 692 (2008) 1975.

Mixed metal oxides modified mesoporous silica with magnetic core: a reusable catalyst for the synthesis of 2-substituted benzimidazoles

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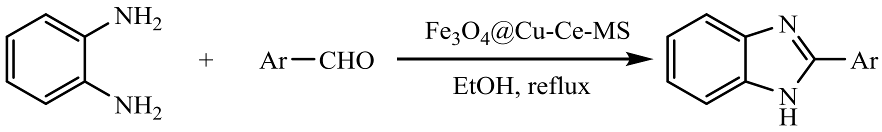
The use of magnetically recoverable catalysts has received considerable importance in organic synthesis because of their ease of handling, simple workup and recoverability. Among the various heterogeneous catalysts, particularly, mesoporuos supported catalysts have advantages of high surface area and 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 benzimidazoles from the reaction of aldehydes and *o*-phenylenediamine in the presence of catalytic amount of mesoporous silica containing Cu and Ce metal oxides with magnetic core (Fe_3O_4@Cu-Ce-MS)[2]



Various types of aldehydes were reacted with *o*-phenylenediamine in the presence of catalytic amount of Fe_3O_4@Cu-Ce-MS at reflux condition and corresponding 2-sudstiuted benzimidazoles 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@Cu-Ce-MS as simple, efficient and eco-friendly catalyst for the synthesis of 2-substituted benzimidazoles. Simple workup and reusability of catalysts are other advantages of this method[3].

References

[1] A.Sch€uuth, J.Wingen, Sauer,Micropor.Mesopor. Mater.44–45 (2001) 465.
[2] A.C Wagvar B.v Panla .v.Martin s.w Martin Zeolites 18 (1997) 469.
[3] Wang, Y.,Sarris., K.Sauer,D.R.,Djuric, S.W. Tetrahedron Lett. 2006, 47, 4823.

Removal of organic dyes pollutants from water by magnetically separable $NiFe_2O_4$/graphene nanohybride

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Organic dyes are widely used in various fields and seriously induce water pollution. Most of the industrial dyes are toxic, carcinogenic, and teratogenic and unfortunately most of them are stable and resistance to photo degradation, biodegradation, oxidizing agents [1,2]. The treatment of industrial effluents is a challenging topic inenvironmental science, as control of water pollution hasbecome of increasing importance in recent years[3]. In this project, the magnetic $NiFe_2O_4$/graphene nanohybride have been synthesized, identified with different analysis such as FT-IR, XRD, SEM, EDAX and then used as an adsorbent for the removal of organic dyes such as methylene blue from aqueous solution.UV–Vis spectroscopy was carried out for analyzing their optical absorption behavior.The efficiency of the organic dyes removal from aqueous solutions, studied by recording adsorption spectra (Fig. 1).Their adsorption capacity was investigated by measuring the removal ofdifferent loading methylene blue from aqueous solutions.

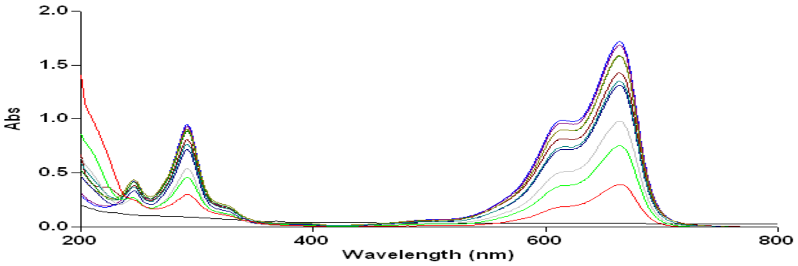

Figure 1. Removal of methylene blue in the presence of$NiFe_2O_4$/graphene

References

[1] S. Qadri, A. Ganoe, Y. Haik, Removal and recovery of acridine orange from solutions by use of magnetic nanoparticles, Journal of Hazardous Materials, 169 (2009) 318-323.
[2] Z. Zhang, J. Kong, Novel magnetic Fe 3 O 4@ C nanoparticles as adsorbents for removal of organic dyes from aqueous solution, Journal of Hazardous Materials, 193 (2011) 325-329.
[3] V. Rocher, J.-M. Siaugue, V. Cabuil, A. Bee, Removal of organic dyes by magnetic alginate beads, Water Research, 42 (2008) 1290-1298.

Solvent-Free Synthesis of 3,4-dihydropyrimidin-2(1*H)*-ones under grauting heating with N,N-dihydroxydiphthalimideas catalyst

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Recently, the interest in synthesis of 3,4-dihydropyrimidin-2(1*H*)-ones (denoted as Biginelli compounds) andtheir derivatives is increasing tremendously because oftheir therapeutic and pharmacological properties andalso because of interesting biological activities of severalmarine alkaloids which contain the dihydropyrimidinenucleus [1-2].Synthetic strategies for thedihydropyrimidine nucleus involves One-Pot to multistepapproaches. The classical Biginelli synthesis is aOne-Pot condensation using dicarbonylcompoundswith aldehydes (aromatic and aliphatic aldehydes) andurea or thiourea in ethanol solution containing catalyticamounts of acid. [3].Here we report on a new procedure for preparing3,4-dihydropyrimidin-2(1*H*)-ones in thepresence of *N,N*-dihydroxydiphthalimide as organocatalyst. We obtained 3,4-dihydropyrimidinonesin high yield by thereaction of various aldehydes with ethyl acetoacetateand urea in the presence of *N,N*-diimideascatalyst under free solvent for 3 h at 120 ^{O}C(Figure 1).

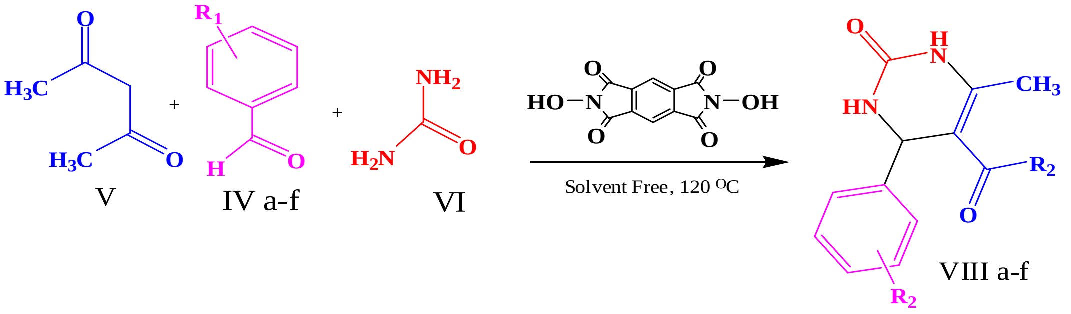

Figure1. Scheme of the reaction.

References

[1] Ma, Y.; Qian, C.; Wang, L.; Yang, M. J. Org. Chem2000, 65, 3864
[2] Big, F., Carloni, S., Frullanti, B., et al., TetrahedronLett., 1999, 40, 3465-3473.
[3] T.N. Akhaja, J.P. Raval, Design. Chin. Chem. Lett. 2012, 23, 446

Photcatalytic green system for reduction of nitroarenes under sunlight and violet LED irradiation

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Heterogeneous photocatalysis by semiconductor materials has been gaining increasing interest in organic synthesis[1].TiO_2, because of its unique chemical and physical properties, such as high efficiency, low cost, physical and chemical stability, widespread availability, and noncorrosive property is broadly used in the fields of solar energy conversion and photocatalysis[2].Li et al. first reported a photoinduced reduction of nitro compounds to the corresponding amines using TiO_2 -P25 as a catalyst under UV light, they used 2 ml of a 0.01M solution of nitrobenzene in the reaction[3].An important problem of heterogeneous photocatalytic reactions is low amount of substrate. Also there aresome limitations for using semiconductors in water, associated with the low solubility of substrates and over-oxidation of organic compounds which are a result of the oxidant species produced (such as $^{\cdot}OH$ and $O_2^{\cdot -}$/$HO_2^{\cdot}$) in a photocatalytic process. Photocatalytic reduction of nitroarenes to amines under sun light and violet LED irradiation in water has been taken in to consideration. To overcome the solubility problem of nitro compounds in water polyethylene glycol-400 was used as cosolvent. The reaction was done using a TiO_2/PEG-400 system in water as solvent. Under sunlight irradiation 0.1 mmol of nitro benzene was used. Very interestingly under violet LED irradiation, 1 mmol of nitro benzene was used in reaction as starting material in water. For other Derivatives of nitrobenzene 0.5 mmol of nitro compound was used.

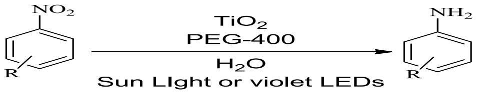

Figure 1. Photocatalytic reduction of nitroarenes in water

References

[1] H. Kisch, Angew. Chem. Int. Ed., 2013, 52, 812.
[2] N. Hoffmann, Aust. J. Chem., 2015, 68, 1621.
[3] F. Mahdavi, T. C. Bruton and Y. Li, J. Org. Chem., 1993, 58, 744.

Visible-Light photocatalytic One-Pot Synthesis of Aldonitrones usingCdS nanorodes

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Photocatalytic reactions by using semiconductors for organic transformation at different conditions such as various solvents, light sources and catalysts are taken in to consideration[1].CdS has been introduced as suitable photocatalyst due to its unique photoelectric properties such as narrow band gap (2.4 eV) and its activity in a wide range of sunlight irradiation[2]. Nitrones as protected form of hydroxylamines are key intermediates for synthesis of biologically active compounds and natural products[3].During the reduction of nitro aromatic compounds, unstable intermediates (e.g. nitroso, hydroxylamine) can be produced. In situ generation of unstable hydroxylamine and its reaction with a carbonyl compound is the mildest and most atom-efficient procedure for nitrone synthesis and also minimizes the synthetic steps.Nanorod CdS photocatalyst has been used for reduction of nitroarenes in water. Reduction of nitro to amines was done in water under green and blue LED irradiation. Also reduction of nitroarenes in the presence of aldehydes for synthesis of nitrones were done successfully under blue LED irradiation. As our best knowledge,this is the first photocatalytic synthesis of nitrone by aldehyde and nitroarenes using a semiconductor as photocatalyst. In this reaction 1mmol of starting materials was used that is very interesting in heterogeneous photocatalysis.

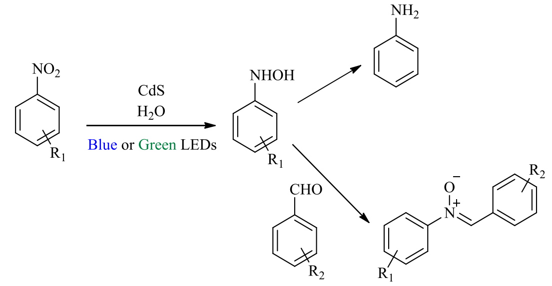

Figure 1. Photocatalytic synthesis of nitrones and amines using nitroarenes and aldehydes in water

References

[1] H. Kisch, Angew. Chem. Int. Ed., 2013, 52, 812-847.
[2] P. Eskandari, F. Kazemi and Z. Zand, J. Photochem. Photobiol., A, 2014, 274, 7-12.
[3] L. Cisneros, P. Serna and A. Corma, Angew. Chem. Int. Ed., 2014, 53, 9306-9310.

Synthesis of benzopyranopyrimidine using nanotriethanolammonium trichloroacetate

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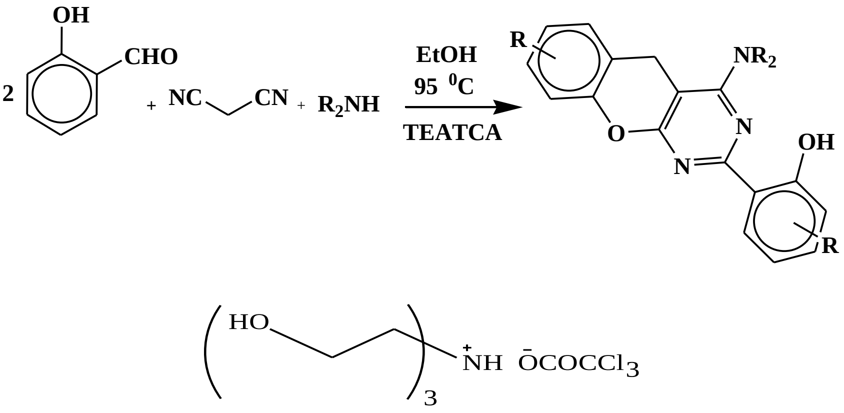
Multi-component reaction(MCR) protocol with environmentally benign solvents and catalytic system is one of the most suitable strategies, wich meets requirements green aspects of chemistry for developing libraries of medicinal scaffold[1]. Benzopyranopyrimidines show interesting features which make them attractive targets for the synthesis via MCR[2]. Benzopyranopyrimidine display a wide range of biological activities including anti-fungicidal, anti-bactericidal[3].Herein, we report an efficient and simple method for the synthesis of newbenzopyranopyrimidineviaapseudo four-component reaction of salicylic aldehydes, malononitrileand various amines in the presence of a catalytic amount of nanotriethanolammoniumtrichloroacetate[TEATCA] in EtOH at 95 ℃ (Figure I).In conclusion, using nontoxic, environmental friendly catalyst and having easy work make this method attractive.



TEATCA

Figure 1. Synthesis of benzopyranopyrimidine in EtOH, at 95^{0}C

References

[1] Dyachenko, V. D., Pugach, Yu. Zh. Obshch. Khim.2012, 82, 844–849.
[2] Kumaravel, k., Vasuki, G. Curr. Org. Chem. 2009, 13,1820.
[3] Zeng, Z. G,. Wan, L. Y., CaO, G. Y., Luo, Y. P. Res. Chem. Intermed. 2012 , 38, 1751–1760.

Synthesis of pyranopyrazole using nano triethanolammonium trichloroacetate

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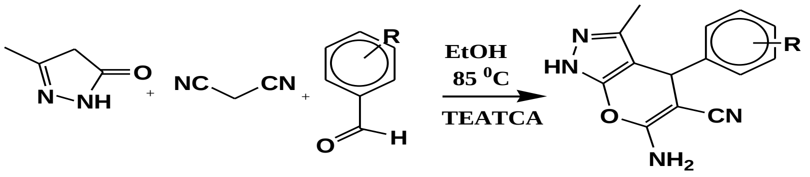
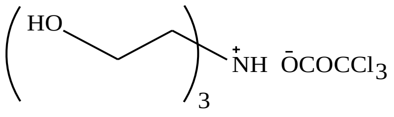
Pyranopyrazole derivatives are important class of hetrocycles due to their wide range of biological and pharmaceutical properties. In addition to fungicidal, bactericidal and herbicidal activities they also exhibit analgesic and anti-flammatory activities and act as hypotensive, hypoglycemic agent vasodilators[1]. Ionic liquids are salts that are liquid at low temperature (<100 degrees C) which represent a new class of solvents with nonmolecular, ionic character. Although ionic liquids have only been studied in depth during the last decades, the field is now maturing to such a degree that the focus is on larger scale applications for use in real processes such as catalysis [2].Herein, we wish to present a green procedure for the synthesis of pyranopyrazole *via* three component reaction of 3-methyl 5-pyrazolon, malononitrile and various aromatic aldehydes in ethanol at 85 °C using nano triethanolammonium trichloroacetate[TEATCA].This method offers several advantages such as inexpensive catalysts, mild reaction conditions and operational simplicity.





TEATCA

Figure 1. Synthesis of pyranopyrazole in EtOH, at 85^{0}C

References

[1] Ghobani-Vaghei, R., Amiri, M., Moshfeghifar, N., Veisi, H., Dadamahaleh, S, A., J. Iran. Chem. Soc. 2009, 6, 754-760.
[2] Lindstro, U. M. Chem. Rev. 2002, 102, 2751.

Volatile Constituents of the Leaves of *Salvia indica L.* Obtained by Microwave Extraction Method

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Salvia, the largest genus of the family Lamiaceae, includes about 900 species widespread all over the world. Sixty species are found in Iran, seventeen of which are endemic [1] .*Salvia* is a knowledged worldwide as an important genus because of the beneficial uses of the essential oils produced by the foliage and many *Salvia* species have been used in folk medicines making members of this genus a popular choice of researchers. Some of these species have been studied in many parts of the world and range of traditional applications of the herbs in domestic medicine seems to be endless, they have been used as a medication against perspiration and fever, as a carminative, a spasmolytic, an antiseptic and also is found to possess antibacterial, antifungal, anti- inflammatory activities [2].In this study the composition of the essential oil from the leaf of *Salvia indica*, (syn: *Salvia brachycalyx* Boiss.), which was collected from Lorestan province, in July 2015, obtained by salventfree microwave extraction method analysed by GC and GC/MS.In *S.indica* oil, thirty-nine components, which representing 91.8% of the total composition, were identified.The leaf oil of *S.indica* consisted of three monoterpene hydrocarbons (1.1%), one oxygenated monoterpene (0.8%), fourteen sesquiterpene hydrocarbons (29.7%), seventeen oxygenated sesquiterpenes (52.1%), two diterpenes (7.5%) and two aliphatic compounds (0.6%). Spathulenol (34.7%) and β-caryophyllene (16.9%) were the major components in this oil followed by sclareoloxide (7.1%), bicyclogermacrene (6.7%), $\beta -$copaen -4-α-ol (5.6%) and cedr-1 (15)-en-9-α-ol (5.0%).

References

[1] V.Mozaffarian, A Dictionary of Iranian Plant Names, Farhang Moaser Publisher, Tehran, Iran (1996) 478.
[2] N.S. Perry, C. Bollen, E.K. Perry, C.Ballard, Pharmacology Biochemistry Behaviour 75 (2003) 651.

Chemical Composition of the Essential Oil from Stems of *Salvia indica L.* Obtained by Steam Distillation

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The genus *Salvia*, including some Iranian species, has been studied chemically and the presence has been reported of terpenoids, even the rare sesterterpenes, essential oils and flavonoids. Fifty-eight species of *Salvia* are found in Iran, 17 of which are endemic [1].

Some species of the genus *Salvia* are used as medicinal, aromatic and ornamental plants.

Tanshen, the rhizome of *S. miltiorrhiza* Bunge.has been used in Chinese traditional medicine for multiple therapeutic remedies. Tanshen has been used primarily for the treatment of coronary heart disease, particularly angina pectoris and myocardial infraction, it has also been included for the treatment of hemorrhage, dysmenorrhea, miscarriage, swelling and insomnia [2].The stems of *S.indica* growing wild in Lorestan province, in Joly 2015.The oil obtained by steam distillation and analyzed by GC and GC/MS.Thirty-six components representing 83.7% of steam distillation oil from stem of *S.indica* were identified. The main compounds of the oil were spathulenol (28.7%), and β-caryophyllene (13.8%).Other notable constituents were caryophyllene oxide(8.9%),bicyclogermacrene(7.3%),sclareoloxide(6.9%) and isopathulenol (5.5%).The oil of the plant was characterized by high amounts of sesquiterpenes(72.2%).The monoterpenes and diterpene fractions were relatively small, representing(0.2% and 9.6%, respectively) of the total oil. β-Caryophyllene(38.4%),followed by germacrene D(11.4%), spathulenol (10.5%) and α-humulene(8.7%) were the main constituents among the 16 characterized, comprising 87.6% of the total,detectedin the oil of *S.palaestina* Benth.In this oil, sesquiterpenes(74.2%) predominated over monoterpenes(12.9%)[3].

References

[1] V.Mozaffarian.A Dictionary of Iranian Plant Names,Farhang Moaser Publisher,Tehran,Iran (1996)478.

[2] X.Wang,S.L.Morris-Natshke, K.H. Lee, Med.Res.Rev27(2007)133.

[3] A.Rustaiyan, M.R.Akhgar,S.Masoudi,F.Nematollahi,J.Essetnt.Oil Res 17(2005)522.

Simple and Efficient Synthesis of Isobenzofurans via Oxidation of Dihydroxyindenobenzofuran Derivatives

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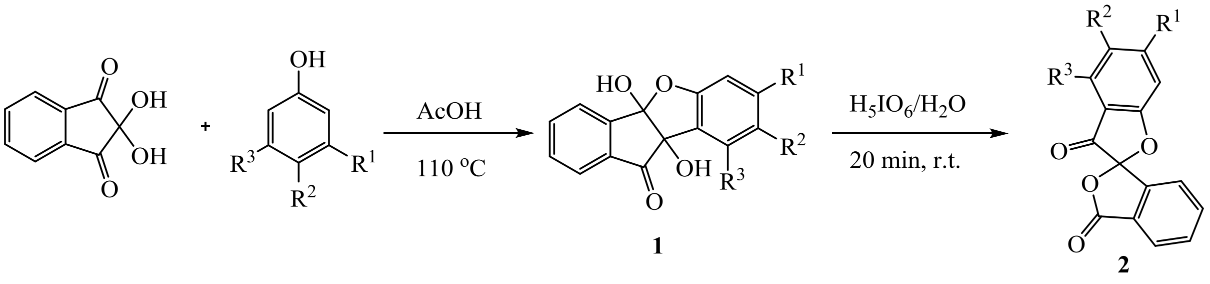
Benzofurans have attracted a great deal of interest because of their presence ina large number of natural products, their biological activities, and their potential applications as pharmacological agents. For example, 5-benzofuranol has potent antiallergic and anti-inflammatoryactivities [1]. Machicen diol, a benzofuran isolated from the extracts of Machilus glaucescens, a folk medicine, has been used in the treatment of asthma, rheumatism, and ulcers. In addition, benzofurans containing 1,3-thiazole derivatives have been reported to possess tuberculostatic, antibacterial, and antifungal activities [2]. As part of our continued interest for the development of newsynthetic methods for spiro-fused compounds [3], we report the oxidationof 4b,9b-dihydroxy-4b,9b-dihydro-10*H*-indeno[1,2-*b*]benzofuran-10-ones1 (Figure 1), as anew and simple route for the synthesis of novel 3*H*,3'*H*-spiro[benzofuran-2,1'-isobenzofuran]-3,3'-dione derivatives 2.dihydroxy indeno benzo furanones1 were simply prepared using addition reaction of ninhydrin with substituted phenols and suffered the oxidative cleavage reaction with H_5IO_6 in aqueous media and at room temperature.The identification of the products 2 were occurred based on theirIR, Mass and NMR Spectra.



8 examples, overal yields: 75-95%

Figure 1. Schemee of the reaction.

References

[1] Lau, C. K.; Belanger, P. C.; Dufresne, C.; Scheigetz, J.; Therien, M.; Fitzsimmons, B. Young, R. N.; Ford-Hutchison, A. W.; Riendeau, D.; Denis, D.; Guay, J.; Charleson, S.; Piechuta, H.; McFarlane, C. S.; Lee Chiu, S. H.; Eline, D.; Alvaro, R. F.; Miwa, G.; Walsh, J. L. J. Med. Chem. 1992, 35, 1299–1318.

[2] Echneiders, G. E.; Stevenson, R. J. Org. Chem. 1979, 44,4710.

[3] Mohammadizadeh, M. R.; Saberi, D.; Taghavi, S.Z. Tetrahedron Lett. 2016, 57, 2064-2067.

Simple, Fast and Efficient Synthesis of 6-Amino-5-(3,4-dioxo-3,4-dihydronaphthalen-1-yl)uracils

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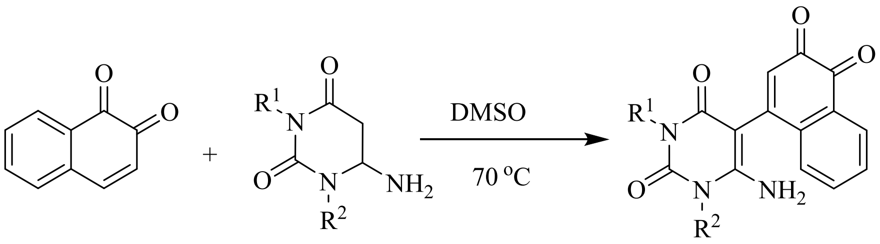
6-Aminouracil derivatives represent very important classes of functionalized uracils. Moreover, 6-amino-uracils find wide applicationsas starting materials for the synthesis of a number of fuseduracils of biological significance, for example, pyrano-, pyrido-,pyrazolo-, pyrimido-, pyridazino-pyrimidines [1]. Uracil derivatives, which have pyrimidine-like structure (uracil = pyrimidine-2,4-dione), have also an elegance role in heterocyclic chemistry. They have aroused much interest owing to their potential applications in medicine and photobiology. Pyrimidine dyes in some cases prepared from 6-aminouracils have found industrial applications in hypnotic drugs, in living cells, in detecting cancer and having pharmacological and biological activities[2].In continues of our interest on chemistry of 6-aminouracils and as a part of our previous research programs on the preparation of biologically potentially importance heterocycles [3], herein, we wish to report a simple and fast procedure for the synthesis of new 6-amino-5-(3,4-dioxo-3,4-dihydronaphthalen-1-yl)uracil derivatives **3***via* reaction of *1,2-Naphthoquinone* ***1*** with 6-aminouracils **2** in DMSO at 70 °C (Figure 1). The reactions were completed within 2-3 hours, affording the corresponding products **3** in good to excellent yields. The structure of these new compounds were undoubtedly characterized by IR, Mass, ^{1}H and ^{13}CNMR Spectra.



1 **2** **3**

Figure 1.simple and highly efficient synthesis of 6-Amino-5-(3,4-dioxo-3,4-dihydronaphthalen-1-yl)uracils

References

[1] A. Agrawal, P. M. S. Chauhan, S.F. Martin. Tetrahedron Lett.46 (2005) 1345.
[2] H. Zeng, Z. P. Lin, A.C. Sartorelli. Biochemical Pharmacology68 (2004) 911.
[3] M.R. Mohammadizadeh, M. Bahramzadeh, S. Z. Taghavi. Tetrahedron Lett.51 (2010) 5807.

Synthesis of pyrimido[4,5-*e*][1,2,4]triazolo[3,4-*b*][1,3,4]thiadiazepine as a Novel heterocyclic system

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Pyrimidine and related fused heterocyclic compounds have attracted the attention of numerous researchers due to their important biological. they have been reported asanticancer, antiviral, antitumor, and anti-inflammatory agents [1-2].Moreover, tetrazoles have found utility in pharmaceuticals as lipophilic spacers and carboxylic acid surrogates, in special explosives, photography and information recording systems[3]. Herein, 2,4-dichloro-5(chloromethyl)-6-methylpyrimidine 1were prepared according to the previous procedure and treated with sodium 1-amino-1H-tetrazole-5-thiolate 2 as abinucleophile in $CHCl_3$. to obtain 5-((2,4-dichloro-6-methylbenzyl)thio)-1H-tetrazol-1-amine3. Compound 3was further cyclized with K_2CO_3 in boiling DMF to give the desired novel tricyclic compound4. Treatment of compound 4 with various secondary amines afforded the corresponding products5a-gin yields(Figure 1). All of these compounds were characterized by FT-IR, ^{1}H NMR, ^{13}C NMR and mass spectrometry.

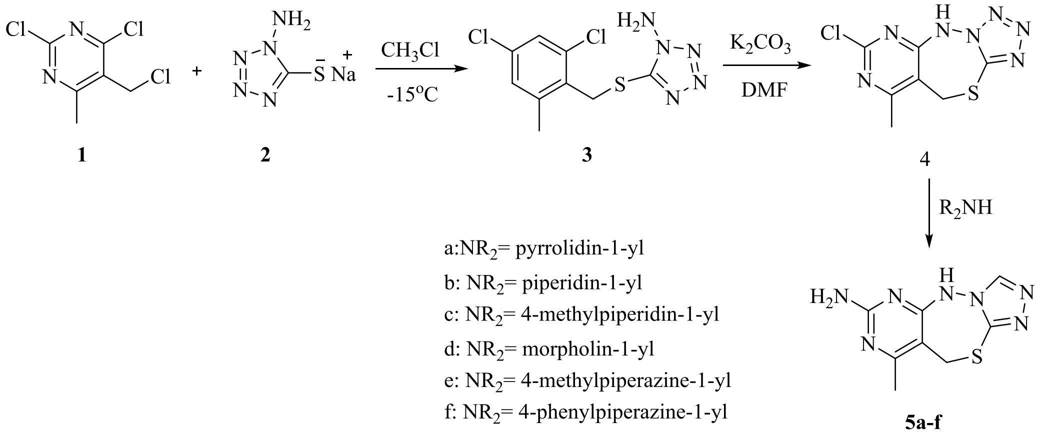

Figure 1. Scheme of the reaction.

References

[1] M.M. Gineinah, M.A. El-Sherbeny, M.N. Nasr and A.R. Maarouf, Arch. Pharm., 2002, 335, 556.
[2] P.G. Baraldi, M.G. Pavani, M.C. Nunez, P. Brigidi, B. Vitali, R. Gambari and R. Romagnoli, Bioorg. Med. Chem., 2002, 10, 449.
[3] S.M. Sondhi, M. Johar, S. Rajvanshi, S.G. Dastidar, R. Shukla, R. Raghubir and J.W. Lown, Aus. J. Chem., 2001, 54, 69.

Polystyrene with the ionic liquid pendant groups based on 1-Methylbezotriazolium cation and some their properties

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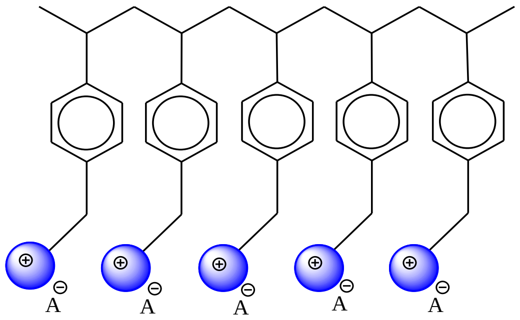
Polymers have an important role in our daily lives and a large amount of polymers produce each year. Polymers have many advantages e.g. Less weight, higher energy efficiency, performance and durability and more flexibility in design and processing [1]. Poly(ionic liquid)s (PILs), are compounds that have an IL species in each monomer repeating unit, that are connected to the polymer backbone and can be afforded through polymerization of IL containing polymerizable groups either in cation or anion, or chemical modification of other polymers. Due to their chemical structure (polymers containing repeating cationic and anionic units that are an electrolyte group), also called poly electrolytes [2]. Styrene is one of the most chemicals that has a wide range of applications from food packaging to automobile segments [3], so much of research is focused on enhancing the properties of polystyrne. In the present work, the styrenic IL monomers based on 1-Methylbenzotriazolium cation were synthesized by linking the 1-Methylbenzotriazol to VBC, then new styrenic ionic liquid based PILs (Figure 1.) were prepared with the free radical polymerization method. The structure of PILs were characterized by IR and^{1}HNMR data.Study of thermogravimetric analysis, and differential scanning calorimetry data showed that the resulting polymers have excellent thermal stability. Solubility of homopolymers in different organic solvents was tested and the electrochemical window of their was investigated for comparison with polystyrene. The styrenic ionic liquid based PILs with the advantage of facile synthesis and the ability to incorporate many desirable functional moieties offer an efficient route to highly functional styrenic PILs.



A: Cl, BF_4, PF_6

Figure 1. Styrenic ionic liquid based PILs.

References

[1] T. Erdmenger, C. Guerrero-Sanchez, J. Vitz, R. Hoogenboom and U. S. Schubert, Chem Soc Rev 39 (2010) 3317.
[2] J. Mythri, B. Anusha and M. S. Reddy, J. Chem. Pharma. Sci. ISSN 974 (2015).
[3] P. Dimitrov-Raytchev, S. Beghdadi, A. Serghei and E. Drockenmuller, J. Polym. Sci. Part A: Polym. Chem. 51 (2013) 34.

A Novel One-Pot Procedure for the Synthesis of 6-Aminouracils

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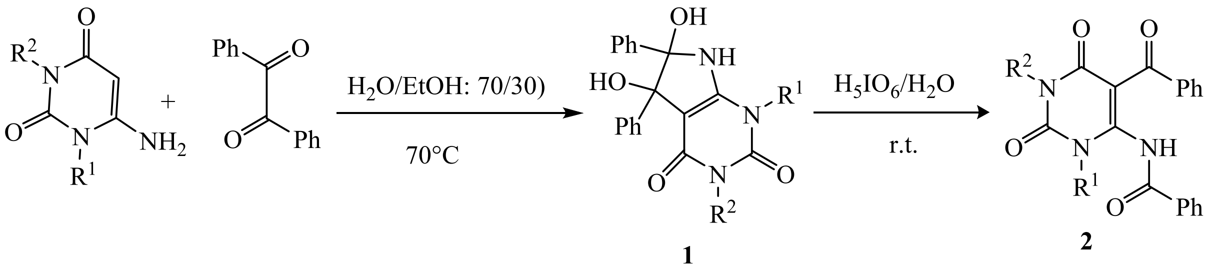
6-Aminouracils are keyintermediates in the synthesis of xanthineswhich constitutethe basic nucleus of various drugs such as caffeine, 6-mercaptopurine, penciclovir, theophylline, theobromine*etc*. 6-Aminouracils are also used as startingmaterials for the synthesisof various fused heterocycles with biological importance, suchas pyrido-, pyrazolo- and pyrimido-pyrimidines [1]. However, many procedures were reported for the synthesis of 6-aminouracils, the basic and most frequently procedures have beeninvolvingthe condensation of ureas with cyanoacetic acid in the presenceof phosphorous oxychloride or acetic anydride, all these procedures suffer from drawbacks such as use of no recovery of catalysts,lack of simplicity in their experimental procedure. Therefore,developing a synthetic method for a One-Pot synthesis of 6-aminouracils using an environmentally friendlysolvents and conditions is desirable [2].In continues of our previous success on the synthesis of biologically potentially importance heterocycles [3], here, we wish to report a novel and efficient procedure for the preparation of substituted 6-aminouracils**2***via* One-Pot synthesis and oxidation of cyclic diols **1**with periodic acid in aqueous media (Figure 1). As shown in the figure1the used oxidant and conditions are in agreement with green aspects of chemistry. The products **2** were characterized based on their IR, Mass and ^{1}H and ^{13}C-NMR Spectra.



5 examples, overal yields: 70-88%

Figure 1. One-Pot synthesis of substituted 6-Aminouracils

References

[1] Kalita, S. J.; Mecadon, H.; Deka, D. C. RSC Adv.2014,4, 32207-32213.
[2] Chavan, S. S.; Degani, M. S. Green Chem.,2012, 14, 296-302.
[3] Mohammadizadeh, M. R., Saberi, D; Taghavi, S. Z.Tetrahedron Lett. 2016, 57, 264–267.

Synthesis of some Dihydro-Dipyrido-Triazine systems from pentafluoropyridine

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Heterocyclic compounds have increasing important in the pharmaceutical industry and the most of important life-science products are contain heterocyclic structures [1,2].Halogen substituents atdifferent positions of heteroaromatic systemsring indicate different reactivity tonucleophiles, for example in pentafluoropyridine order reactivity toward nucleophilic attack follow the sequence 4-F> 2-F > 3-F [3-4]. In this work we report the synthesis of some dihydro-dipyrido-triazine Systems via reaction of 1,6- diamino- 2- oxo- aryl- 1,2-dihydropyridine- 3,5- dicarbonitrile (**1**)with pentafluoropyridine(**2**) in the presence of potassium carbonate in CH_3CN at reflux temperature (Figure 1). All fluorinated products were confirmed with NMR Spectra.

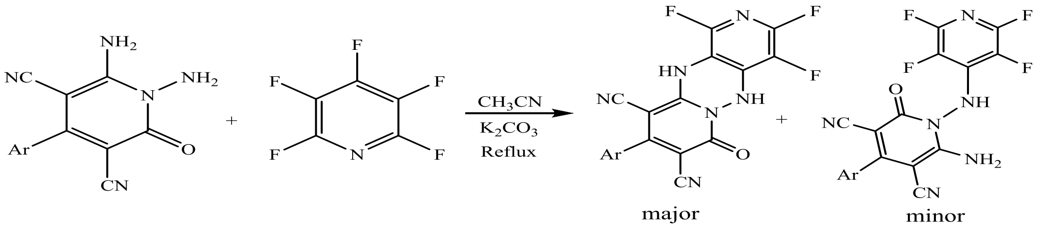

Figure 1. Synthesis of dihydro-dipyrido-triazin systems.

Reference

[1] Pozharskii, A. F.; Soldantenkov, A. T.; Katritzky, A. R. Heterocycles in Life and Society; John Wiley and Sons: New York, NY, 1997.

[2] Katritzky, A. R.; Rees, C. W. Comprehensive Heterocyclic Chemistry; Pergamon: Oxford, 1984; Vols. 1–8.

[3] R.D. Chambers, C.R. Sargent, Adv. Heterocycl. Chem. 28 (1981) 1.

Design, synthesis and antibacterial activity of some pyrrolo[3,4-b]quinolin-2(3*H*)-yl)benzamide derivatives

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Emerging infectious diseases and the increasing number of multi-drug resistant microbial pathogens still make the treatment of infectious diseases an important and challenging problem[1]. Therefore, there is an urgent need for development of new antibacterial and antifungal agents with divergent and unique structure and with a mechanism of action possibly different from that of existing antimicrobial agents[2]. The pyrrolo[3,4-b]quinoline ring system is present in compounds associated with a wide variety of pharmacological properties as is exemplified with hypnotic and cytotoxic effects, and with analgesic and antiviral activities [3].In this study, a series of new pyrrolo[3,4-b]quinolin-2(3H)-yl)benzamide derivatives (**7a-g**) was synthesized by reaction of benzohydrazide derivatives (**6a-g**) with 9-phenylfuro[3,4-b]quinoline-1,3-diones (**5a-b**) in the presence of Et_3N and evaluatedfor their antibacterial activity against various bacterial strains using in vitro disc diffusion methodby measuring the zone of inhibition. Most of the compounds exhibited potential antibacterial activity against gram-negative (*Escherichia coli*) and gram-positive bacteria (*Streptococcus* and *Enterococcus*).

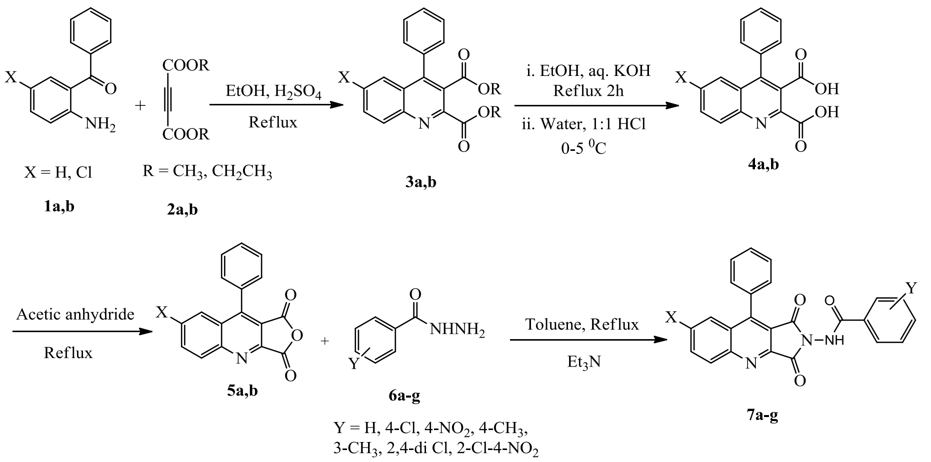

Figure 1. Scheme of the reaction.

References

[1] A.K. Zafer, T.Z. Gulhan, O. Ahmet, R. Gilbert. European Journal of Medicinal Chemistry 43 (2008) 155.
[2] A. Khalafi-Nezhad, M.N.S. Rad, H. Mohabatkar, Z. Asrari, B. Hemmateenejad. Bioorganic and Medicinal Chemistry 13 (2005) 1931.
[3] Q. Z. Zheng, K. Cheng, X. M. Zhang, K. Liu, Q. C. Jiao, H. L. Zhu. European Journal of Medicinal Chemistry 45 (2010) 3207.

Chemical Composition of the Essential Oil From Leaves and Flowers of *Teucrium hyrcanicum L.* Grown Wild in Iran

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Teucrium genus belonging to the Lamiaceae family comprises about 300 species, 12 are described in the flora of Iran, among which three are endemic [1]. A wide number of *Teucrium* species are rich in strongly – bioactive phenolic compounds and are used in folkloric medicine, in the food industry and in pharmacies for their antimicrobial, antinociceptive, antioxidant, hypolipdemic, anti- inflammatory and hypoglycemic properties. Due to the wide spectrum of their biological activities, several essential oils from *Teucrium* aromatic plants play an important role to treat various human diseases [2]. Water distilled oil obtained from the aerial parts of *T. persicum* have been the subject of our previous studies. epi - α - Cadinol (23.2%) and α - pinene (17.3%) were the main components [3].In this study the composition of the essential oil from leaves and flowers oil of *T. hyrcanicum* which was collected from Gilan province, In July 2015, obtained by hydrodistillation were analyzed by GC and GC/MS.In *T. hyrcanicum* oil, thirty- six components, which representing 93.5% of the total composition, were identified. The leaf and flower oil of *T. hyrcanicum* consisted of one monoterpene hydrocarbon (4.8%), five oxygenated monoterpenes (16.1 %), one sesquiterpene hydrocarbon (8.3 %), three oxygenated sesquiterpenes (8.8 %), one diterpene (0.6 %) and 25 non terpenoid compounds (54.8 %).(Z) -β- Farnesene (8.3%), liguloxide (8.0 %), p-tert- butyl - α- methyl hydro cinnamaldehyde (6.8 %), linalool (6.6 %) and n- hexyl salicylate (5.3 %) were the major components in this oil, followed by limonene (4.8 %) citronellol (4.5 %) and phenyl ethyl alcohol (4.3 %).

References

[1] V.Mozaffarian, A Dictionary of Iranian Plant Name, Farhang Moaser Publisher, Tehran, Iran (1996) 543.
[2] M. Roghayeh, Z. Sepehri, M. Jahantigh, F. Javadian, Int .J. Adv. Biol. Biomed.Res 3 (2015) 149.
[3] S.Masoudi, Z. Aghajani, A. Rustaiyan, A. Feizbakhsh, A. Motavalizadeh, Journal of Essential Oil Research 21 (2009) 5.

Volatile Constituents of the Stems of *Teucrium hyrcanicum L.* Grown Wild in Iran

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The genus*Teucrium* which belongs to the family Lamiacea, includes 300 species widespread all around the world. In flora of Iran, this genus represented by 12 species, among which three are endemic [1]. The genus *Teucrium* is one of the richest sources of diterpenes, with a neoclerodane skeleton: more than 220 diterpenes have been described up to now, and many of these are particulary interesting because of their ecological role as antifeedants against different species of insects and for their role in the medicinal properties of the plants [2]. *Teucrium polium* and *T. gnphalodes* are two medicinal plants endemic to the Iberian Peninsula. The stems of *T. hyrcanicum* was collected from Rostam Abad, Gilan Province, in July 2015. The essential oil obtained by hydrodistillation using a Clevenger type apparatus from the stem of the plant and analyzed by GC and GC/MS. Twenty – seven components representing 86.2% of the stem oil of *T. hyrcanicum* were identified. The main compounds were hexadecanoic acid (29.4 %) and ligoloxide (17.3 %). Other notable constituents were ethyl hexanoate (8.9 %), 6,10,14- trimethyl- 2 - pentadecanone (6.8 %), and 1- octen- 3- ol (4.2 %). The oil of the plant was characterized by large amounts of aliphatic compounds (62.7 %).

References

[1] V. Mozaffarian, A Dictionary of Iranian Plant Names, Farhang Moaser Publisher, Tehran, Iran (1996) 543.

[2] F. Piozzi, M. Bruno, S. Rosselli, A. Maggio, Heterocycles 65 (2005) 1221.

Malva parviflora L. Leaf Aqueous Extract Assisted Green Synthesis of Gold Nanoparticles at Room Temperature and Cytotoxicity Evaluation of Nanoparticles on Cell Culture

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Recently, noble metal nanoparticles such as Au, Ag, Pt, and Pd are widely developed due to their special physiochemical properties in biological applications. Among these, gold nanoparticles have been considered as an important area of research due to their unique and tunable surface plasmon resonance and their applications in biomedical science [1]. Plant mediated synthesis of AuNPs is gaining more importance over other processes because the synthetic methods involve various chemicals that may lead to the presence of toxic chemical species, which may have adverse effects in biological applications. Currently a lot of research studies leading to novel methods of green synthesis of AuNPs have been carried as these methods are cost effective, free of hazardous reagents and involve only mild reaction conditions [2, 3].

In this study, green synthesis of gold nanoparticles (AuNPs) from aqueous $AuCl_4^-$ solution using aqueous extract of *Malva parviflora* L. was successfully carried out. The leaf aqueous extract of *Malva parviflora* was prepared using ultrasound-assisted extraction method. The obtained *Malva parviflora* L. extract is capable of in situ synthesis of red-purple color AuNPs at ambient conditions. The reaction process was monitored by using UV–vis spectrophotometry. Further characterizations of nanoparticles were carried out using TEM image and particle size analysis. The surface plasmon absorption spectrum of AuNPs exhibits only a single peak at around 545 nm. The TEM image showed that the highly dispersed AuNPs with less than 20 nm size and spherical shape were prepared which effectively considered as single particles. The effect of different variables on the biosynthesis and plasmon absorbance of AuNPs such as various volumes of extract, time and pH were studied. The results indicated that the red color AuNPs with 8 nm size and intensified plasmon absorbance bands were observed at alkaline media. Furthermore, cytotoxicity evaluation of nanoparticles denoted that the green synthesized AuNPs have low toxicity in comparison with chemically prepared AuNPs using citrate.

References

[1] A. Lakshmanan, C. Umamaheswari, N.S. Nagarajan. Journal of Nanoscience and NanoTechnology 2 (2016)76.
[2] M. M.H. Khalil, E. H. Ismail, F. El-Magdoub. Arabian Journal of Chemistry 5 (2012) 431.
[3] Ch. Jayaseelan, R. Ramkumar, A. Abdul Rahuman, P. Perumal. Industrial Crops and Products 45 (2013) 423.

A theoretical study of aromatics with AIM and Gaussian softwares

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Aromaticity is one of the cornerstones of modern organic chemistry, aromaticity is a manifestation of electron delocalization in closed circuits,either in two or in three dimensions,The properties derived from topological analysis of electron density at the ring critical point, RCP, have been used to model four different aromaticity indices. The intercorrelations between various aromaticity indices and some properties extracted from the RCPs of 9 aromatic rings have been investigated. It was found that individual RCP properties cannot be considered as reliable quantitative characteristics of π electron delocalization in heterocyclic compounds.

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References

[1] L.T. Scott, J.S. Siegel, Tetrahedron 57 (2002) 9.
[2] E. Matito, F. Feixas, M. Solà, J. Mol. Struct.Theochem 811 (2007) 3.
[3] M. Güell, J. Poater, J.M. Luis, O. M◌́, M. Yلّez, M. Solà, Chem. Phys. Chem.6(2005) 2552.

Preparation of (N,N-dimethylaminoethyl)methacrylate containing metronidazole and investigation of the effect of croslinker on swelling ratio and drug delivery

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Hydrophilic gels called hydrogels are cross-linked materials absorbing large quantities of water without dissolving. Capacity to store water or aqueous soloutions make hydrogels as an unique matrix of drug delivery system. Crosslinked poly(2-N,N-dimethylaminoethyl methacrylate) were synthesized using ammonium persulfate (APS)/ Tetramethylethylendiamine (TEMED) as an initiator/accelerator system in the presence of tetraethylenglycol diacrylate (TEGDA) as crosslinker in water at 60˚ C. The synthesized samples were confirmed by various techniques and then were investigated as a carrier for gastroretentive delivery of Metronidazole (MTZ), an effective antibiotic administered in peptic ulcer therapy. The parameters such as pH, irradiation time on the swelling behavior of products were studied. The results of swelling studies in artificial gastric and intestine media exhibited higher swelling ratio in lower pH for gastroretentive drug delivery (GDD). The aim of this work was the development of a versatile route for the preparation of pH-responsive hydrogel. Swelling rate of synthetized polymer was studied in simulated gastric fluid (SGF) and simulated intestinal fluid (SIF) mediums. The results show that the developed hydrogle system shows a potential application for pH-senstive oral drug delivery**.**

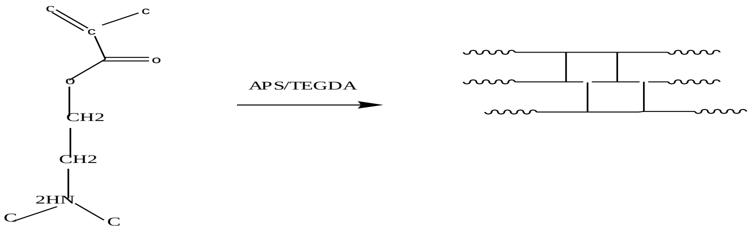

Figure 1. Scheme of the reaction.

Refrences

[1] Rezanejadeh bardajee,G,;pourjavadi,A.;Soleiman, A.Colloida and Surfaces A;Physicochem. Eng.Aspects 20011 392, 16-24
[2] Gurdag,G;Çavus,S. Polym.Adv.Technol.2006;17:878-883
[3] BGupta,P.;Vermani,p.;Garg,S.DDT Vol.7 ,No. 10 May 2002

Synthesis of 2-amino-4-azido-5-phenylfuran-3-carbonitrile derivatives viamulti-component reactions from arylglyoxals and malononitrile and Sodium azide

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Due to the high importance of furans in biologically active molecules, a number of synthetic approaches have been devised and published as alternatives to the classical methods represented by the Knorr, Paal-Knorr, and Hantzschprotocols [1-3].

In this communication, we report synthesis of furan derivatives from arylglyoxals and malononitrile, in the presence of sodium azide in water as solvent at room temperature. The product was identified by IR, ^{1}H-NMR and ^{13}C-NMR Spectra.

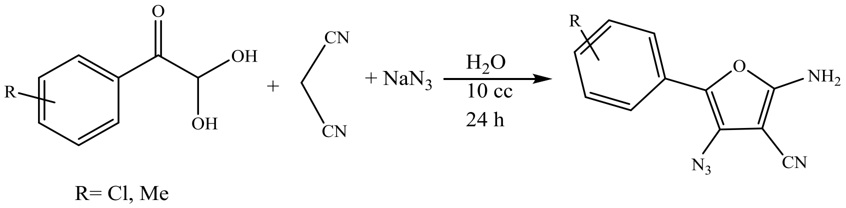

Figure 1. Scheme of the reaction.

Reference

[1] (a) Knorr, L. Chem. Ber. 1884, 17, 2863. (b) Paal, C. Chem. Ber. 1884, 17, 2756. (c) Hantzsch, A. Ber. Dtsch. Chem. Ges.1890, 23, 1474.

[2] Recent reviews on pyrrole and furan synthesis: (a) Russel, J. S.; Pelkey, E. T.; Yoon-Miller, S. J. P. Prog. Heterocycl.Chem. 2009, 21, 145. (b) Hou, X.-L.; Yang, Z.; Yeung, K.-S.; Wong, H. N. C. Prog. Heterocycl.Chem. 2009, 21, 179.

[3] Representative examples of alternative strategies: (a) Kobatake, T.; Yoshida, S.; Yorimitsu, H.; Oshima, K. Angew. Chem., Int. Ed. 2010, 49, 2340. (b) Liu, W.; Jiang, H.; Huang, L. Org. Lett. 2010, 12, 312. (c) Mizuno, A.; Kuzama, H.; Iwasawa, N. Angew. Chem., Int. Ed. 2009, 48, 8318. (d) Wang, J.-Y.; Wang, X.-P.; Yu, Z.-S.; Yu, W. AdV. Synth. Catal.2009, 351, 2063. (e) Lygin, A. V.; Larionov, O. V.; Korotkov, V. S.; Meijere, A. Chem.sEur. J. 2009, 15, 227. (f) Liu, X.-T.; Huang, L.; Zheng, F.-J.; Zhan, Z.-P. AdV. Synth. Catal.2008, 350, 2778. (g) Martin, R.; Larsen, C. H.; Cuenca, A.; Buchwald, S. L. Org. Lett. 2007, 9, 3379.

Synthesis of New Dye for using in Sensitized Nanostructured Solar Cell

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In recent years, energy demands and universal warming havearoused intense attention in clean and renewable solar energy sources.In this context, dye-sensitized solar cells have attractedconsiderable attention as they offer the possibility of low-costconversion of photovoltaic energy. The search for novel dyesin the con text of dye-sensitized solar cells has gainedmuchimpetus since the first reportin1991 by O'Regan.[1] Thereare twokindsof dyes,metal-complexandmetal-free types.Importantmetal- complexdyesareruthenium complexes.[2]Although the conventionalruthenium-based sensitizers hold the record of the solar-energy-to-electricity conversionefficiencies of 11%, they are expensive andhard to purify relative to metal-free organic sensitizers. In view of the limite davailability an denvironmentalissues associatedwithrutheniumdyes,metal-freedyesareconsideredto be analternativeforuseindye-sensitized solar cellsbecausetheyhavehighmolar absorptioncoefficients andcanbepreparedmoreeasily and economically. Thus, organicsensitizers have emerged as competitive alternatives to theRu-based counterparts because various organic chromophoreswith high molar extinction coefficients can be facilely synthesized. Thus, considerable progress has been made on the design oforganic dyes, which favor high performance in dye sensitized solar cells. Herein, we synthesized a new organic dye employing diphenyl amine following by alkylation, vilsmeierformylationand wittig reaction which was used as sensitizers in dye-sensitized solar cells. Figure 1 shows the synthesis of this new organic dye.

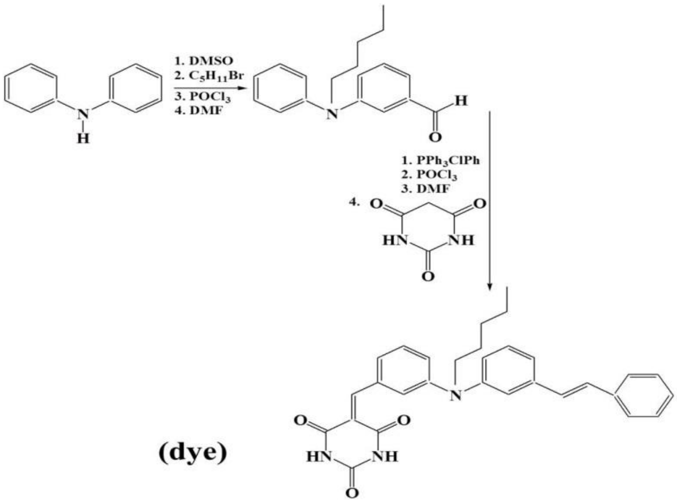

Figure 1. Synthesis of new organic dye

References

[1] H. Zhou, P. Xue, Y.Zhang, X. Zhao, J. Jia, X. Zhang, X. Liu, R. Lu.Tetrahedron67 (2011) 8477.
[2] Z. Tian, M. Huang, B. Zhao, H. Huang, X. Feng, Y. Nie, P. Shen. Dyes and Pigments87 (2010) 181.

Oxidative Desulfurization of Dibenzothiophene over Nano Polyoxometalate Supported on Nano MoO_3 and Nano MCM -41

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Sulfur organic compounds comprise the bulk of the content of sulfur crude oil. sulfurOrganic compounds in crude oil content in Iran between 0.25 to 3.23 weight percent is estimated, so Iran is among the countries with the highest amount of Sulfur organic compounds in its oil reserves. Combustion of fuels get from petroleum like diesel and gasoline produced and emissions from sulfur oxides that cause to environmental pollution and acid rains and are chemical catalyst deactivation. Also acid rain causing to solve construction materials, toxic lake and loss of jungles [1]. ODS is considered as one of the leading processes to reduce the total sulfur content of fuels due to its potential advantages over HDS. First, it requires no hydrogen, and, second, this process can be carried out at relatively mild conditions (usually 313-373 K and 0.1-0.2 MPa). In fact, the ODS is a kind of desulfurization technology in which oxidants oxidize organic sulfur and the reaction products are eliminated by absorption or extraction [2]. ODS is conducted at atmospheric pressure where temperature is usually below 100ºC. Regarding the recent studies, oxidative desulfurization can reduce the sulfur content of diesel and gasoline with 1500 ppm to less than 5 ppm while its cost is less that of traditional hydrotreater plants [3].M41S is the generic term for the various types of MCM (Mobil Composition of Matter) materials in the mesoporous rang. MCM-41 is the most widely studied M41S material [4].This is due to thesimplicity and ease in its preparation with negligible pore-networkingand pore-blocking effects [5].It consists of an amorphous(alumino, metallo)-silicate framework forming hexagonalpores. MCM-41 has high surface areas of up to 1200 m^2/g and largepore volumes. The pores are very uniform causing narrow pore sizedistributions[6].Inthis study, a kind of ternary acidic solid catalysts that include POM / MoO_3 / MCM - 41 is used. Using this nano-catalysis POM / MoO_3 / MCM- 41 is in desulfurization. The advantage of using this nano-catalysts is having a relatively large surface area and volume, which is a good alternative to Theconventional catalysts. The required Tests to prove Nanvshdn such as Sem, FT-IR, XRD and The BET test to obtain specific surface area of the catalyst weredone. Then optimizing parameters such as molar ratio of O / S, temperature, time and catalysts to achieve maximum conversion rate rate was done.

References

[1] Anbia. M, Hariri, S. A. Desalination 2010, 261, 61-66
[2] J. A. Kadijani, E. Narimani, H. A. Kadijani 2014, 56, 116-123
[3] G. Zhang, Yu. F. Wang 2009, 51, 196

Chemical Composition of the Methanolic Extract From the Aerial Parts of *Ferula haussknechtii Wolff ex Rech.f.* From Iran

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The genus *Ferula* is represented in the Flora of Iran by 30 species, including 15 endemic [1]. The resins of the plant have been used in China as a remedy for malaria and dysentery and also as an insecticide. Othermedical uses are also reported, such as sedative, antispasmodic, for toothache, asthma, cough, epilepsy, fever, irritable colon, as an antihystericfor feminine sterility, and against rheumatism. A large number of studies have concerned the genus *Ferula* and reported newly identified compounds extracted by solvent. The reported compounds are mainly coumarin derivatives and sesquiterpene alcohol esters, most of which are aromatic esters bearing the daucane skeleton [2]. Few studies have reported the chemical composition of *Ferula* essential oils. The aerial parts of *Ferula haussknechtii* was collected from Ilam, in July 2015. Voucher specimens have been deposited at the Herbarium of the Research Institute of Forests and Rangelands (TARI), Tehran, Iran.The methanolic extract of the air-dried aerial parts of the plant was obtained by percolation method. The extract was analyzed by GC and GC/MS. Sixteen components were identified in the extract of *F.haussknechtii* representing 85.4% of the total components detected. The major compounds of methanolic extract were (Z) -α- atlantone (20.8%) and (E) -α- atlantone (19.2%) followed by iso menthyl lactate (7.9%), neo- menthyl lactate (5.9%), (Z) – menthyl jasmonate (5.7%) and hexadecane (5.4%).Water distilled oil obtained from the aerial parts of *F. szowitsiana* has been the subject of our previous studies. α- Pinene (12.6%), germacrene D (12.5%) and β- pinene (10.1%) were found to be the major constituents [3].

References

[1] V. Mozaffarian, A Dictionary of Iranian Plant Names, Farhang Moaser Publisher, Tehran, Iran (1996) 228.
[2] G. Appendio, G.Ctavotto, O. Sterner, M. Ballero, J. Nat. Prod 64 (2001) 393.
[3] Z. Habibi, H.R. Aghaie, R. Ghahremanzadeh, S. Masoudi, A. Rustaiyan, Journal of Essential Oil Research 18 (2006) 503.

The adsorption of tetrazole derivatives at the surface of TiO_2 anatase for dye-sensitized solar cell application: a periodic density functional theory study

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Dye-sensitized solar cells (DSSCs), which have been considered as one of the most promising and low-cost alternatives to conventional inorganic silicon-based solar cells, have attracted considerable attention since reported by O'Regan and Grätzel in the 1990's [1-3].In this work, we have selected four typical additives, 2H-tetrazole (2HTz), 2H-tetrazole-5-thiol (5TTz), 2H-tetrazole-5-amine (5ATz) and TBA, to investigate their interaction modes and mechanisms with TiO_2anatase (101), (100) and (001) surfaces in both vacuum and acetonitrile conditions by a periodic DFT method. The results are analyzed by means of adsorption modes and energies, band structures, total and partial density of states (TDOS and PDOS). We find that the additive adsorption can strongly affect the geometric and electronic structures of three different TiO_2 surfaces. Moreover, the solvent environment and the adsorption density of additive molecules are also important and influential to the structural, energetic and electronic properties of additive-anatase systems so as to influence the conversion efficiency of DSSC. Table 1 shown key adsorption and electronic structure parameters of both bare and additive sensitized TiO_2anatase (101) surfaces with and without solvent condition.

Table 1.

Adsorbate	**N-Ti bond length (°A)**	**Hydrogen bond length H...O_{2c} (°A)**	**Adsorption energy E_{ad} (kcal mol^{-1})**	**Fermi energy (eV)**	**ΔFermi energy (eV)**	**Band gap (eV)**
Vacuum						
Bare				-6.546		2.61
2HTz	2.307	1.751, 2.868	26.225	-6.546	0.000	2.42
5ATz	2.249	1.743, 2.219	31.897	-6.008	0.538	1.44
5TTz	2.288	1.696, 2.117	57.357	-6.080	0.466	1.39
TBP	2.301	2.065, 2.326	31.374	-6.023	0.523	2.59
Acetonitrile						
Bare				-6.447		2.61
2HTz	2.2823	1.744, 2.883	19.075	-6.398	0.05	2.59
5ATz	2.211	1.769, 2.213	15.302	-5.914	0.54	1.44
5TTz	2.364	1.689, 2.086	15.628	-5.971	0.48	1.52
TBP	2.278	2.083, 2.349	27.893	-6.200	0.25	2.37

References

[1] M. Grätzel, Nature414 (2001) 3.
[2] B. Hosseinzadeh, A. S. Benia, A. N. Chermahini, R. Ghaharyc, A. Teimouri,Synthetic Metals 209 (2015) 1.
[3] Y. Qin, M. Li, C. Yan, S. Liu, W. Dai1, M. Li,Journal of Materials Science: Materials in Electronics 27 (2016) 3974.

Theoretical studies of triazolinedionesas reusable reagents for the oxidation of 1,4-dihydropyridines and dihydro-1*H*-pyrazoles via an anomeric based oxidation

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The modeling of the reactions of 4-propyl-1,2,4-triazole-3,5-dione as oxidizing agent for theoxidation of 1,4-dihydropyridines and 4-(*p*-chloro)phenyl-1,3,4-triazole-3,5-dione as an effective oxidizing agent for the oxidation of 1,4,5-triphenyl-4,5-dihydro-1*H*-pyrazole was performed on the basis of the anomeric based effect (Figures 1 and 2). The modeling and the appropriate calculations on the structures of the precursors, the different positions of the transition states (TS) of the reactions, intermediates and the products have undertaken by DFT-B3LYP/6-31G* method [1]. The theoretical study shows that stepwise anomeric based oxidation (ABO) have suitable structures than concerted pathway. The different aspects of this study were investigated and the obtained resultsare presented.

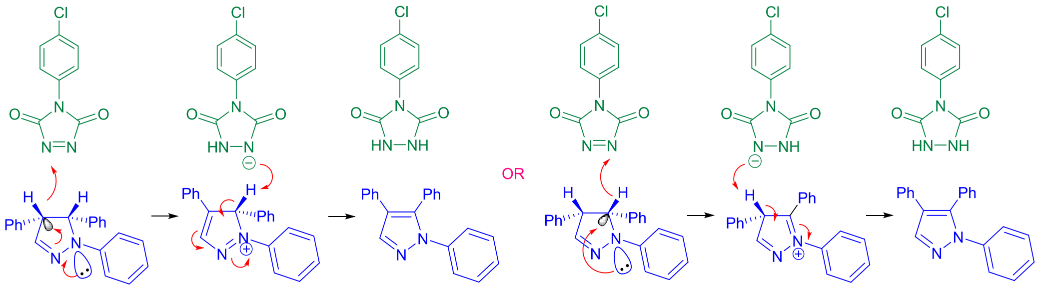

Figure 1. Stepwise anomeric based oxidation mechanism in the synthesis of 1,3,5-trisubstituted pyrazolines

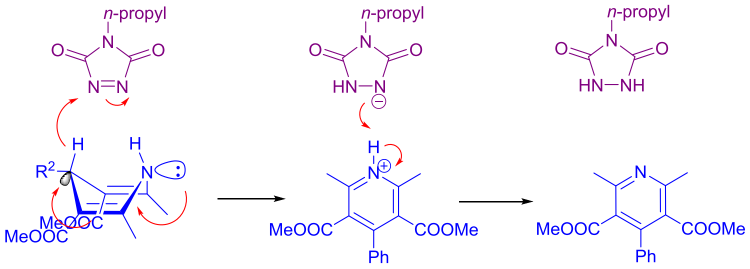

Figure 2. Stepwise anomeric based oxidation mechanism in the synthesis of 1,4-dihydropyridines

References

[1] All of the calculations were performed by: *Spatran '10*-Quantum Mechanics Program: (PC/x86) 1.1.0v4. 2011, Wavefunction Inc., USA.

Superparamagnetic $Fe(OH)_3@Fe_3O_4$ nanoparticles: An efficient and recoverable catalyst for transamidation of primary carboxamides, phthalimide, urea and thiourea with amines

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The amide bond formation is an important functional group in chemistry and nature due to its presence in polymers, dyes, peptides, and protein structures [1]. Transamidation of amides with amines is an attractive method for exchanging the constituents of two different amide groups. Due to the high stability and easy separation of the catalyst from the reaction mixture by using an external magnet, magnetic nanoparticles-supported catalysts have been successfully deployed in a variety of important organic reactions [2]. As part of our continuing interests in using magnetic nanoparticles as catalyst support in organic reactions, we have recently reported the results obtained for the tandem oxidative amidation of alcohols with amine hydrochloride salts using superparamagnetic $Fe(OH)_3@Fe_3O_4$ nanoparticles catalyst [3].To further establish other organic transformations with our catalyst, herein, we describe an inexpensive, magnetically recoverable and environmentally friendly catalytic system ($Fe(OH)_3@Fe_3O_4$) for the transamidation of primary carboxamides, phthalimide, urea and thiourea with amines (Figure 1).

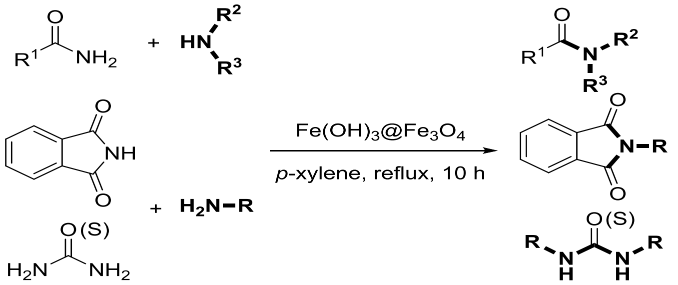

Figure1. $Fe(OH)_3@Fe_3O_4$ catalyzed transamidation of primary carboxamides, phthalimide, urea and thiourea with amines.

References

[1] (a) W. Wrasidlo and J. Augl, Journal of Polymer Science Part A-1: Polymer Chemistry, 1969, 7, 321-332; (b) J. Szadowski and Z. Niewiadomski, Dyes and pigments, 1993, 21, 123-133; (c) J. M. Humphrey and A. R. Chamberlin, Chem. Rev., 1997, 97, 2243-2266.
[2] M. B. Gawande, P. S. Branco and R. S. Varma, Chem. Soc. Rev., 2013, 42, 3371-3393.
[3] M. Arefi, D. Saberi, M. Karimi and A. Heydari, ACS Comb. Sci., 2015, 17, 341-347.

Studies on the Preparation, Structure and Characteristics of Magnetic Nanohydrogels by Modified Starch as Crosslinker for Anticancer Drug Carriers

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Within the past two decades, the use of magnetic micro- and nanoparticles in biomedical applications has attracted more and mor attention. In this respect, the design of polymeric (nano-)carrier materials is a key part of *de novo* drug delivery systems (DDSs). Among them multi-stimuli responsive biodegradable polymeric nanocarriers for targeted and controlled drug delivery are particular of interest, in part due to their good biocompatibility, high drug loading capacity, adequate stability in the bloodstream, long circulation properties, and selective accumulation at the site of action together with a suitable drug release profile [1-2].

For this purpose, the starch end-caped itaconatmacromonomer (StIAM) was adsorbed onto the surface of Fe_3O_4 nanoparticles, and then copolymerized with NIPAAm*via* a ‘free’ radical initiated polymerization technique (MNHG). The chemical structures of sample as representatives were characterized by means of FTIR and ^1H NMR spectroscopies. The LCST, morphologies, elemental compositions, and magnetic properties of the synthesized MNHGwere examined. Finally loading efficiency and release rate of methotrexate were assessed.

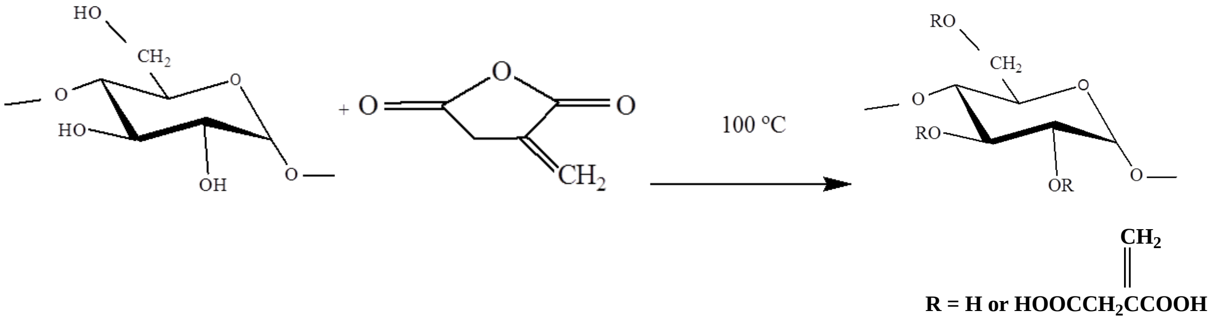

Figure 1. Scheme of the reaction.

References

[1] Zhao, S.; Wang, D.; Zhang, K.; Zhang, H. Int. J. Polym. Mater.Polym. Biomater64 (2015) 792.

[2] Ding, S.; Shen, Y.; Walters, K. B.; Chen, J.; Jin, Y. Int. J. Polym. Mater.Polym.Biomater 63(2014) 487.

[3] Tay, S.H., Pang, S.C., Chin, S.F..Carbhy.Polym. 88 (2012)1195.

Synthesis of Star-Shaped Terpolymer Hyperbranched Polyester–PCL-PANI as a Biodegradable–Conductive Polymer

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The conductive polymers such as polyaniline (PANI), and its derivatives have been witnessed an immense interest for the fabrication of conductive scaffolds due to its simple synthesis, chemical and electronic properties[1]. In this respect, hyperbranched aliphaticpolyesters(HAP) and polycaprolactone(PCL) may be appropriate candidates for improvement of aniline properties, in part due to their biocompatibility, biodegradability, their highly branched structure and wide range of practical, technological, and biomedical applications [2-3]. The HAP were synthesized by the meltpolycondensation reaction and poly(ε-caprolactone) arms have been grown on some of its end hydroxyl groups (HAPCL) by the ring opening polymerization. The synthesized macromonomer (HAPCL) subsequently were employed in chemical oxidation copolymerizations with aniline monomers to produce star-shaped PANI (S-PANI) with (HAPCL)core.Theterpolymer ,HAPCL and HAP were characterized by FT-IR,^{1}HNMR,scanning electron microscopy and cyclic voltammetry.

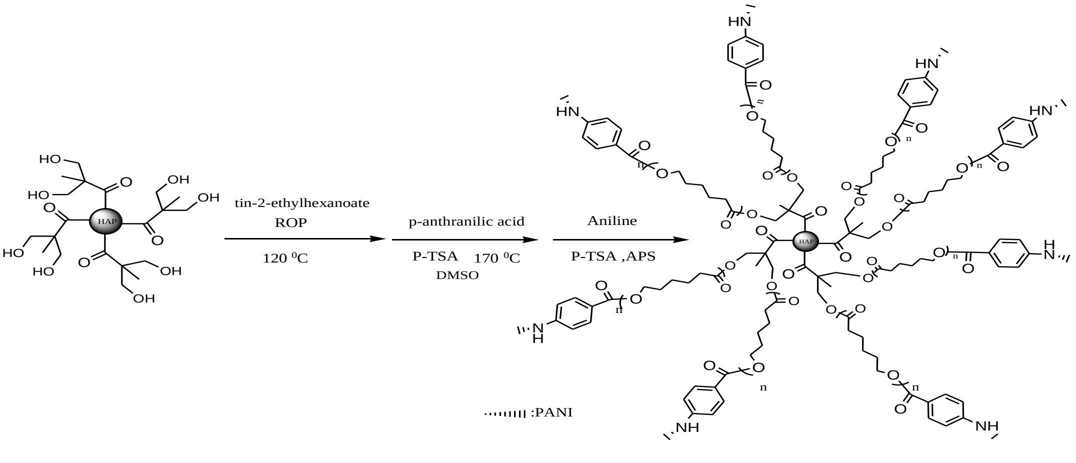

Figure 1. Scheme of the reaction

Refrences

[1] Xin Zhao, Peng Li, BaolinGuo, Peter X. Ma, ActaBiomaterialia 26 (2015) 236.

[2] Jean-d'Amour, K. Twibanire, T. Bruce Grindley.Polymers 4(2012) 794.

[3] Adrian M. Tomuto, Xavier Fernandez-Francos, FrancescFerrando, Xavier Ramis and Angels Serra.Polym.Adv.Technol 24(2013) 962.

Synthesis of Amphiphilic Hydrogels Based on Polyethylene glycole and Polycaprolactone for Drug Delivery Application

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Hydrogels are presently under investigation as matrices for the controlled release of bioactive molecules, in particularpharmaceutical proteins, and for the encapsulation of living cells [1]. Hydrogels based on poly ethylene glycol (PEG) in combinationwith a biodegradable polyester have the advantages of biocompatibility and degradability and have thus found applications inbiomedical systems [2]. In this research, azide-functionalized polycaprolactone (PCL) and poly ethylene glycole were synthesized, separately. Afterwards, pentaerythritol was functionalized by alkyne groups by using of propargyl bromide. The functionalization of precursor was confirmed by IR and H-NMR spectroscopy. In the final step amphiphilic hydrogels were synthesized by coupling of azide and alkyne groups of precursors in the presence of Cu (I) and sodium ascorbate catalyst system (Click Chemistry). The amount of hydrophobic (PCL) and hydrophilic (PEG) parts of hydrogels were 25%-75%, 50%-50%, and 75%-25%, respectively. The results show, with increasing of PEG percentage in hydrogels structure, the swelling increased in water.

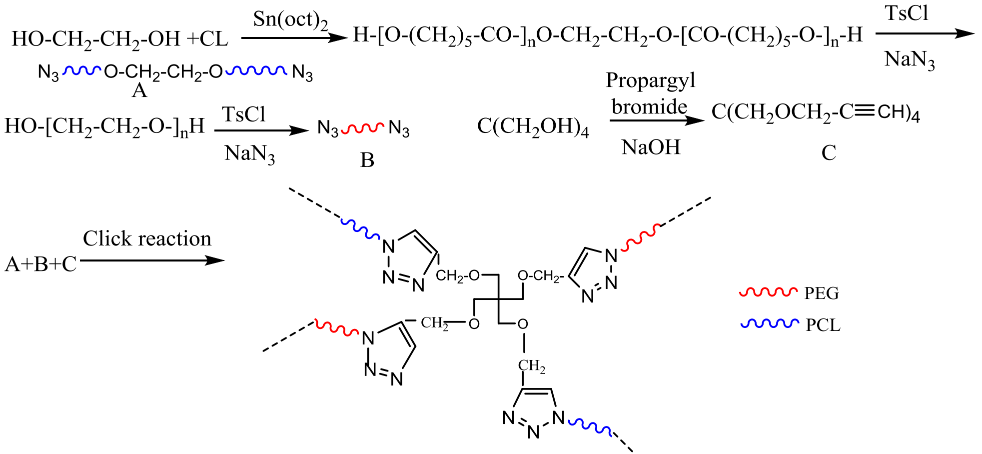

Figure 1. Scheme of the reaction

References

[1] W.E Hennink, C.Van Nostrum, Novel crosslinking methods to design hydrogels. Advanced drug delivery reviews.64 (2012), 223.

[2] L. Klouda,A.G. Mikos, Thermoresponsive hydrogels in biomedical applications. European Journal of Pharmaceutics and Biopharmaceutics, 68(2008), 34.

Development of a Control Release System for Co-delivery of 5-Fluorouracil and Folic Acid based on Natural Polymer-Montmorillonite Composites

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In recent years, the discovery of new drug delivery systems based on biomaterials has attracted much attention for treatment of cancer diseases. Widely used biomaterials for the controlled release of anticancer drugs include natural polymers, such as alginate (Alg), chitosan (CS), and cellulose derivatives [1]. Chitosan, a cationic polysaccharide consisting of d-glucosamine and *N*-acetyl glucosamine, has been extensively applied in drug delivery systems, because it is biodegradable, biocompatible, non-immunogenic, non-carcinogenic, anti-bacterial and mucoadhesive. The use of polyelectrolyte complexes (PEC) between the anionic polymers such as Alg and cationic CS has been widely studied for the controlled delivery of drugs [2]. Among chemotherapeutic compounds in the treatment of cancer diseases, 5-fluorouracil (5-FU) is one of the most widely used antineoplastics drugs for the treatment of different cancer diseases. However, it metabolizes so fast that the biological half-life is only 10-20 min [3]. Studies on the applications of clays to carry out specific functions such as delaying and/or targeting drug release, improving drug dissolution, increasing drug stability and modifying drug delivery patterns have been reviewed. Among layered silicate materials, montmorillonite (MMT), has attracted a great deal of attention due to its ability to release drugs in a controlled manner, mucoadhesiveness to the pharmaceutical formulations, ability to cross the gastrointestinal barrier and orally bioavailability [4]. In this study to develop a control drug release system for 5-FU, and the synergitic effect of folic acid in cancer chemotherapeutic compounds, drugs were loaded on montmorillonite layers by intercalation method. In order to control the drug release, the prepared nanocomposites was compounded with Alg, and further coated with CS. This novel drug delivery system was characterized by Fourier transform infrared spectroscopy (FT-IR), X-ray diffraction (XRD), and scanning electron microscopy (SEM) analyses. By in vitro experiments the effects of MMIT contents and pH of the release media on the release rate of the drugs were investigated. According to the results, the prepared nanocomposite system is suitable for co-delivery of 5-FU and folic acid with a controlled manner.

References

[1] H. Xu, H. Ma, P. Yang, X. Zhang, X. Wu, W. Yin, H. Wang, D. Xu. Colloids and Surfaces B: Biointerfaces 136 (2015) 729.
[2] G. Rassu, A. Salis, E. P. Porcu, P. Giunchedi, M. Roldo, E. Gavini. Carbohydrate Polymers 136 (2016) 1338.
[3] N.S. Rejinold, K.P. Chennazhi, S.V. Nair, H. Tamura, R. Jayakumar. Carbohydrate Polymers 83 (2011) 776.
[4] M.G. Apps, A.J. Ammit, A. Gu, N. J. Wheate. Inorganica Chimica Acta 421 (2014) 513.

Mk tvsjhnl Evaluation of Anticancer Properties on Synthesized (Z)-Methyl 2-(1-(benzo[d]thiazol-2-yl)-2-oxo-1,2-dihydroimidazo[2,1-a]isoquinolin-3(10bH)-ylidene)acetate on TC-1 cell line)

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Most of the drugs which are currently used were detection by organic chemistry reactions. In recent years, synthesis of fused heterocycles are of interest due to their medicinal activities. Dihydroimidazoisoquinoline and its derivatives are very important multi-ring compounds due to their pharmacological and biological activities [1-4].

In this study evaluation of anticancer properties of synthesized (Z)-methyl 2-(1-(benzo[d]thiazol-2-yl)-2-oxo-1,2-dihydroimidazo [2,1-a] isoquinolin-3(10bH)-ylidene)acetate on TC-1Cell Line is described [5].

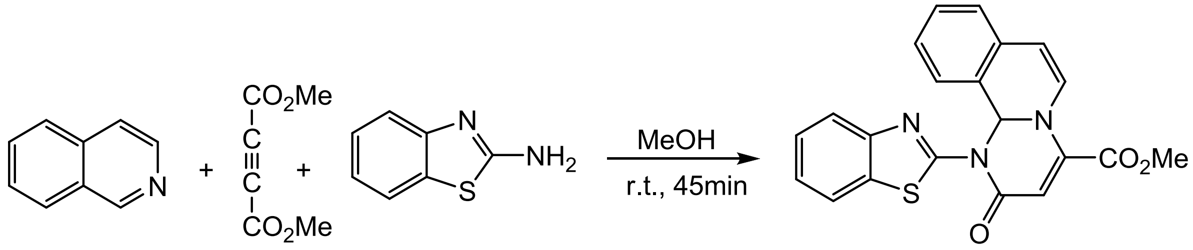

Figure 1. Scheme of the reaction.

References

[1] M. Chang, M.H. Wu. Y.L. Chen. Tetrahedron Letters 53 (2012) 4146.
[2] V. G. Brunton, P. Br. Workman. Journal of Cancer 1993, 67, 989.
[3] G. D. Ho, W. M. Seganish, A. Bercovici, D. Tulshian, W. J. Greenlee, R. D. V. Rijn, A. Hruza, L. Xiao, D. Rindgen, D. Mullins, M. Guzzi, X. Zhang, C. Bleickardt, R. Hodgson, Bioorganic Medicinal Letters 2012, 22, 2585.

Synthesis of Silver Nanoparticles via Poly (Acrylamide),Chitosan g-poly (Acrylamide) Hydrogel Networks by use of $NaBH_4$ and Glucose as Reducing Agent and use them for Antibacterial Application

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Nanoparticles (NPs) and nanostructured materials areconsidered as an important class of materials that have foundfascinated interest in biomedical, catalytical, opticaland electronic as well as quantum-size domain applications. A number of methods have been suggested anddeveloped for the synthesis of non-agglomerated nanoparticles. These include polymers, biological macromolecules, latex particles, mesoporous inorganicmaterials dendrimers, microgels or hydrogels, colloidal systems, and others. Most of theabove mentioned systems provide a good stability for nanoparticles, but microgel or hydrogel network template/carriersystems can act in a similar way. In addition, these make itmore convenient for producing smaller size nanoparticles.However, these make it more convenient for producing smallersize nanoparticles [1]. Poly (Acrylamide),Chitosan g-poly (Acrylamide) hydrogel had synthesized according to Kim et al [2] and Pourjavadi et al [3]. Briefly after synthesizing hydrogels they placed in $AgNO_3$ solution for 24 hours and after that they transferred to $NaBH_4$ and Glucose with NaOH solutions with different concentrations. Effect of hydrogel kind, reducing agent species and their concentrations on the size of silver nanoparticles have been studied. The formationof silver nanoparticles has been confirmed with ultraviolet visible (UV–Vis) spectroscopy, dynamic light scattering (DLS), TEM, SEM, Fourier transform infrared (FT-IR) spectroscopy, X-ray diffraction (XRD) analyses. Thermogravimetric analysis (TGA)provides the amounts of silver nanoparticles exist in the hydrogel networks. In conclusion, we have demonstrated that controlled sized silver nanoparticles with 10-40 nm were synthesized inside the hydrogeltemplates. The nano-composites exhibitfair anti-bacterial action against E. coli and B.cereus as model bacteria.

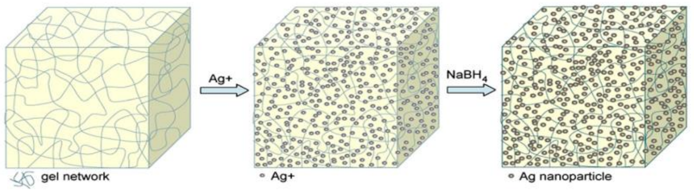

Figure 6. Schemeatic representation for the Ag nanoparticles formation in the hydrogel network [1]

References

[1] Y.M. Mohan, K. Lee, T. Premkumar, K.E. Geckeler, Polymer 48 (2007) 158.
[2] A. Pourjavadi, G.R. Mahdavinia, Turkish Journal of Chemistry 30 (2006) 595.
[3] S. Kim, G. Iyer, A. Nadarajah, J.M. Frantz, A.L. Spongberg, International Journal of Polymer Analysis and Characterization 15 (2010) 307.

Synthesis and characterization of Ni-Cr-NO_3 layered double hydroxide prepared by co-precipitation at hydrothermal conditions

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Layered double hydroxides are nanostructured materials with positive charge which can form nanobiohybrids in combination with biomolecules with negative charge (such as vitamins, drugs and DNA strings). In this research project Ni-Cr-LDH was synthesized with metal ratio of 3:1by co-precipitation method at hydrothermal conditions. These solutions were kept at pH 10.5. The optimal operating conditions was reported T=65°c and time=24 h.The prepared LDH was characterized by X-ray diffraction (XRD), fourier transform infrared spectrometer (FT-IR), ultra violet (UV), cyclic voltametery (CV) and scanning electron microscopy (SEM). The XRD patterns exhibit the characteristic reflections of LDH which are sharp and symmetric at low 2θ angle. In the FT- IR spectra an intense and broad adsorption band located at 3510 cm^{-1} was observed, which was attributed to the OH stretching due to the presence of hydroxyl groups and interlayer water molecule of LDH. λ_{max} of Ni and Cr salts were different with λ_{max} of LDHin the UV spectra.The electrochemical investigations in different pH revealed that the obtained electrode can be used as a sensor and was used in presence of 2-nitro phenol electrocatalysis.

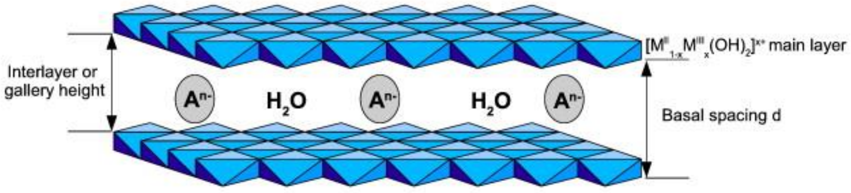

Figure 1. structure of LDH

References

[1] P. Nalawade, B. Aware, V. Kadam, R. Hirlekar, Layered double hydroxides: A review, J. Sci. Ind. Res, 68 (2009) 267-272.

[2] E.T. Thostenson, C. Li, T.-W. Chou, Nanocomposites in context, Composites Science and Technology, 65 (2005) 491-516.

Nano TiO_2/SiO_2: An Efficient and Recyclable Catalyst for the Synthesis of 1-Amidoalkyl-2-naphthols

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Amidoalkylnaphthols are observed in the structure of some nucleoside antibiotics and HIV protease inhibitors. They have also possess useful biological and pharmacological properties such as adrenoceptor blocking, antihypertensive, and Ca^{2+} channel blocking activities [1]. Amidoalkylnaphthols are also important synthetic building blocks and are used as precursors for the synthesis of cardiovascular-active 1-aminomethyl-2-naphthols [2], and 1,3-oxazines [3]. Recently nano catalyst pay attended special interest because of the vast area that elevated their efficiency. In this work, the preparation of some novel amidoalkylnaphthols using nano TiO_2/SiO_2 as an efficient nano catalyst is described via the three-component reaction of 2-naphthol, various aldehydes, and (thio)amides in the presence of catalytic amount of nano TiO_2/SiO_2 under thermal solvent-free conditions. This simple protocol offer advantages such as short reaction times, simple work-up procedure, excellent yield, and recovery and reusability of the catalyst.

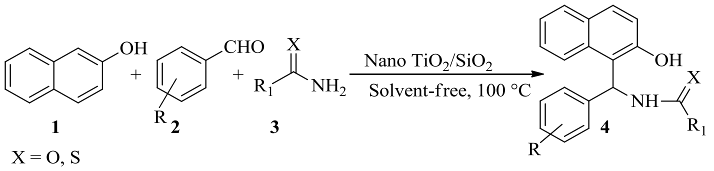

Figure 1. Synthesis ofamidoalkylnaphthols using nano TiO_2/SiO_2.

References

[1] S.A. Karnail, B.C. O'Reilly, E.P. Ruby, Ch.F. Turk, G. Aberg, M.M. Asaad, J.L. Bergey, S. Moreland, J.R. Powell, J. Med. Chem. 30 (1987) 627-635.
[2] A.Y. Shen, C.T. Tsai, C.L. Chen, Eur. J. Med. Chem. 34 (1999) 877-882.
[3] B.P. Mathew, A. Kumar, Sharma, P.K. Shukla, M. Nath, Eur. J. Med. Chem. 45 (2012) 1502-1507.

Synthesis of new antibacterial nanocomposite based-Cubane and its application in combination cancer therapy

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Explosives and Drugs are two completely different categories so that one destroys and the other cures. But now it has been proved that these two different manners exist in an eight-carbon box-shape compound called cubane simultaneously. The first usage of the cubane in medicinal chemistry returns to a patent in 1971.The mentioned compounds in this report were the potent antiviral agents [1]. Resistance of cancer cells to chemotherapy drugs is the most challenging part of cancer therapy that could be omitted when multiple drugs are delivered simultaneously; though, different drugs target different components of the cancer cell. The combined therapy from more than one anticancer drug can produce the optimal therapy effect [2].On the other hand, the body's immune system under chemotherapy become weak and susceptible to infectious diseases, so the during of chemotherapy for these patients, antibiotics are prescribed. Regardless of great amount of antibiotics and chemotherapeutics accessible for medical use, meanwhile the growing number of multi-drug resistant microbial pathogens produced in the last decades revealed an extensive medical requirement for novel antimicrobial agents [3]. In this study based-silica polymeric nanocarrier with anticipating the anti-bacterial properties was designed and developed as dual anticancer drug delivery system. The chemical structure, stimuli responsive co-delivery of anticancer drugs, anti-bacterial and anti-tumoral property of the developed system was fully characterized.

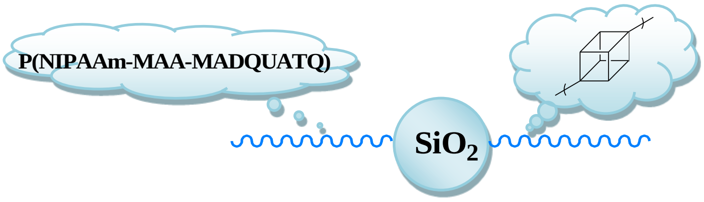

Figure 1. Structure of nanocomposite

References

[1] Biegasiewicz K. F., Griffiths J. R., Savage G. P., Tsanaktsidis J., Priefer R.; Chem. Rev. 115 (2015) 6719−6745.
[2] Ouahab A, Shao C, Shen Y, Tu J.; Drug Dev Ind Pharm. 40 (2014) 860-8.
[3] Rizzotto M. INTECH Open Access Publisher; (2012).

Dual anticancer drug delivery by smart antibacterial nanocomposite based-tetrazol

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Tetrazole is a cyclic and aromatic compound including a carbon and four nitrogen atoms in a five-membered ring. In the category of heterocyclic compounds, tetrazole derivatives, in particular 5-substituted tetrazoles, are successfully utilized in medicine, biochemistry, agriculture and fine organic synthesis. Also a large number of medicinally important tetrazole heterocyclic incorporated drugs such as antihypertensive, antihistamine, diuretics, antiparasitic, anticancer drugs, inhibitors of thrombosis, and drugs with anti-inflammatory, anesthetic, antifungal, tuberculostatic and antiviral activity approved by the FDA [1].Smart carriers can increase the penetrance and survival of drugs in tumors and decrease the side effect and toxicity related with most anti-cancer drugs. Introducing different stimulus-responsive properties to DDSs is an efficient way to achieve these goals [2].Cancer cells can develop resistance to chemotherapy drugs, but are less likely to develop resistance when multiple drugs are delivered simultaneously. However, different drugs target different parts of the cancer cell [3].In this research a novel antibacterial polymeric nano-system was developed for combination cancer therapy. The synthesized nanocarrier was fully characterized and its antibacterial activity was assessed by MIC values against some bacterias and funguses.DOX and MTX as anticancer drugs were conjugated concurrently to nanocarrier with an encapsulation efficiency of about 95% and sustained the release of both drugs up to 20 days with apparent pH-triggered controlled release manner. Cell viability tests affirmed that the co-administration of DOX with MTX lead to an efficient anticancer performance to MCF7 cell lines verified by MTT assay test.

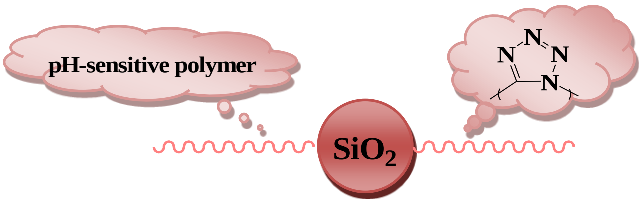

Figure 1.structure of nanocomposite

References

[1] Wei C-X., Bian M., Gong G-H.; Molecules. 20 (2015) 5528-5553.
[2] Wang C-F., Mäkilä EM., Kaasalainen MH., et al.; Acta biomaterialia.;16 (2015) 206-214.
[3] Kang L., Gao Z., Huang W., Jin M., Wang Q.; Acta Pharm Sin B. (2015).

Novel approach for curcumin analogues synthesisas overcoming drug resistance in cancer therapy using EDAHS as recyclable catalyst

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Generally the classical synthetic methodologies involve expensive reagents and catalysts, which are not easily available and require harsh reaction conditions. Thus there is need to replace such reagents and catalysts. The threat to ecological and environmental synthesis due to the damages caused by the chemicals has put forward a new area of the so called “Green Chemistry” that ionic liquids are incncept. Currently protic ionic liquids (PILs) have got popularity due to their extensive liquid temperature range, ionic conductivity and high thermal stability, which is ample for practical applications PILs, usually synthesized by the neutralization reaction of Bronsted acid and base, establish one of the most vital classes of ILs [1]. The development of new anti-cancer treatments with greater efficacy and fewer side effects remains a significant challenge of modern scientific and medical research. Curcumin, a natural polyphenol found in the dietary spice turmeric, has been demonstrated to inhibit cancer cell survival and proliferation, and to induce apoptosis without promoting the development of side effects[2].

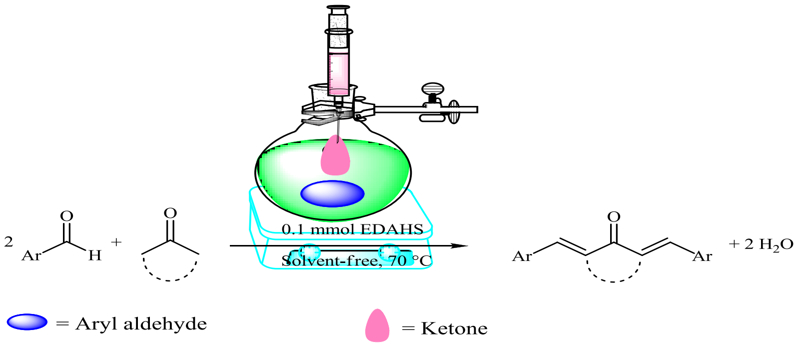

Figure 1. Reaction of ketone and aromatic aldehyde derivatives in EDAHS

We have successfully developed a simple and an efficient method for the synthesis of curcumin derivatives under solvent-free conditions by the condensation of various aromatic aldehydes, using cheap and readily available EDAHS as a protic ionic liquid catalyst. For this purpose, a mixture 4-methylbenzaldehyde (0.24 mL, 2 mmol) and 1,3-diketones (0.13 mL, 1 mmol) was treated with EDAHS (0.026 gr, 0.1mmol) at 70 °C for 40 min.When the starting aldehyde had completely disappeared, the reaction mixture was quenched by adding H_2O (10 mL) and filtered.

References

[1] R. Xiang, F. Chen, L. Wu, S. Li, Q. Chen, *Electrochimica Acta*, 56 (2011) 7503.
[2] A. Scharstuhl, H. Mutsaers, S. Pennings, W. Szarek, F. Russel, F. Wagener, *J. Cell. Mol. Med,* 13 (2009) 712.

The Electron Affinity Energy of Aromatic Hydrocarbon; Rylenes

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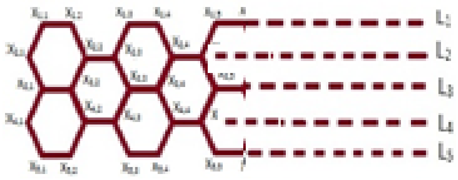
Aromatic hydrocarbon from the root of benzene can provide suitable environments for electron transition due to p orbitals, upper and lower electron clouds, and resonance phenomenon. Rylenes is a family of organic molecules with the chemical formula of $C_{10n}H_{4n+4}$which is focused in nanomedicines.Topological Indices, introduced in chemistry science using molecular graphs, are real numbers and constant [1]. The RRR index (Reduced Reciprocal Randic) has been firstly defined by Ivan Gutman in 2014 [2].Consider simple graph of Rylenes ($C_{10n}H_{4n+4}$) as presented in Figure 1. It is first tried to produce a relationship between the RRR indexesbased on the number of rings (n) as the following:

$$RRR(G) = (16 + 4\sqrt{2})n - 8 \qquad (1)$$

Then RRR index is measured for Rylenes usingequation (1). The electron affinity energy (E_{aff}) of Rylenes was calculated using Gaussian 09 software and data were compared with those mentioned in valid papers[3]. Figure 2 shows the changes in E_{aff} ofRylenesaccording to the RRR index. Therefore, E_{aff} ofRylenescould be well predicted by the following equation:

$$E_{affinity} = 1.1516 ln(RRR) - 3.1243 \qquad (2)$$



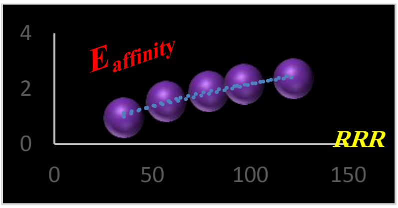


Figure1. Simple molecular graph of Rylenes.**Figure2.** E_{aff} of Rylenes according toRRR index.

References

[1] N. Trinajstic, Chemical Graph Theory. 2nd Edition, CRC Press, Boca Raton (1992).
[2] I. Gutman, B. Furtula and C. ElphickThree, MATCH Commun. Math. Comput. Chem., 72, (2014).
[3] G. Malloci, G. M ulas, G. Cappellini and C. Joblin, Chem. Phys. 340 (2007).

Aerobic Photo Oxidation of Alcohols by Tetrabutylammonium Tribromide (TBATB)

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The oxidation of alcohols to the corresponding carbonyl compounds is a key reaction in organic synthesis. The selective oxidation of alcohols to aldehydes orketones is a very important organic transformation, especially in preparing of some important precursors and intermediates for drugs, fine chemicals, vitamins and fragrances [1]. Acyclic and cyclic acetals of various carbonylcompounds were obtained in excellent yields under a mildreaction condition in the presence of trialkyl orthoformateand a catalytic amount of tetrabutylammonium tribromide(TBATB) in absolute alcohol [2]. In this work, we reported aerobic photo oxidation of alcohols by TBATB to corresponding carbonyl compound at room temperature. The carbonyl compound was characterized by ^{1}HNMR,^{13}CNMR, Gas Chromatography (GC) and FT-IR. This method presented high yield, chemoselective, and safe, operationally simple under mild reaction conditions, fast and cost-effective. Also, this investigationshowed that we used light as a green and available source.

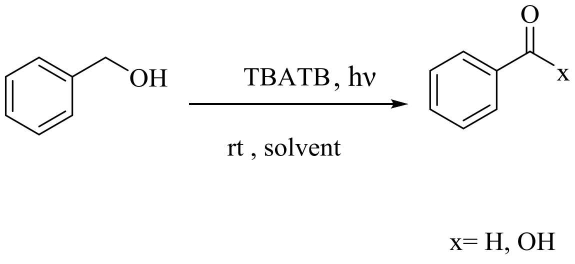

Figure 1. Aerobic photo oxidation of alcohols.

References

[1] J. Muzart, Tetrahedron 59 (2003) 5789.
[2] R. Gopinath, B.K. Haqueand Patel, Journal of Organic Chemistry 67 (2002) 5842.

Phytochemical Content of Aerial Parts of *Salvia Limbata* From Sabzevar-Iran

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Salvia limbata is one species of the genus *salvia* which is belongs to the family of lamiaceae[1]. The wide variety of secondary metabolites such as flavonoids, tannins, and terpenoids were found in the essential oil of the plant that investigated for their pharmacological properties like analgesic; anti-inflammatory;hemostatic; antioxidant; antimicrobial and as an antitumor remedy[2]. Inthis study, we investigate the presence of some phytochemical compounds such as phenolic, flavonoid, alkaloid, anthraquinone, terpenoid, and steroids compounds in the extracts of aerial parts of *S.limbata.*The plant was collected from Sabzevar in May 2015. First of all, the plant part of *S. limbata* include flower and leaf were dried at room temperature, gritted, and steeped in methanol for 72 hours at room temperature. Then thecrude extract was condensed with rotary and fractionated with n-hexane,ethyl acetate and water, respectively. Finally different reagents were applied on TLC or extracts solution to screen of the presence of group of compounds. Wagner regent (I_2+KI) for alkaloids(produce of brownish precipitate); $H_2SO_4$and $CHCl_3$ for steroeids and terpenoids compounds (formation two phase); $FeCl_3$ (1%) for phenolic compounds; KOH (5%) for anthraquinons, and $AlCl_3$ (1%) for flavonoids(dark green, red, and yellow points on the TLC profile respectively)[3].The results are shown in Table 1.

Table1: Phytochemical content of the aerial parts of Salvia limbata

Plant Parts	**Fractions**	**Compounds**				
		Phenolic	Flavonoid	Alkaloid	Anthraquinone	Steroid and Terpenoid
Flower	n- Hexane	-	-	-	-	-
	Ethyl acetate	✓	✓	-	-	-
	Water	-	✓	✓	-	-
Leaves	n- Hexane	-	-	-	-	-
	Ethyl acetate	✓	✓	-	-	-
	Water	-	-	✓	-	-

Reference

[1] S.E. Sajjadi, Z. Shahpiri. Journal of Pharmaceutical Sciences, 12 (2004) 94.
[2] M. Karami, E. Hossini, N. S. Majd, M. A. Ebrahimzadeh, S. Alemy, Journal of Clinical Excellence 3 (2015) 1.
[3] H. Harlina, A. Prajitno, E. Suprayitno, H. Nursyam, Aquatic Science and Technology 1 (2013) 15.

Green Synthesis of Silver Nanoparticles Using Aqueous Extract of *Salvia Limbata*

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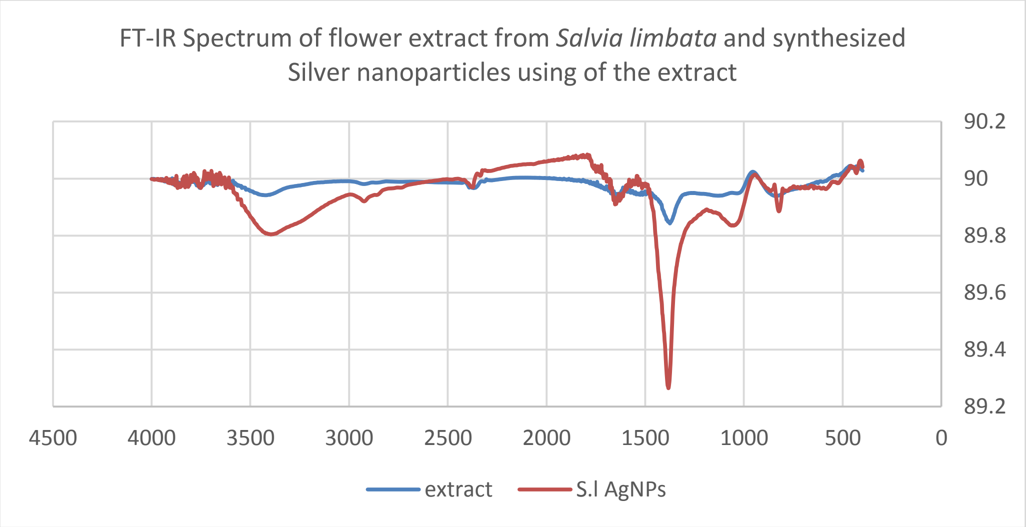
Silver nanoparticles have unique properties in molecular diagnostic and are also used in several aspects. AgNPs are used as anti-bacterial agents, catalyst, and optical sensors. [1]. Physical and chemical methods are the major ways to synthesis of silver nanoparticles (AgNPs); but the procedures are toxic, environmentally hazardous, and expensive [2]. Using of microorganisms and plant extracts is an alternative methods, which stands in green chemistry scope. In this study we synthesis the AgNPs using water extract of *salvia limbata* and also evaluate the effect of temperature on the synthesis of AgNPs. First, The flower of plant was collected, driedand milled. 100 g of the dried powder of the plant partwas added to 200 ml of double distilled water and boiled for 5 min. The obtained extract was filtered. Finally 5 ml of the extract was added to 100 ml of 1mM aqueous $AgNO_3$ solution. The mixture was stirred for 24 h at different temperatures (30, 40, 50, 60, and 70 °C). The maximum yield of Ag NPs were obtained at 30°C. Formation of nanoparticles were characterized by Uv-Vis., FT-IR spectroscopy, X-ray, AFM, and SEM.



Reference

[1] S. Prabhu, E.K. Poulose. International Nano Letters 2 (2012) 1.

[2] A.M. Awwad, N.M. Salem, A.O. Abdeen, International Journal of Industrial Chemistry 4 (2013) 1.

A One-Pot synthesis of oxazepine-quinazolinone bis-heterocyclic scaffolds via isocyanide-based three-component reactions

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To date, the development of new methods for the synthesis of heterocyclic compounds has been and remains a hot topic in organic chemistry, due to their importance in biologically active natural products and synthetic materials.The well-known biological properties of benzoxazepines[1] and quinazolinones[2] prompted us to synthesize molecules in which both nuclei exist. As a part of our ongoing research program on the isocyanide-based MCRs,[3] herein, we report the synthesis of oxazepine-quinazolinone *bis*-heterocyclic scaffolds **4** by an Ugi One-Pot three-component four-center reaction of 2-(2-formylphenoxy)acetic acid **1** as a bifunctional reagent, 2-aminobenzamide **2**, and an isocyanide **3**. The target compound is obtained without using any catalyst in excellent overall yields. It is worth mentioning that in the course of our reaction, one C-C bond, several C-N bonds, one amide group, a benzoxazepine ring and a quinazolinone ring are newly formed. These new structures broaden the scaffolds that are accessible through Ugi reactions, and may represent interesting pharmacophores.

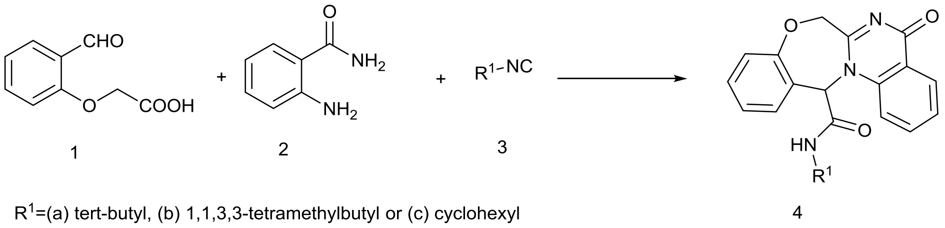

Figure 1. Synthesis of oxazepine-quinazolinone*bis*-heterocyclic scaffolds 4.

References

[1] H. Agirbas, B. Kemal, F. Budak. Med. Chem. Res. 20 (2011) 1170.
[2] K. Nepali, S. Sharma, R. Ojha, K. L. Dhar. Med. Chem. Res. 22 (2013) 1.
[3] S. Shaabani, A. Shaabani, S. W. Ng. ACS Comb. Sci. 16 (2014) 176.

Copper(I) Oxide Nanoparticles Supported on Magnetic Casein as a Bio-Supported and Magnetically Recoverable Catalyst for Aqueous Click Chemistry Synthesis of 1,4-Disbustituted 1,2,3-Triazoles

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As is well known, nanoparticles with small sizes tend to aggregate in solution. To avoid uncontrolled growth or aggregation in the preparation of nanoparticles, the stabilizer such as polymers, surfactants or small organic molecules is often used[1]. Casein, a proline rich globular protein which is readily available in milk, can be thought as block copolymers consisting of blocks with high levels of hydrophobic or hydrophilic amino acid residues[2]. As a part of our ongoing research program on the development of new catalytic systems with emphasise on green and natural supports[3], herein, we present a successful preparation and excellent catalytic activity of copper(I) oxide nanoparticles supported on magnetic casein (Cu_2O/Casein@Fe_3O_4NPs). One-Pot three-component reaction of various alkyl halides, sodium azide and various alkynes was carried out under environmentally-friendly conditions with excellent yields in short reaction time at room temperature (Figure 1). To the best of our knowledge, this work is presented as the first example to demonstrate the usefulness of casein as a support for copper(I) oxide nanoparticles and it is a novel catalyst with unique properties for the Huisgen 1,3-dipolar cycloaddition to prepare 1,4-disubstituted-1,2,3-triazoles.

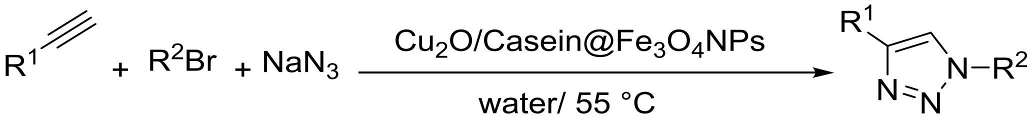

Figure 1. Synthesis of 1,2,3-triazoles by Cu_2O/Casein@Fe_3O_4NPs as catalyst.

References

[1] Y. Weizmann, D. M. Chenoweth, T. M. Swager. J. Am. Chem. Soc. 132 (2010) 14009.
[2] Y. Liu, R. Guo. Biomacromolecules 8 (2007) 2902.
[3] A. Shaabani, S. Shaabani, H. Afaridoun. RSC Adv. 6 (2016) 48396.

Preparation of nanoparticles of cobalt and nickel nanoparticles from cobalt(II) and nickel(II) complexes with ligands based on salicylidene

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In this research cobaltnanoparticles of average diameter (30 -70) nm and nickel nanoparticles average diameter (30 -50) nm by thermal decomposition.[Bis (salicylidene) cobalt(II)] and [Bis (salicylidene) nickel (II)] were used as precursor. Metal particles smaller than100nmprimary particle diameter are generally considerd as nanoparticles. Such metal nanoparticles often exhibit very interesting electronic,magnetic, optical, and chemical properties. For example, their high surface-to-volume rations have large fractions of metal atoms at surface availablefor catalysis. The different combinations of triphenyl phosphine ($C_{18}H_{15}P$) and oleylamine ($C_{18}H_{37}N$) were added as surfactants to control the particle size. The resultant samples are characterized by X-ray diffraction (XRD) and scanning electron microscopy (SEM) to depict the decreased of size and morphology.

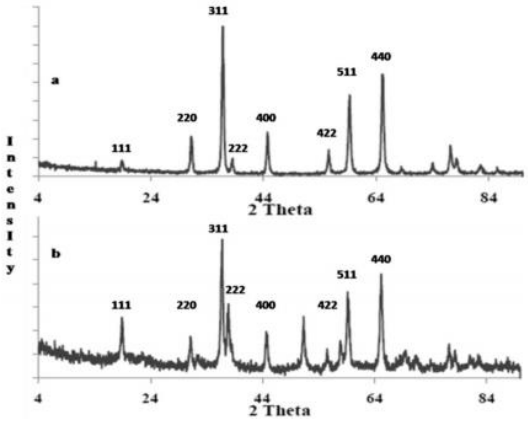

Figure 1. PXRD patterns of Co and Ni nano particles

References

[1] C.P. Chen , T.H. Chang , T.F.Wang , Ceram . Int. 27(2001) 925.
[2] M. Salavati– Niasari , M .Shaterian , M.R,Ganjali, P.Norouzi , J. Mol . Catal.A 261(2007) 147.

Phytofabrication of silver nanoparticles assisted by fruit of Nopal and its free radical scavenging property

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Development of biologically inspired experimental processes for the synthesis of nanoparticles is evolvinginto an important branch of nanotechnology. An eco-friendly synthesis of inorganic nanoparticle is afast growing research in the limb of nanotechnology [1-3]. In the present study, it is reported that Nopal fruit mediated synthesis of silver nanoparticles by the reduction of Ag ions. The color change in reaction mixture (pale yellow to dark brown)was observed during synthesis process. Biosynthesized silver nanoparticles showed surface Plasmonresonance at around 450 nm.The morphology and structure of synthesized silver nanoparticles were characterized on Scanning Electron Microscopy (SEM) equipped with a Thermo EDAX attachment, TransmissionElectron Microscopy (TEM), X-ray diffraction (XRD), (FT-IR), Dynamic Light Scattering (DLS) whichreveals that the Ag nanoparticles are spherical and the average particle size is 17.96 nm.Crystalline natureof the nanoparticles is confirmed from the XRD pattern. FTIR spectrum indicates that the biomoleculesof carboxyl, amine and hydroxyl functional groups involved in the reduction of silver nanoparticles. The biosynthesized silver nanoparticles displayed considerable antioxidant capacity.

References

[1] P. Mukherjee, A. Ahmad and D. Mandal, Nano Letters1(10), (2001), 515.
[2] F. Li JL, L. Wang and X. Y. Liu, Cancer Letters274(2), (2013), 319.
[3] S. Ashokhumar, S. Ravi, V. Kathiravan, S. Velmurgan, Spectrochimica Acta Part A: Molecular and Biomolecular Spectroscopy134**,** (2015)**,** 34-39.

Preparation of tetra star-shaped conducting polymers based on polyaniline , and blend with polycaprolactones for preparation of nanofibers via electrospinning method

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Among the known organic conducting polymers, polyaniline (PANI) has attracted special attention. Several methods have been developed to improve the processibility of PANI[1-2]. In this work, we used PEG because of its good properties such as hydrophilicity and biodegradability to synthesis of A_2BA_2 tetraarm star-shaped polymer with A= PANI and B= PEG. In the first step, PEG (M_n~2000 g/mol) was capped by an epoxy group at the ω-position by the reaction with epichlorohydrin. Then, the epoxy ring was converted into two hydroxyl groups by hydrolysis. At the next step, these hydroxyl groups were esterified with 4-amino benzoic acid. Finally, the star polymer was prepared by reaction of this end functionalized PEG with ammonium persulfate as initiator for polymerization of aniline monomers. In this step, both polyaniline homopolymer and star polymer were formed. We seprated them upon their solubility. Thene the blends of copolymers and polycaprolactone prepared by electrospinning method and are converted into the fibrs.. The chemical structure of star polymer was determined by FT-IR and ^{1}H NMR spectroscopy. Cyclic voltammetry (CV) stedies showed that this star polymer is electroactive. Morphology star polymer and fibers was investigated by scanning electron microscopy (SEM). This novel system opens up new and interesting opportunities for applications such as electroactive scaffold for tissue engineering.

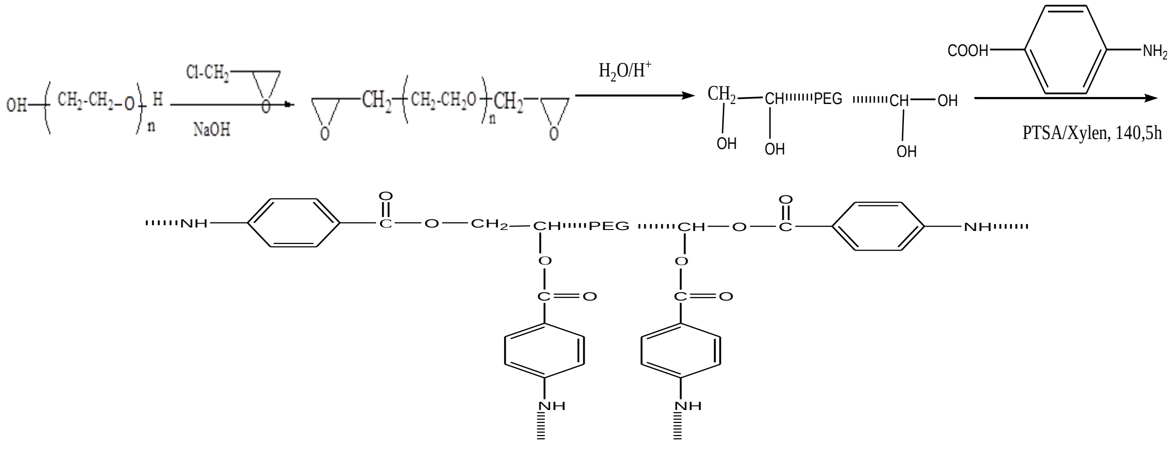

Figure 1. Scheme of the reaction

References

[1] Kerileng M.Molapo, Peter M. Ndangili, Rachel F. Ajayi, Milua Masikini, J. Electrochem. Sci.,2012.

[2] Higashihara,T., Hayashi,M., Hirao,A., 2011, Progress in Polymer Science, 36: 323.

Efficient synthesis of aryloylamido coumarins derivatives via three-component coupling of 4-hydroxycoumarin, aryl glyoxal, and amides catalyzed by ZnO nanoparticles

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Modern synthetic design demands high efficiency in terms of minimization of synthetic steps together with maximization of complexity [1]. One of the ways to fulfill these goals is the development and use of multicomponent reactions which consist of several simultaneous bond-forming reactions and allow the high efficient synthesis of complex molecules starting from simple substrates in a One-Pot manner [2].Coumarin and chromene and their derivatives have attracted considerable attention from organic and medicinal chemists for many years as a large number of natural products contain this heterocyclic nucleus. They are widely used as additives in food, perfumes, cosmetics, pharmaceuticals and optical brighteners and dispersed fluorescent and laser dyes. Thus the synthesis of derivatives of this nucleus is of much interest [3].We herein describe a practical and inexpensive method for the preparation of aryloylamido coumarins derivatives via a three-component condensation reaction between 4-hydroxycoumarin, aryl glyoxal, and amides or in the presence of ZnO nanoparticles as catalyst under thermal and solvent-free conditions.

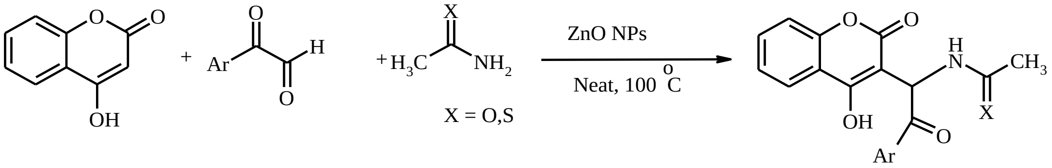

Figure 1. Scheme of the reaction.

References

[1] B. M. Trost, Science. 254 (1991) 1471.
[2] H.Bienayme, C.Hulme, G. Oddon, P.Schmidt, Chem.sEur. J. 6 (2000) 3321.
[3] A. J.von Wangelin, H.Neumann, D.Go¨rdes, S.Klaus, D.Stru¨bing, M.Beller, Chem.sEur. J.9 (2003) 4286.

Phthalocyanines@ magnetic chitosan: As an efficient nanocatalyst for selective aerobic oxidation of alkyl arenes and alcohols

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Oxidation is the second largest industrial process that plays an important role in organic chemistry [1]. The synthesis of the valuable oxygen-containing compounds (ketones, aldehydes, esters, and acids) from hydrocarbons in the aerobic oxidation conditions is an important challenge for the chemical industry and a large number of homogeneous and heterogeneous catalytic systems have been developed for aerobic oxidation processes.

Phthalocyanines (PCs) are important compounds that have attracted considerable attention due to their excellent properties and have many applications in dye-synthesized solar cells, photodynamic therapy, pigments, dyes, and biomimetic catalyst. Various supports such as silica, activated carbon, metal-organic frameworks and biopolymers as a support have been used for immobilization the phthalocyanines [2]. Recently, we have showed that phthalocayanines immobilized onto graphen and cellulose were efficient catalysts for organic transformations. Within our program on sustainable organic transformations and nanocatalyst [3], we have introduced the phthalocyanines@ magnetic chitosan as an efficient nanocatalyst for an aerobic oxidation of various alkyl arenes and alcohols.

References

[1] Z. Guo, B. Liu, Q. Zhang, W. Deng, Y. Wang, Y. Yang, Chem. Soc. Rev., 43 (2014) 3480.
[2] A.B. Sorokin, Chem. Rev., 113 (2013) 8152.
[3] A. Shaabani, M. Borjian Boroujeni, M.S. Laeini, Appl. Organomet. Chem., 30 (2016) 154.

A Stimuli-Responsive ABC Triblock Copolymer Based on P(SEMA-*b*-NIPAM-*b*-VEA): RAFT synthesis and “Schizophrenic” Micellization

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This article describesthe synthesis of ABC, Stimuli-Responsive triblock copolymers were prapared via reversible addition-fragment chain transfer (RAFT) polymerization. In this work, we report a systematic study of how morphological changes of poly[(succinic ethyl methacrylate)-b-poly(N-isopropylacrylamide-b-poly(N-4-vinylbenzyl),N,N-diethylamine); P(SEMA-b-NIPAM-b-VEA)]occurred with combined stimulus of temperature and pH . The “schizophrenic” behavior of PSEMA-b-PNIPAM-b-PVEA was observed by means of Fourier transform infrared (FTIR), and ^{1}H nuclear magnetic resonance (NMR) spectroscopies, dynamic light scattering (DLS). The synthesis is accomplished by first polymerizing 2-hydroxyethylmethacrylate and N-isopropylacrylamide as a hydrophilic block in pH=4 and polyvinylethylamine as hydrophobic block in pH=10.The zeta potential measurements at various pHs demonstrated that the synthesized P(SEMA-b-NIPAM-b-VEA) triblock copolymer has zwitterionic properties .It is expected that the synthesized P(SEMA-b-NIPAM-b-VEA) triblock copolymer considered as a prospective candidate in nanomedicine applications such as drug delivery.

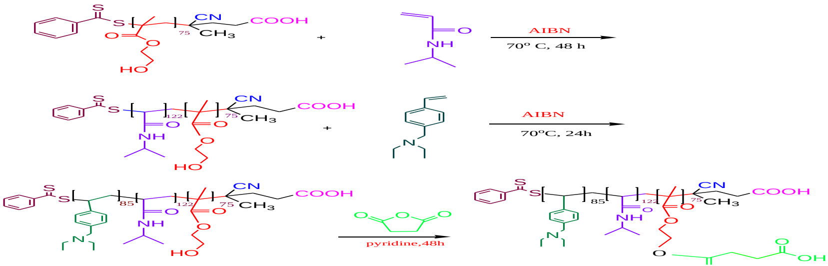

Figure 1.scheme of the reaction

References

[1] Adam E. Smith, Xuewei Xu, Stacey E. Kirkland-York, Daniel A. Savin, Charles L. McCormick, “Schizophrenic” self-assembly of block copolymers synthesized via aqueous RAFT polymerization: From micelles to vesicles. Macromolecules 2010, 43, 1210–1217.

[2] Zhang Q, Hong JD, Hoogenboom R. A triple thermoresponsive schizophrenic diblock copolymer. Polym Chem 2013; 4(16):4322–4325.

Vanadium(V)-Promoted Sulfoxidation in the Presence of Schiff Base of Glucosamine

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A series of Schiff-base ligands derived from 6-aminoglucose and various salicylaldehyde derivatives introducing different electronic and steric effects were synthesized and fully characterized. These ligands were used in vanadium-promoted sulfoxidation reactions and tested for their influence on the activity of the employed catalytic system. Generated catalysts perform superior to pre-prepared complexes.

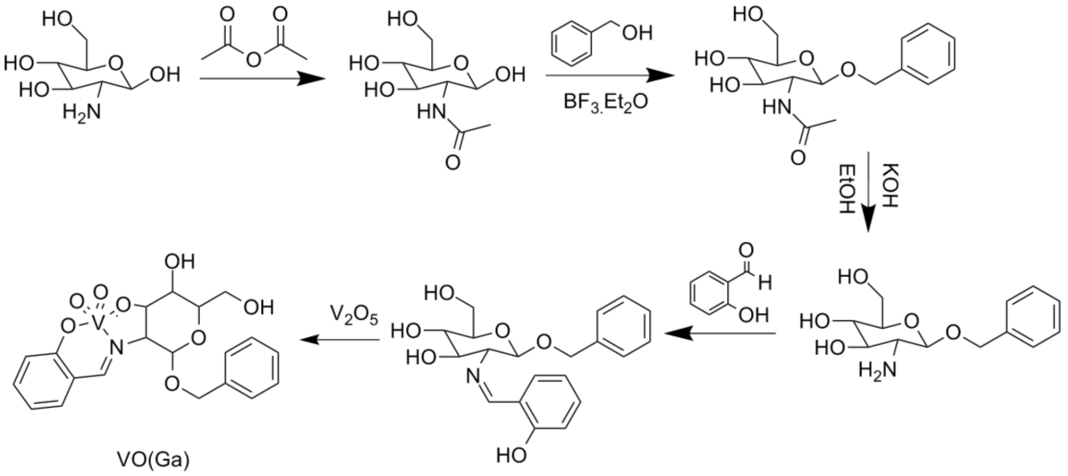

Figure 7. Vanadium complexation of schiff base synthesis of glucosamine.

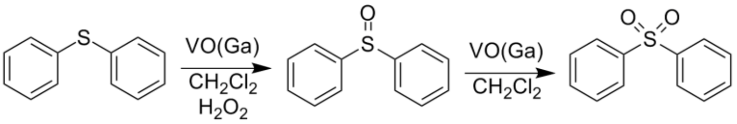

Figure 8. Vanadium-promoted sulfoxidation reaction

References

[1] G. Mohammadnezhad, R. Debel, W. Plass, Journal of Molecular Catalysis A: Chemical 410 (2015) 160.

Stereoselective synthesis of chiral aminonitriles by multicomponent Strecker reaction

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Multicomponent reactions have huge potential for the rapid generation of small molecules libraries. However, there is a continuous need for designing and carrying out the reactions with novel starting materials in organic synthesis[1].

Strecker reaction is one of the most important multicomponent reactions in organic chemistry for direct One-Pot synthesis of α-amino nitriles and other biologically relevant molecules[2]. Asymmetric strecker reaction could be done using chiral starting materials or chiral catalysts.

Layered double hydroxides (LDHs) are mineral and synthetic materials with positively charged brucite type layers of mixed metal hydroxides. LDHs have technological importance in catalysis, separation technology, medical science and nanocomposite material engineering[3].

In this approach, we would like to introduce chiral α-amino nitriles as an intermediated for novel α-amino acids. The reaction was carried out in presence of catalytic amount of LDH. Herein, we wish to report diastereoselective synthesis of α-amino nitriles with 2 chiral centers.

References

[1] Schreiber, S. L. Nature 457 (2009) 153.
[2] Enders, D.; Shilvock, J. P. J. Chem.Soc. Rev. (2000) 359.
[3] Nalawade, P.; Aware, B.; Kadam, V. J.; Hirlekar, R. S. J. Sci. Ind. Res. 68 (2009) 267.

An efficient synthesis of functionalized 3-(α-amidobenzyl)-4-hydroxycoumarin derivatives by nanoSiO$_2$-BF$_3$ promoted condensation reaction between aromatic aldehyde, 4-hydroxycoumarin, and amides

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Recently, multi-component and domino reactions are efficient and effective methods in the sustainable synthesis of heterocycles. Due to atom economy and simplicity of One-Pot procedures, multi-component reactions occupy a superior position compared with other reactions. These reactions are widely applied in pharmaceutical chemistry for producing different structures and combinatorial libraries for drug discovery [1-2].

Coumarin and chromene and their derivatives have attracted considerable attention from organic and medicinal chemists for many years as a large number of natural products contain this heterocyclic nucleus. They are widely used as additives in food, perfumes, cosmetics, pharmaceuticals and optical brighteners and dispersed fluorescent and laser dyes. Thus the synthesis of derivatives of this nucleus is of much interest [3].

Herein we have researched three-component coupling of 4-hydroxycoumarin 1, aryl aldehydes 2, and amides 3, in the presence of NanoSiO$_2$-BF$_3$ as heterogeneous catalyst to the synthesis of 3-(α-amidobenzyl)-4-hydroxycoumarin derivatives 4.

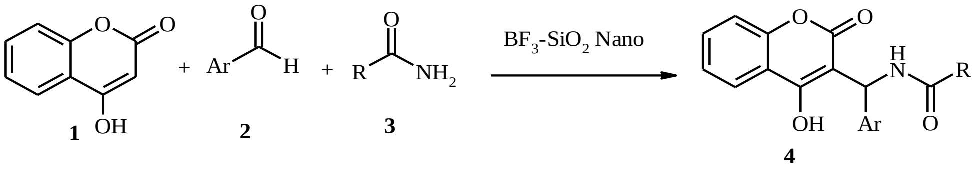

Figure 1.synthesis of functionalized 3-(α-amidobenzyl)-4-hydroxycoumarin derivatives

References

[1] S. L. Dax, J. J. McNally, M. A. Youngman, Curr. Med. Chem. 6, (1999). 255.

[2] R. W.. Armstrong, A. P. Combs, P. A. Tempest, S. D.Brown, T. A. Keating, Acc. Chem. Res. 29, 123(1996).

[3] A. J.von Wangelin, H.Neumann, D.Go¨rdes, S.Klaus, D.Stru¨bing, M.Beller, Chem.sEur. J.9 (2003) 4286.

Synthesis of substituted pyrrole derivatives in solvent free media with molybdenum complex supported on magnetic nanoparticles as recyclable catalyst

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Metal complexes immobilized onto metal nanoparticles are a category of relatively new promising materials for catalysis and analytical chemistry [1-2]. A magnetically recoverable catalyst consisting of molybdenum complex was prepared. The synthesized catalyst was characterized by X-ray powder diffraction (XRD), vibrating sample magnetometry (VSM), inductively coupled plasma atomic emission spectroscopy (ICP-AES) and Fourier transform infrared (FT-IR). The immobilized catalyst was shown to be an efficient heterogeneous catalyst for the synthesis of substituted pyrroles [3]. The catalyst could be easily and efficiently isolated from the final product solution by magnetic decantation and be reused for 5 consecutive reactions without showing any significant activity degradation.

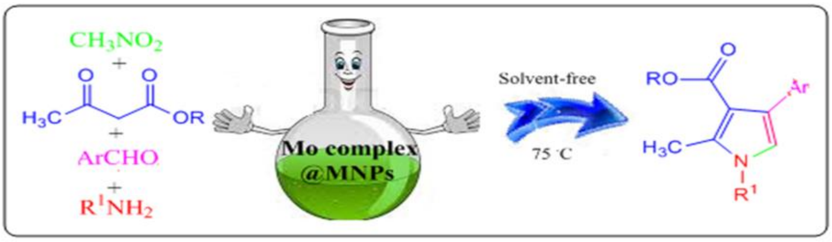

Figure 1. Mo complex@MNPs mediated synthesis of substituted pyrroles under solvent-free condition.

References

[1] M. Y. Zhu, C. J. Wang, D. H. Meng and G. W. Diao, J. Mater. Chem. A, 1 (2013) 2118-2125.
[2] V. Polshettiwar, R. Luque, A. Fihri, H. Zhou, M. bouhara and J. M. Basset, Chem. Rev., 111 (2011)3036-3075.
[3] D. M. D’Souza, T. J. J. Muller, Chem. Soc. Rev., 36 (2007) 1095–1108.

Synthesis of magnetic molecularly imprinted polymers for selective release and take up of thiopental barbiturate

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Molecular imprinting is known as a technique for creation oftailor-made binding sites with memory of the shape, size andfunctional groups of the template molecules. Molecularly imprinted polymers (MIPs) can be synthesized by copolymerization of the functionalmonomers and cross-linkers in the presence of template molecules. After removal of the template molecules, recognitioncavities complementary to the template molecule in shape,size and chemical functionality were formed in the highlycross-linked polymer matrix, which can selectively rebindthe template molecules from a mixture of closely related compounds, as shown below[1].

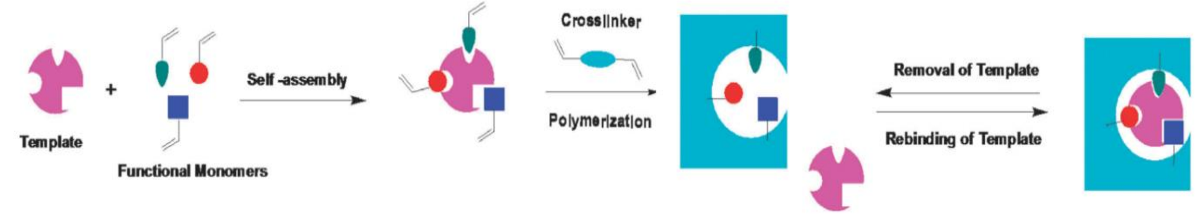

Figure 1. Preparation of MIP.

Surface imprintingapproach has advantages in comparision with the traditional MIPs (e.g. complete template removal, high bindingcapacity, fast kinetics and mass transfer).

In this work, surface imprinting was formed on magnetic nanoparticles (MNPS) so that a core shell structure was achieved (Core: MNPs, Shell: MIP network). Thanks to this hybrid system, not only the advantages of the surface imprinting approach, but also the desired properties of MNPs can be exploited [2].Barbiturates, belong to anticonvulsant drugs and having sedative and hypnotic properties, are used as template molecules.Furthermore, they are frequent drugs of abuse and their abuse is now widespread [3]. MNPs (Fe_3O_4) was synthesized by coprecipitationusing $FeCl_2.4H_2O$ and $FeCl_3.6H_2O$ as raw materials. Then theMNPs modified and functionlized with with a functional silica layer through sol-gel method. Then, the prepared functional MNPs, thiopental (as template and an anesthesia drug), methacrylic acid (as a functional monomer), ethyleneglycoldimethacrylate (EGDMA) as cross-linker and finally AIBN were copolymerized.The structure, morphology, release and rebind properties of the resultant MIPs have been completely characterized.

References

[1] L. Chen, S. Xu, J. Li, Chem. Soc. Rev, 2011, 40, 2922–2942.
[2]S. Wang,B. Wang, H. Si, J. Shan, X. Yang, RSC Adv, 2015,5, 8028-8036.
[3] N. Funaya, H. Matsunaga, J. H. Aginaka,Chromatography 2015, 36, 39-44.

Synthesis and Characterization of Fe_3O_4@Au@Molecularly Imprinted Polymers (Fe_3O_4@Au@MIP) for Selective Release and Uptake of Thiopental Barbiturate

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Fe_3O_4@Au nanoparticles (core:Fe_3O_4, shell:Au) have received considerable attention because of their advantageous properties arisen from both individual Au and Fe_3O_4 nanoparticles. Specially, the coating of the magnetic Fe_3O_4nanoparticles to the biocompatible metal, gold, prevents not only the chemical and enzymatic degradation of the Fe_3O_4core, but also seems to be suitable for further binding of various types of compounds (especially sulfur-containing ones) and functionalization. Molecularly imprinted polymers (MIPs) that provide a surface for recognizing and binding a specific therapeutic substance, has an enormous potential to revolutionize the performance of drug delivery systems. MIPs can provide other advantages, such as tailored predefined drug recognition systems with binding site functionality, allowing for precise control of drug release or up take [1,2].

To benefit advantages of both Fe_3O_4@Au nanoparticles and MIPs, in this study, we prepare MIP network on Fe_3O_4@Au nanoparticles (Fe_3O_4@Au@MIP; core:Fe_3O_4, middle layer:Au, shell: MIP). Barbiturates, the most common drugs used in the practice anesthesiology, were used as template. In order to synthesize Fe_3O_4@Au@MIP, firstly Fe_3O_4@Auwas synthesized by three-step method; Fe_3O_4 nanoparticles were prepared by co-precipitation and reduced to Fe_2O_3 by nitric acid, and then Fe_2O_3 nanoparticles were used as seeds in sodium citrate solution to reduce the $HAuCl_4$,then, Fe_3O_4@Ausurface was functionalized with thiol compounds. Secondly, MIP was prepared by using of thiopental as a template, methacrylic acid as the functional monomer, ethylene glycol dimethacrylateas the cross-linker and AIBN as initiator. The resulting nanoparticles were characterized using TEM, FTIR, UV–Vis, XRD and their release and rebind behaviors were studied.

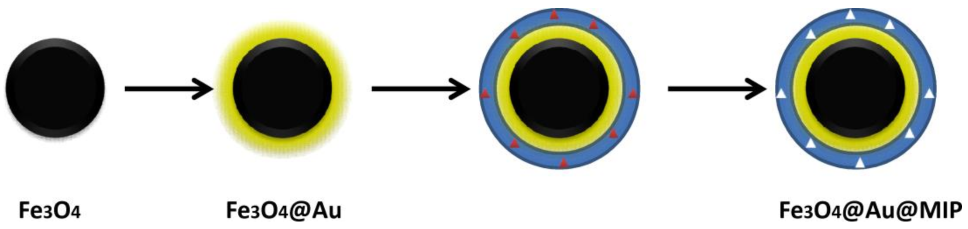

Figure 1. prosidure of MIPsynthesis

References

[1] S. M. Silva, R.Tavallaie, L. Sandiford, R.D. Tilley, J. J. Gooding, Chem. Commun, 2016, 52, 7528-7540.
[2] Pavel Štarha, David Smola, Jiří Tuček, Zdeněk Trávníček.Int. J. Mol. Sci. 2015, 16, 2034-2051.

Effect of surface-modified SiO_2 nanoparticles on termal and mechanical properties of DGEBA-IPD epoxy network

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In the last recent years, many researches have been registered about the surface modification of inorganic nanoparticles and their loading process in organic polymers thattheir reportages are seen in some review articles. [1-3]

In this investigation, silica nanoparticles are linked with Isocyanate-functionalized polyether through urethane linkages (Figure 1).

The resulting modified nanoparticles spread in-situ in a polymer matrix produced by the reaction between diglycidyl ether of bisphenol A (DGEBA, epoxy resin) and isophorone diamine (IPD) hardener.

The nanocomposites obtained with different amount of modified silica nanoparticles are verified by TGA‹SEM‹XRD‹FT-IR and DMA techniques.

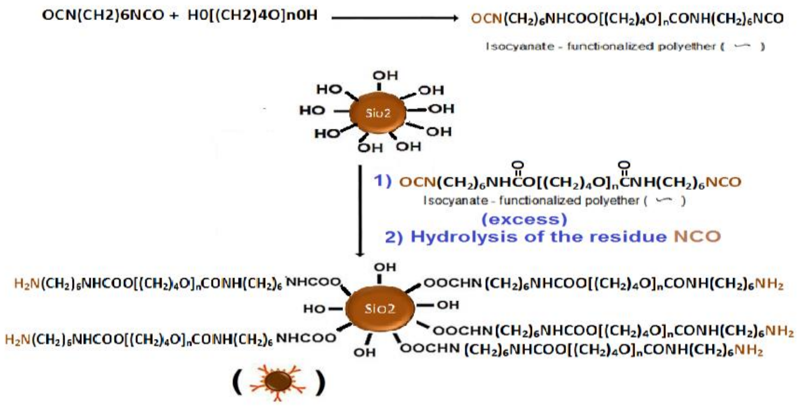

Figure 1.Modification of nanosilica

References

[1] R.Bagwe, L.Hilliard, W.Tan (2006). "Surface Modification of Silica Nanoparticles to Reduce Aggregation and Nonspecific Binding." American Chemical Society., 22 (9).

[2] S. Kangoa, S.Kaliab, A.Celli, J.Njugunad, Y.Habibie, R.Kumara (2013). "Surface modification of inorganic nanoparticles for development of organic–inorganic nanocomposites—A review." Progress in Polymer Science., 38.

[3] R.A.Sperling, W.J.Parak (2010). "Surface modification, functionalization and nanoparticles bioconjugation of colloidal inorganic." royal society publishing., 368.

PTMO-cured epoxy composites loaded by PTMO-coated silica nanoparticles

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Polymer nanocomposites have drawn considerable research interest due to significant enhancement in thermomechanical, electrical and morphological properties as compared to the pristine polymer matrix [1-3].

In the present study poly (tetramethylene glycol) (PTMG) is converted to the corresponding NH_2-terminated poly (tetramethylen oxide)(PTMO). Amine-functonallized PTMO (H_2N-PTMO-NH_2) is used both as the hardener of diglycidyl ether of bisphenol A resin to reach the related epoxy network and as the surface-modifier of silica nanoparticles. The resulting PTMO- derived epoxies are prodused in the presence of PTMO-coated silica nanoparticles, as shown in figure 1.

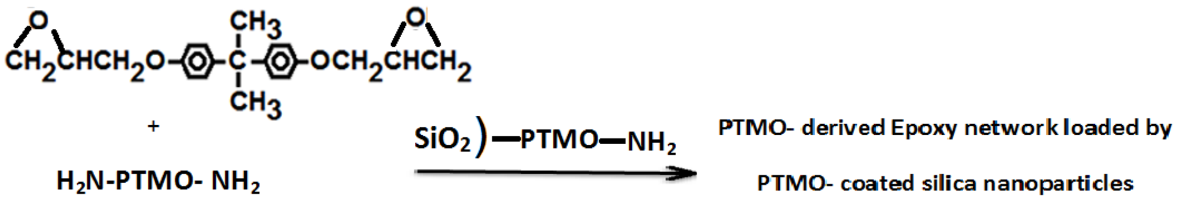

Figure 1. Schematic pregentation of Nanocomposites Synthesis

References

[1] S.S.Ray, M.Okamoto, Prog in Polym Sci 2003; 28: 1539-1641.

[2] Vikas Mittal, Materials 2009; 2: 992-1057.

[3] S.BJagtap, D.Ratna, eXpress Polym Lett 2013; 7: 329-339.

Greener synthesis of N-heterocyclic compounds in deep eutectic solvent under mild reaction conditions

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Deep eutectic solvents (DESs), as an advanced ionic liquid (ILs), obtained by the simple complexion of quaternary ammonium salts and the most frequently choline chloride with hydrogen bond donors (e.g. Urea, amide, acid, or polyol [1].

Multicomponent reactions (MCRs) are not only a powerful tools in organic, combinatorial and medicinal chemistry; they also represent an excellent framework of green chemistry [2].

Operationally simple, atom economical, and scalable synthesis of imidazoles from 1,2-diketones, aldehydes and amines and indolo[3,2-a] carbazoles from 1,2-diketones and indoles is shown to proceed readily in deep eutectic solvent with good yield. The scope of the reaction is quite broad; a variety of aromatic and aliphatic, activated and unactivated aldehydes as well as amines and indoles have all been shown to be viable substrates for this reaction.

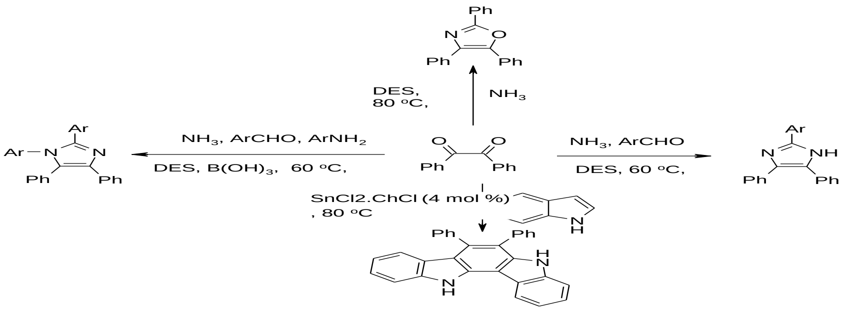

Figure 1. Synthesis of imidazole, oxazole and carbazoles

References

[1]Azizi, N. Aryanasab, F. Torkiyan, L. Saidi, M.R. J. Org. Chem. 2006, 71, 3634.
[2] Azizi, N. Torkiyan, L. Saidi, M.R. Org. Lett. 2006, 8, 2079.
[3] Acknowledgements: Financial support of this work by Chemistry and ChemicalResearchCenter of Iran is gratefully appreciated.

Preparation of nickel nanoparticles from spent catalyst

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In this project, a mild solvothermal method has been employed to successfully synthesize nanocrystalline zinc oxide and its covalent modifications with dithiopeptides and aminoacides which is a kind of novel and high-efficiency absorbent for the removal of acid dye methyl orange, metal from aqueous solution. In order to achieve further improvement of absorbent activity, the surface of ZnO was effectively modified with selected dithiocarbamate functionalities. We demonstrate for the first time dithiopeptides and aminoacides based DTC surface immobilization on ZnO and the application of this hybrid material for various propose. Different microscopic and spectroscopic techniques as well as size, surface and elemental composition analyses were employed to prove these modifications. The as-prepared products were characterized by transmissionelectron microscopy (TEM), scanning electron microscopy (SEM), X-ray diffraction (XRD), X-ray photoelectron spectroscopy (XPS), Fourier transform infrared spectroscopy (FTIR), Brunauer, Emmet, and Teller (BET), and Zeta potential measurements.

References

[1] A. McLaren, T. Valdes-Solis, G. Li and S. C. Tsang, J. Am. Chem. Soc. 2009 131 12540–12541.
[2] E. S. Jang, J. H. Won, S. J. Hwang and J. H. Choy, Adv. Mater. 2006 18 3309 – 3312 .
[3] K. S. Leschkies, R. Divakar, J. Basu, E. Enache-Pommer, J. E. Boercker, C. B. Carter, U. R. Kortshagen, D. J. Norris and E. S. Aydil, Nano Lett. 2007 7 1793–1798.

Synthesis and Molecular Docking of Some Xanthine Oxidase Inhibitors

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New drugs for the inhibition of the enzyme xanthine oxidase are in development and they have to be screened before being considered for preclinical and clinical evaluation. In order to understand the mechanism of ligand binding and to identify potent xanthine oxidase inhibitors, a study involving molecular docking and virtual screening has been performed[1]. The objective of the current study is to evaluate the xanthine oxidase inhibitory activity of three compounds using in silico docking studies. In this perspective, quercetin , allopurinol and a 1.4- dihydropyridine derivative were selected[2]. Allopurinol, a known xanthine oxidase inhibitor was used as the standard. In Silico docking studies were carried out using AutoDock 4.2, based on the Lamarckian genetic algorithm principle[3]. The two important parameters like binding energy and inhibition constant were determined. The results showed that all three selected compounds showed binding energy ranging between -7.0 kcal/mol to -4.4kcal/mol. The binding energy energy of , quercetin , 1.4 dihydropyridine derivative and allopurinol were -7.03 kcal/mol ,-5.20 kcal/mol and -4.4 kcal/mol respectively and inhibition constant were 6.85 μM , 360μM and 1040 μM respectively. The images of ligplot software showed that quercetin has three additional H-bonds comparing to other compounds. Regarding the data obtained for binding energies with docked target, docking outputs supported that higher binding energy of quercetincan be interpreted by additional H-bonds with the active sites of the receptor. These molecular docking analyses could lead to the further development of potent xanthine oxidase inhibitors for the prevention and treatment of gout and related inflammatory conditions.

References

[1] Muthuswamy Umamaheswari, Arumugam Madeswaran, Kuppusamy AsokkumarDiscovery of potential xanthine oxidase inhibitors using *in silico* docking studies, Der Pharma Chemica, 2011, 3 (5): 240-247

[2] Vivek Parashar Pandey , Surendra Singh Bisht , Mridul Mishra , Ashutosh Kumar ,Mohammad Imran Siddiqi , Aditya Verma c, Monika Mittal , Shraddha A. Sane , Suman Gupta ,Rama P. Tripathi , Synthesis and molecular docking studies of 1-phenyl-4-glycosyl-dihydropyridines as potent antileishmanial agents, European Journal of Medicinal Chemistry 45 (2010) 2381-2388.

[3] Hadi Adibi, Javid Shahbazi Mojarrad, Hadi Asgharloo, Gholamreza Zarrin, Synthesis, in vitro antimicrobial and antioxidant activities of chalcone and flavone derivatives holding allylic substitutions, Med Chem Res (2011) 20:1318–1324.

Synthesis, characterization and thermal study of some new nano-structure zinc(II) halide/pseudohalide complexes

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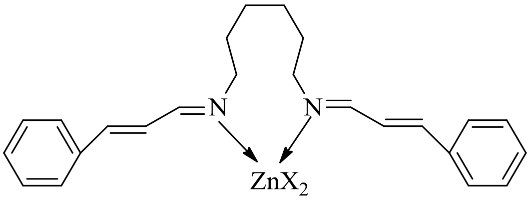
Nowadays nanostructure compounds are of interest because of notable properties with respect to bulk ones. Nanometer-size particles of metal coordination complexes enhance their physical and chemical properties that may be due to the large number of surface molecules when are compared with non-nanostructure compounds [1]. Schiff bases are the most widely utilized chelating ligands in the development of coordination chemistry. Schiff base compounds containing an imine group are usually formed by the condensation reaction between a primary amine and an active carbonyl. Because of the possible variety of the initial reactants for the synthesis of Schiff bases ligands, these compounds show a wide variety of chemical structures with different physicochemical properties [2]. In addition Schiff base metal complexes have been extensively investigated because of their potential applications in fields of science and technology such as catalysis area, medicine, optical industries, bioinorganic chemistry, polymer industries, and microbiological utilities [3].

In this work, we report synthesis, spectroscopic and thermal characterization of some new nano-structure zinc(II) coordination compounds of a bidendate Schiff base ligand entitled as (N^1E,N^6E)-N^1,N^6-bis((E)-3-phenylallylidene)hexane-1,6-diamine (Figure 1).The prepared compounds have been characterized by UV–visible, FT-SSIR, ^{1}H-NMR and ^{13} C-NMR spectra. Moreover the zinc complexes were prepared in nanostructure size under ultrasonic conditions that confirmed by XRD, SEM, and TEM analyses.



(X= Cl, Br, I, SCN, N_3)

Figure 1. The structure of complexes

References

[1] Z. Rashidi Ranjbar, I. Sheikhshoaie, Z. Bagheri, International Journal of Nano Dimension 5 (2014) 409.
[2] M.H. Habibi, E. Shojaee, G.S. Nichol, Spectrochimica ActaPart A 98 (2012) 396.
[3] M.B. Halli, R.B. Sumathi, Journal ofMolecular Structure. 1022 (2012) 130.

Synthesis, spectroscopic, and thermal studiesof some new nano-structure Cd(II) coordination compoundsofN,N-bis[(E)-3-(phenylprop)-2-enylidene]hexanediamine

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Schiff base metal complexes are in a field of coordinationchemistry with increasing interest. These compounds haveplayed a major role in the development of the inorganiccoordination chemistry due to easily preparation, diversity ofstructures, and providing the effects of steric interactions oncoordination geometries [1].In recent years, the Schiff base complexes have been found as oneimportant group of the coordination compounds dueto their valuable biochemical, analytical and antimicrobial properties. Moreover in organic methodology, Schiff base complexes have key role in catalysis of a variety of organic reactions such as metathesis process, reductive carbonylation, polymerization, decarboxylation and oxidation [2]. The study of nano structure compounds is an extremely popular field because of their unique properties that are absolutely different with respect to them in bulkphase that is related to the large numbers of surface molecules. Choosing the proper synthetic process is an important factor incontrol of the size of materials at the sub micrometer scale so thatselecting a proper method is a serious step in nanotechnology field [3].

In this research we report the synthesis, physical and spectral characterization, and thermal investigation of a new ligand and their complexes with generalformula $CdLX_2$in which X=Cl^- ,Br^-,I^-, SCN^- and $N_3^-$and L=N,N-bis[(E)-3-(phenylprop)-2-enylidene]hexanediamine. The nano-structure cadmium complexes were also prepared under ultrasonic irradiation and were characterized by various analyses such as FT-IR, UV–visible,^{1}H and^{13}C NMR spectra, XRD, SEM and TEM.

References

[1] V. Alexander, ChemicalReviews 95 (1995) 273.

[2] M. Montazerozohori, M. Sedighipoor, Sh. Joohari, International Journal of ElectrochemicalScience7 (2012) 77.

[3] H. Zhang, D.R. Yang, D.S. Li, X.Y. Ma, S.Z. Li, D.L. Que,Crystal Growth&Design5 (2005) 547.

Synthesis of PAMAM Dendrimer as a new carrier in cancer drug delivery

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Dendrimers are the emerging polymeric architectures that are known for their defined structures, versatility in drug delivery and high functionality whose properties resemble with biomolecules. Controlled drug delivery systems have various advantages compared to conventional treatment ways, such as high efficacy, reduced toxicity, and improved quality of life of patient. Dendrimers offer advantages including a lower polydispersity index, multiple sites of attachment, and a controllable, well-defined size and structure that can be easily modified to change the chemical properties of the system[1]. Procarbazine HCl is a ‘nonclassical’ oral alkylating anticancer agent that was first synthesized in the late 1950s. It has been used in the treatment of many cancers, but its main use is in the treatment of Hodgkin’s lymphoma and brain tumors and, to a lesser extent, Non-Hodgkin’s lymphoma and primary central nervous system lymphoma. Procarbazine is a prodrug that undergoes metabolic transformation into active intermediates that are thought to inhibit DNA, RNA, and protein synthesis[2] The aim of this study synthesis of new polyamidoamine (PAMAM) dendrimer having polyethylene glycol grafts as novel drug carrier for procarbazine delivery. In this study we successfully synthesized and conjugated PEGylated PAMAM dendrimers with procarbazine. Cytotoxicity was measured by MTT assay on A549 cell line. In this study, the second generation polyamide amine(PAMAM) dendrimers were synthesized by divergent method[l]. Then The carboxyl terminal functional groups of PEG activated with DCC and Conguated with G2PAMAM. Their positive ammonium surfaces were modified and , the drug is covalently attached to the periphery of the dendrimer to form dendrimer prodrugs[3]. Moreover surface were characterization of PEGylated PAMAM dendrimers was carried out TEM micrographs. Further physiochemical , physiological and biological properties such as drug entrapment , drug release, characterization of structures and cytotoxicity were carried out by UV,FTIR, NMR and MTT assay techniques for PEGylated and non PEGylated PAMAM dendrimer. The results showed that The physicochemical and biopharmaceutical properties of PEGylated G2PAMAM dendrimer better than and non PEGylated G2PAMAM dendrimer.

References:

[1] Aliasghar Hamidi, Mohammad R. Rashidi, et.al. Novel Aldehyde-Terminated Dendrimers; Synthesis and Cytotoxicity Assay, BioImpacts, 2012, 2(2), 97-103.
[2] Jean-Pierre Armand, Vincent Ribrag, Jean-Luc Harrousseau, Lauren Abrey, Reappraisal of the use of procarbazine in the treatment of lymphomas and brain tumors, Ther Clin Risk Manag. 2007 Jun; 3(2): 213–224.
[3] Ruth Duncan, Lorella Izzo, Dendrimer biocompatibility and toxicity, Advanced Drug Delivery Reviews 57 (2005) 2215– 2237.

Thin Film Formation of Pd/CDS nanoparticles at Oil–Water Interface as an Effective Catalyst for Suzuki–Miyaura reaction in Water

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Palladium is the most widely utilized catalysts for the formation of C−S, C−N and C−C bonds in both industry and academia [1]. Alloying is a strategy that has been used to find non-Pd catalysts that are effective and less expensive for the Suzuki-Miyaura cross-coupling [2]. Pd/CdS nanoparticles (NPs) thin film was synthesized by the reduction of an organopalladium(II) complex, [$PdCl_2$(cod)] (cod = cis,cis-1,5-cyclooctadiene) and a semiconductor of CdS at an oil–water interface. The structure and morphology of the as-prepared NPs was characterized with X-ray diffraction (XRD) and transmission electron microscopy (TEM). Catalytic activity of the prepared NPs was investigated in the Suzuki–Miyaura cross-coupling reaction in H_2O. Pd/CdS thin filmexhibited higher catalytic activity compared to Pd thin film in the Suzuki–Miyaura coupling reaction due to the appropriate interaction between palladium and CdS.Comparedto the classical reactions, this method consistently has the advantages of a green solvent, low catalyst loading, short reactiontimes, high yields and reusability of the catalyst.

References

[1] L. Yin, J. Liebscher, Chemical Review 107 (2007)133.

[2] S.J. Hoseini, A. Zarei, H. Rafatbakhsh Iran, Applied Organometallic Chemistry 29 (2015) 489.

Diastereoselective synthesis of *Z*-gem-bromonitrochromenes

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Chromenes are an important heterocyclic skeleton with extended biological activities. These compounds are widespread in plants and also some active compounds. Some chromenes that contain nitro moiety are inhibitors of the proliferation of cancer cells, antihypertensive drugs, and important intermediates in the synthesis of medically active 2H-benzopyrans [1].

There are some aaproaches for the synthesis of these compounds. But there are some limitation for the synthesis, such as low yield, harsh reaction condition. Meanwhile, using the basic reaction condition could cause the racemization. Carrying out the reaction in a soft media is an interesting demand in organic synthesis. We describe here a method for synthesis of *Z*-gem-3-nitrochromene through the reaction of 2-hydroxy benzaldehyde derivatives and *β*-bromo-nitrostyrene in the presence of base [2].

The product was formed as diastereoselective with good to high yield and easy work up. The structure of the product especially the diastereoselectivity of the product was confirmed based on the NMR Spectroscopy, HR-MS and X-ray crystallographic data.

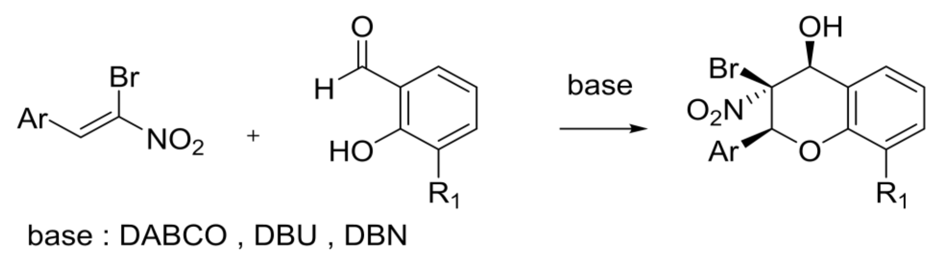

Figure 1. Reaction of (Z)-gem-Bromonitroalkenes and o-Hydroxybenzaldehydes

References

[1] G. X. Wang, N. X. Wang, T. Shi, J. L. Yu, X. L. Tang. Progress in Chemistry 20 (2008) 518.
[2] R.G. Soengas, H. Rodriguez-Solla, A.M. S. Silva, R. Llavona, F.A. Almeida Paz. J.org.chem. 78 (2013) 12831.

Encapsulation of Pd(II) into superparamagnetic nanoparticles grafted with EDTA and their catalytic activity towards reduction of nitroarenes and Suzuki–Miyaura coupling

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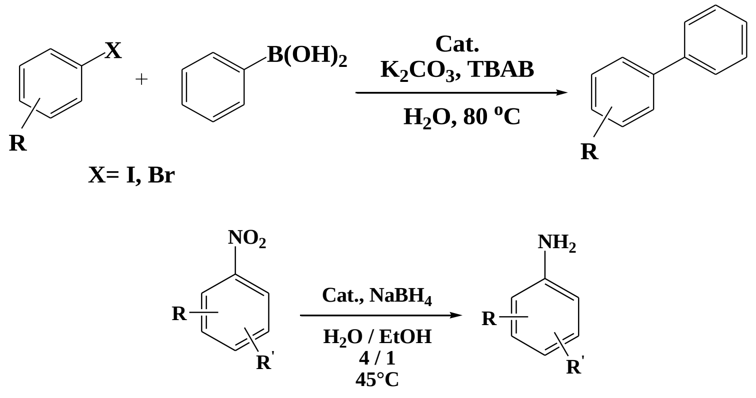
A robust, safe and magnetically recoverable palladium catalyst was synthesized by anchoring Pd(II) onto ethylenediaminetetraaceticacid-coated Fe_3O_4 (Fe_3O_4@EDTA) magnetic nanoparticles. The Fe_3O_4 magnetic nanoparticle-supported Pd(II)–EDTA complex catalyst thus obtainedwas characterized using scanning and transmission electronmicroscopies, thermogravimetric analysis, vibrating sample magnetometry, X-ray diffraction, and inductively coupled plasma atomic emission and Fourier transform infrared spectroscopies. Fe_3O_4@EDTA–Pd(II) was screened for the Suzuki reaction and reduction of nitro compounds in water. The Pd content of the catalyst was measured to be 0.28 mmolPd g^{-1}. In addition, the Fe_3O_4@EDTA–Pd catalyst can be easilyseparated and recovered with an external permanent magnet. The anchored solid catalyst can be recycled efficiently and reused five times with only a very slight loss of catalytic activity.



Cat. : Fe3O4@EDTA-Pd

Figure 1.reduction of nitroarenes and Suzuki–Miyaura coupling through catalytic method

References

[1] K. Azizi, A. Heydari, RSC Adv. 2014, 4, 8812.
[2] K. Azizi, A. Heydari, RSC Adv. 2014, 4, 6508.
[3] K. Azizi, M. Karimi, F.Nikbakht, A. Heydari – Appl.Catal.A., 2014, 482, 336.

Furanocomarin from the root of *ferulago carduchorum (Boiss.& Hausskn.)*

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Ferulago carduchorum is a perennial herb of Apiaceae, which is endemic of Iran distributed in central part of Iran.chevil, is the common name for the plant in Iran [1]. Ferulago carduchorum has been used throughout history as sedative tonic and for treatment of ulcers, hemorrhoids, spleen disease, digestive panics, headache, and snake bite [2]. In the present work, the plant materials were collected from Kuhkiloye ve Boyer Ahmad province.Airdried and powdered plant roots were extracted with n-hexan, dichloromethane and methanol, respectively, using a soxhlet apparatus. The n-hexan extract was fractioned with VLC technique and after primary test with analytical TLC, best fraction was extracted with column chromatography (CC).In next stage, best fraction was subjected to preparative thin layer chromatography.

(P-TLC) using chlorophorm: aceton (91:9) as solvent system to yield one linear furanocoumarin named prantschimgin.The structure of isolated compound was elucidated by spectroscopic data such as HNMR,CNMR,UVand IR.Up to our knowledge, this is the first report on root phytochemicals of F.carducrum.It was assumed that biological and pharmacological activities of the plant might be contributed to the presence of furanocoumarins.The comparison of our results with the literature showed that prantschimginispresented in other species of the genus and could be used as a chemotaxonomic marker of the genus.

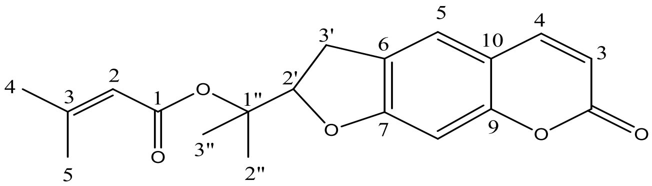

Figure 1.scheme of the reaction

References

[1] S.M.Razavi,M, A.Hajiboland. Dormancy breaking and germination of prangos ferulaceae seeds.(2009) 3,78-83.

[2] M.Taran, H.R.Ghasempour, E.Shirinpour.Jundishapurjournal of Microbiology, (2010) 3(1):10-14.

Conversion of 3-Substituted 1,2,4-Oxadiazoles in the present of Fe_3O_4 to symmetric 1,2,4-Oxadiazole

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The chemistry of heterocyclic compounds is an important research area in organic chemistry due to their use in pharmaceuticals and their presence in natural products as well as new materials[1].Oxadiazoles are five-membered heterocyclic compounds that occupy a special place due to thegrowing importance of these heterocycles for the design ofbiologically active compounds and for materials construction [2].

Among oxadiazoles 1,2,4-oxadiazole derivatives have gained importance inmedicinal chemistry.Several methods havebeen reported in the literature for the synthesis of 1,2,4-oxadiazoles. In general, synthesis of 1,2,4-oxadiazoles involves first the O-acylation step of an amidoximeby an activated carboxylic acid derivatives, followed by cyclodehydration. It has been found that cyclizationcould be effected by treating an O-acylamidoxime withNaH or NaOEt at room temperature, pyridine withheating [3].

This work we syntheses symmetric oxadiazole with Fe_3O_4 as an catalyst.

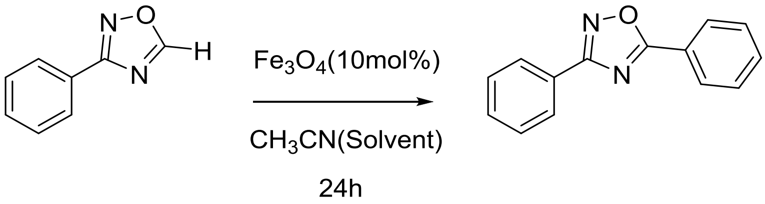

Figure 1.scheme of the reaction

References

[1] Kaboudin, B.; Kazemi, F.; Pirouz, M.; Khoshkhoo, A. B.; Kato, J.; Yokomatsu, T. Synthesis (Stuttg).2016.

[2] Bostrom, J.; Hogner, A.; Llinas, A.; Wellner, E.; Plowright, A. T. J. Med. Chm. 2012, 55, 187.

[3] Kaboudin, B.; Saadati, F. Tetrahedron Lett. 2007, 48, 2829–2832.

Poly(4,4'-oxydiphenylene-pyromellitimide) incorporated by Poly(tetramethylene oxide) coated silica nanoparticles: Synthesis and thermo-mechanical properties

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Polyimides are known as unique high temperature polymers [1]. Numerious studies have been focused on polyimide-matrix nanocomposites [2]. This work describes synthesis and thermo-mechanical properties of a number of new nanocomposites composed of polyimide-matrix, namely poly(4,4'-oxydiphenylene-pyromellitimide) (POPI), and silica nanoparticles (NP's) surface modified by amine-functionalized poly(tetramethylene oxide) (PTMO) (Figure 1). The resulting polyimide matrix nanocomposites are charecterized by FT-IR, XRD, FE-SEM, TGA and DMA measurments.

Hexamethylenediisocyanate (HDI) reacts with PTMO in mole ratio of 2. The NCO-terminated PTMO obtained is used for surface modification of SiO_2NP's. Next, Pyromelliticdianhydride(PMDA)/4,4'-Oxydianiline(ODA) polyimides are synthesis in the presense of PTMO-coated SiO_2NP'sin different contents, i.e. 5.0, 7.5 and 10.0 wt%.

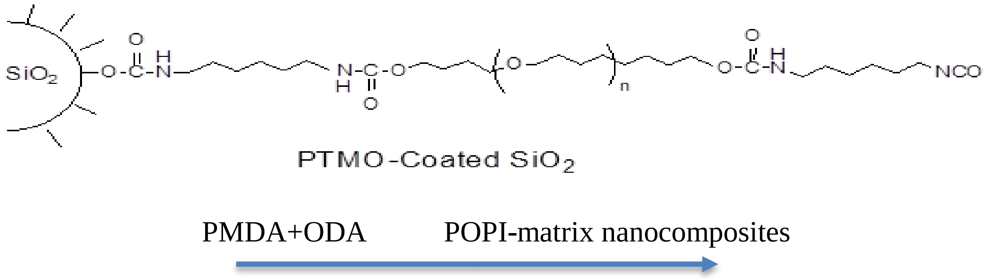

Figure 1. Schematic representaition of new POPI-matrix nanocomposites.

References

[1] Der-jangLiaw, Kung-Liaw, Kung-Li Wang, Ying-Chi Huang, Kueir-Ram Lee, Juin-Yih Lai, Chang-Sik Ha. (2012). “Advanced polyimide materials: synthese, physical properties and applications.” Progress in polymer science, 37.

[2] Young-Jae, K. Jong- Heon, K. Shin- Woo, H. Dongil, K. Jin-Kyu, L. (2014). “polyimidenanocamposites with functionalized SiO2 nanoparticles: enhanced processability, thermal and mechanical properties.” Royal society of chemistry, 4.

Organo-modification of SiO_2 coated magnetite nanoparticles, and their loading into segmented polyurethane matrix

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Due to the magnetite nano-particles have a tremendous influence on magnetic behavior of polymers, their loading into polymer (thermoset or thermoplast) matrix has a significant importance, therefore it has been widely studied.If the magnetite nanoparticles are coated in an organic or inorganic shell, they maintain magnetic properties and also reach enormous stability[1-2]. Firstly, Fe_3O_4 nano particles (NP's) are prepared by coprecipitation method. Then, silica shell is produced on the Fe_3O_4 core via reaction withTetraethyl orthosilicate. The resulting Fe_3O_4@SiO_2 NP'sare organically modified by OCN-terminated Polytetramethylene oxide (PTMO). Segmented PU matices are synthesized in the presence of Fe_3O_4@SiO_2@PTMO NP's in different contents (Figure 1).

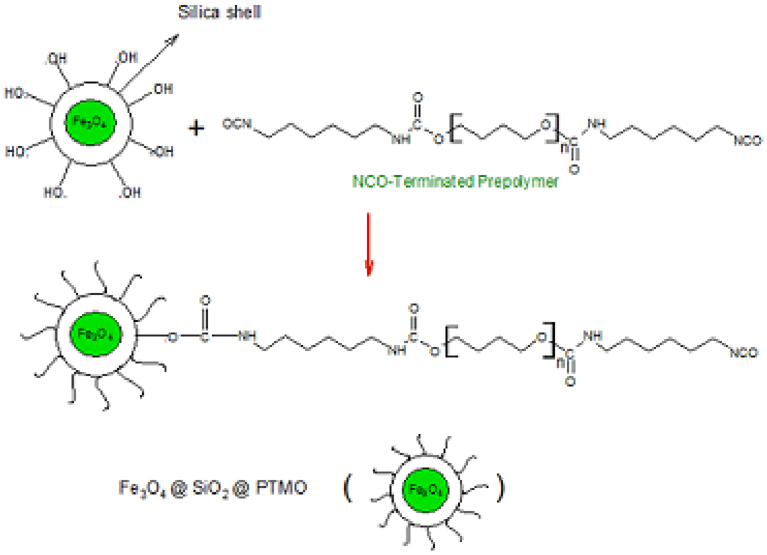

Figure 1.Synthesis of Fe_3O_4@SiO_2@PTMO@SPU nanocomposites.

Fe_3O_4@SiO_2@PTMO@SPU nanocomposites are characterized by FT-IR, XRD, SEM, TGA and DMAtechniques.

References

[1] Lu, A. H. Salabas, E. L. and Schuth, F. (2007) "Magnetic Nanoparticles: Synthesis, Protection, Functionalization, and Application", Angew. Chem. Int. Ed, 46.

[2] Li, Y. S. Church, J. S. Woodhead, A. L. and Moussa, F. (2010) "Preparation and characterization of silica coated iron oxide magnetic nano-particles", Spectrochimica Acta Part A, 76.

A highly efficient and green synthesis of 1,2,3,4-tetrahydropyrimidines under solvent-free conditions

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In recent years, the interest in Dihydropyrimidines has increased rapidly because of the structural resemblanceof DHPM with clinically important Hantzsch pyridines [1,2].Pyrimidine derivatives comprise a diverseand interesting group of drugs which are extremely important for their biological activities [3,4]. A mild, simple and efficient procedure for the preparation of 1,2,3,4-tetrahydropyrimidins is described using BSA as an acidic and efficient catalyst under solvent-free conditions. Simple methodologies, easy work-up procedure, easy preparation of the catalyst, excellent yields and very short reaction times are among the other advantages of this work. Further, the catalyst can be reused and recovered for several times without significant decrease in its activity.

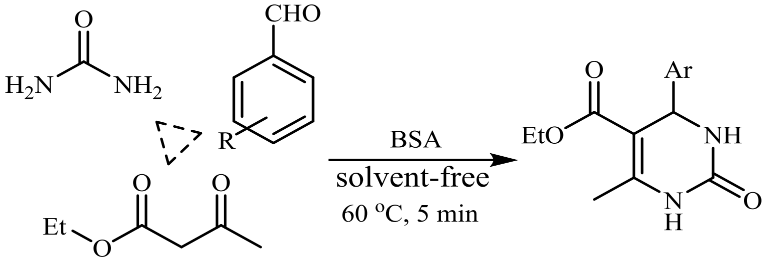

Figure 1. Preparation of tetrahydropyridines.

References

[1] K.S. Atwal, G.C. Rovnyak. J. Schwartz, Journal of Medicinal Chemistry 33 (1990) 1510.
[2] C.O. Kappe Molecules 3 (1998) 1.
[3] D.J. Triggle, R.A. Janis Annu Rev PharmacolToxicol 27 (1987) 347.
[4] B. Desai, D. Sureja, Y. NaliaparaBioorganic & Medicinal Chemistry 9 (2001) 1993.

Synthesise of nanophytosome based on saponins

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Saponins are one of the most important chemical compounds that widely distributed in nature. Saponins have a wide range of properties due to their extensive structural diversity, including hepatoprotective, anti-ulcer, antimicrobial, adjuvant, anti-inflammatory and anti-tumor activities [1]. While the individual use of saponins as antitumor agents has been extended the scientific scanner for more than 40 years, no single clinically relevant saponin with sole status as a pharmaceutical agent has been approved by the US Food and Drug Administration, due to high cytotoxic effect [2]. Among of Iranian plants, zizyphus spina-christi (sidr) is saponin-rich. In this work, saponins were extracted from Zizyphus spina-christi using ethanol and then fractionated using chloroform, ethyl acetate and finally with water-saturated butanol. Then nanophytosom was prepared using saponins and emulsified with soybean lecithin and cholesterol solution [3]. Properties of the samples were investigated by FTIR, NMR, DLS, Zeta potential and SEM analyses.

References

[1] A. D. P. Barbosa, "AN OVERVIEW ON THE BIOLOGICAL AND PHARMACOLOGICAL ACTIVITIES OF SAPONINS," International Journal of Pharmacy and Pharmaceutical Sciences, vol. 6, pp. 47-50, 2014.
[2] M. Thakur, M. F. Melzig, H. Fuchs, and A. Weng, "Chemistry and pharmacology of saponins: special focus on cytotoxic properties," Botanics: Targets and Therapy, vol. 1, pp. 19-29, 2011.
[3] Y. Ye, H. Xing, and Y. Li, "Nanoencapsulation of the sasanquasaponin from Camellia oleifera, its photo responsiveness and neuroprotective effects," International Journal of Nanomedicine, vol. 9, pp. 4475–4484, 2014.

An Efficient Synthesis of 1,8-Dioxo-octahydro-xanthene Derivatives Containing Chromone Moiety

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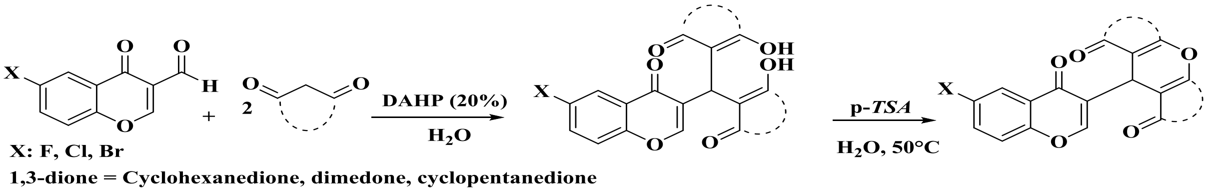
1,8-dioxo-octahydro Xanthenes are known as biologically active heterocyclic skeleton with extended activities. The suitable method for the synthesis of these compounds is the reaction between benzaldehyde derivatives and 1,3-dione in acid. There are different reaction media and catalyst for the synthesis of these compounds.[1-3] 3-Formyl chromone is a heterocyclic compound with 3 positions for nucleophilic addition and was used in different multicomponent reactions in our research group. Herein, we wish to report the synthesis of 1,8-dioxo-octahydro xanthene derivatives through the reaction of 3- formyl chromone and two equivalent1,3-dione in water in the presence of diammonium hydrogen phosphate. The intermediate was separated and heated in water in the presence of catalytic amount of *para*-toluene sulfonic acid led to the desired 1,8-dioxo-octahydroxanthenes contained chromone skeleton.

The structure of the products was confirmed based on ^{1}H&^{13}C NMR spectroscopy, HR-MS and also X-ray crystallographic data. Due to the existence of chromone skeleton in the structure of the product, the product has a high potential for further reaction. The work for further reactions is in progress in our laboratory.



DAHP= diammonium hydrogen phosphate, p-TSA= para –toluene sulfonic acid

Figure 1.scheme of the reaction

Refrences

[1] Chen, X.; Pardhan, T.; Wang, F.; Seung Kim, J.; Yoon, J.;Chem. Rev., 2012, 112, 1910-1956.
[2] Vasas, A.; Hohmann J.; Nat. Prod. Rep., 2011, 28, 824-842.
[3] Venkatesan, K.; Pujari, S.; Lahoti, R.J.; Srinivasn, K.V.; Ultrasonics Sonochemistry, 2008, 15 548-553.

Poly vinyl Sulfonic acid supported on nano rice husk silica: an efficient catalyst for the One-Pot synthesis of 1*H*-indazolo[2,1-b]-Phthalazinetrione

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Phthalazine derivatives are an important class of heterocyclic compounds due to their wide range of pharmaceutical and biological activities.[1] Phthalazine derivatives was reported to possess anticonvulsant; antifungal, anticancer, and vasorelaxant activities.[2] Therefore, considerable effort has been devoted toward finding an efficient synthesis of phthalazine derivatives.

In this research, sodium silicate was produced from the rice husk by acidic titration and burning process and then converted to nano silica under acidic conditions. The polyvinyl sulfonic acid was easily prepared by the reaction of polyvinyl alcohol and chloro sulfonic acid and supported on the extracted nano silica by simple grinding.

The catalytic activity of this solid acid nanocomposite, NanoSilica/PVSA, was probed through the One-Pot synthesis of 1H-indazolo[2,1-b]-Phthalazinetrione via three-component couplings of phthalhydrazide, aromatic aldehydes, and dimidone. In this reactions NanoSilica/PVSA shows a highly catalytic nature, easy to handle procedure, easy workup, recycle exploitation, good to excellent isolated yields and the elimination of solvent that is a relatively environmentally important.

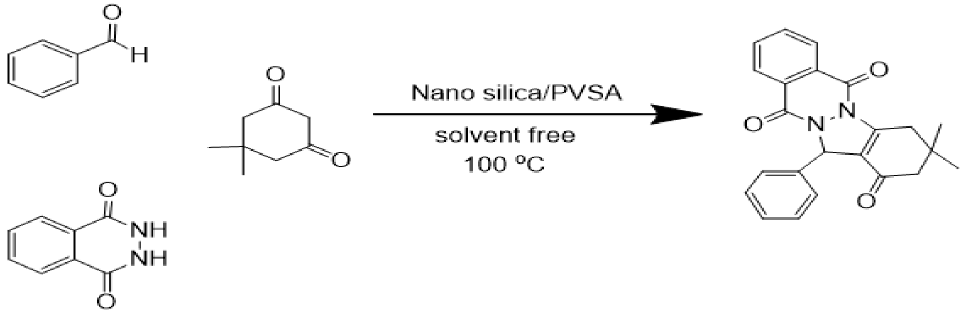

Figure 1.: One-Pot synthesis of 1H-indazolo[2,1-b]-Phthalazinetrione

References

[1] R. P. Jain and ,J. C. Vederas, Bioorg, Med. Chem. Lett. 14 (2004) 3655.
[2] S. Grasso, G. DeSarro, N. Micale, M. Zappala, G. Puia, M. Baraldi, and C. Demicheli, J. Med. Chem. 43 (2000) 2851.

An efficient route to the One-Pot synthesis of 1*H*-indazolo[2,1-b]-Phthalazinetrione catalyzed by β-Cyclodextrin sulfunic acid supported on nano rice husk silica

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The synthesis of new heterocyclic compounds has always been a subject of great interest due to their wide applicability. Among a large variety of heterocyclic compounds, heterocycles containing phthalazine moiety are of interest because they show several pharmacological and biological activities. Phthalazine derivatives, which have two bridgehead nitrogen atoms in a fused ring system, possess cytotoxic, antimicrobial, anticonvulsant, antifungal, anticancer and anti-inflammatory activities. Moreover, these compounds exhibited good promise as new luminescent materials or fluorescence probes.[1,2] By having these facts in minds, in this research β _cyclodextrin sulfunic acid was easily prepared by the reaction of β _cyclidextrin and chloro sulfunic acid in dry chloroform ($CHCl_3$) at room temprature, and to modified its efficiency, supported on nano silica. nano silica extracted from rice husk by acid treatment and then combustion.The size of nano silica was determined by SEM microscopy.The capacity of solid acid was determined by acid_base titration. The catalitic ability of this acid in the three components condensation reaction of a varity of a aromatic aldehyde with electron donating and electron with drawing groups with phethalhydrazide and dimidone was investigated. According to the results, this solid acid act very efficient and produced 1H_indazolo [2,1-b]-Phthalazinetrione derivatives in good isolated yields in short reaction time.

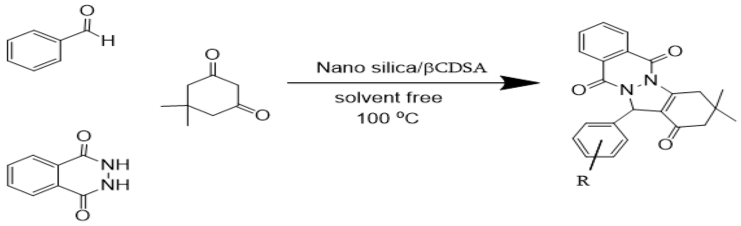

Figure 1.: One-Pot synthesis of 1H-indazolo[2,1-b]-Phthalazinetrione

References

[1] F. Al-Assar, K. N. Zelenin, E. E. Lesiovskaya, I. P. Bezhan, B. A. Chakchir, Pharm .Chem. J. 36 (2002) 598.
[2] R. P. Jain, J. C. Vederas, Bioorg. Med. Chem. Lett. 14 (2004) 3655.

Covalently immobilization of palladium(II) tetrasulfophthalocyanine on keratin protein grafted graphene oxide nanosheets: a new high–performance catalyst for C–C coupling reactions

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Palladium–catalyzed cross–coupling reactions as extraordinary powerful and widespread methods are found in all areas of chemistry which used to construct carbon–carbon and carbon–heteroatom bonds.[1-3]Since irreversible precipitation of palladium in the reaction media affected its catalytic activities, to settle the matter, a controlled and reversible release of palladium from macrocyclic complexes as a novel method was proposed.In this study, wool keratin protein as amphiphilic biomaterial was extracted from natural wool and used to modify the surface of graphene oxide nanosheets. An aqua soluble palladium(II) complex with a phthalocyanine ligand possessing covalently binding ability was immobilized on keratin protein grafted graphene oxide nanosheets. The covalently supported palladium(II) tetrasulfophthalocyanine complex revealed efficient catalytic reactivity by controlled temporary release of active species for Heck and Sonogashira coupling reactions in aqueous solution. Heck coupling of styrene and Sonogashira coupling of phenylacetylene with different aryl halides wassuccessfully catalyzed by the synthesized palladium(II) tetrasulfophthalocyanine covalently supported on keratin protein grafted graphene oxide nanosheets as a novel catalyst precursor. The controlled release of palladium active species prevents the formation of inactive palladium agglomerates under harsh conditions and consequently this controlled release leads to high catalytic performances.

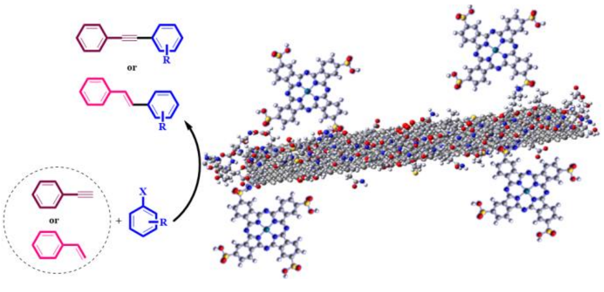

Figure 1.scheme of the reaction

References

[1] R. Chinchilla, C. Nájera, Recent advances in Sonogashira reactions., Chem. Soc. Rev. 40 (2011) 5084–5121.
[2] Q. Wang, Y. Su, L. Li, H. Huang, Transition-metal catalysed C-N bond activation., Chem. Soc. Rev. 45 (2016) 1257–1272.
[3] A. Shaabani, M. Mahyari, PdCo bimetallic nanoparticles supported on PPI-grafted graphene as an efficient catalyst for Sonogashira reactions., J. Mater. Chem. A, 1 (2013) 9303-9311.

Cr– and Zn–Substituted Cobalt Ferrite Nanoparticles Supported on Guanidine–Modified Graphene Oxide as Two Efficient and Recyclable Catalysts for Catalytic Applications

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Graphene is an exciting material for applied catalyst research because of its distinct properties, such as high surface area, high mechanical strength and electrical conductivity, intrinsic low mass, high water dispersibility, easy surface modifications, and oxygen–carrying functionalities.[1-3]In this study, we synthesized and characterized two new graphene–based catalysts and applied for the aerobic oxidation of various organic compounds. Functionalization of graphene oxide with guanidine lead to uniformly dispersing of $CrCoFeO_4$ and $Zn_{0.5}Co_{0.5}Fe_2O_4$ nanoparticles. The distribution of $CrCoFeO_4$ and $Zn_{0.5}Co_{0.5}Fe_2O_4$ on the surface of guanidine–grafted graphene oxide nanosheets gave the active catalytic systems with high catalytic activity and selectivity in the aerobic oxidation of the alkyl arenes and alcohols to the corresponding aldehydes and ketones without any over oxidation. Guanidine–grafted graphene oxide nanosheets as support for immobilization of $CrCoFeO_4$ and $Zn_{0.5}Co_{0.5}Fe_2O_4$nanoparticlesenhance the catalytic activity of the prepared systems in the aerobic oxidation of indane and 1–indanol due to π–π interaction between graphene support and benzene skeleton of the reactants and consequently the adsorption of aromatic reactants on the surface of G–GO support. Also, the oxidative synthesis of 2-phenylbenzo[*d*]oxazole derivativesby employing inexpensive and readily available aromatic hydrocarbons of petroleum naphtha(toluene and three xylene isomers)as aldehyde precursors was catalyzed successfully in the precense of $CrCoFeO_4$@G–GO and $Zn_{0.5}Co_{0.5}Fe_2O_4$@G–GO catalysts.

References

[1] S. Sabater, J. A. Mata and E. Peris, ACS Catal., 4(2014) 2038–2047.

[2] Q. Huang, L. Zhou, X. Jiang, Y. Zhou, H. Fan and W. Lang, ACS Appl. Mater. Interfaces, 6 (2014) 13502–13509.

[3] A. Shaabani, Z. Hezarkhani, M.KeramatiNejad, AuCu and AgCu bimetallic nanoparticles supported on guanidine-modified reduced graphene oxide nanosheets as catalysts in the reduction of nitroarenes: tandem synthesis of benzo[*b*][1,4]diazepine derivatives, RSC Adv., 6 (2016) 30247-30257.

Experimental design method for removal of blue 5 from aqueous solutions by ozone photocatalyst process

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Due to the toxicity effects and endocrine disrupting properties of aromatic compounds, their removal from water and wastewater has gained widespread global attention. In this study, the photocatalytic degradation of blue acid 5 in the presence of titanium dioxide (TiO_2) nano-particles and ozone was investigated. A full factorial design consisting of three factors at three levels was used to examine the effect of pH, amount of catalyst and various concentrations of blue acid 5 on the apparent degradation rate constant. The individual effect of TiO_2 amount (50, 150 and 250 mg/L), pH (3, 7 and 11) and initial concentration (100, 150 and 200 mg/L) on the apparent degradation rate constant was determined. A regression model was developed to relate the apparent degradation constant to the various factors. The apparent degradation rate constant trend was as follows: $O_3/UV/TiO_2$ > $O_3/$ TiO_2> O_3/UV> O_3> UV/TiO_2 . The data indicated no significant interaction between the experimental factors. The lowest activation energy was observed for UV/TiO_2 degradation. A maximum degradation rate constant of 0.0138 min−1 was recorded for $O_3/UV/TiO_2$ process at pH=11 and a TiO_2 amount of 250 mg/L at an initial concentration of 100 mg/L. The response model adequately related the apparent degradation rate constant to the factors within the range of factors under consideration.

References

[1] kolekar Y.M ,2008, Decolorization and Degradation of Disperse Blue 79 and Acid Organge 10 by Bacillus fusiformis KMK5 Isolated from the Textile Dye Contaminated Soil, Bioresour. Technol.99,8999.
[2] Gomez, V.Larrechi, M.S. Callo, M. P. 2007, Kinetic and Adsorption Study of Acid Dye Removal Using Activated Carbon,Chemosphere ,69,1151.
[3] Wang C.-T., Chou W.-L, Chung M-H, Kuo Y.-M,2010 , COD removal from real dyeing wastewater by electro-Fenton technology using an activated carbon fiber cathode, Dwsalination,253:129.

An Efficient Approach for the Synthesis of Panobinostat as Anti-Cancer Drug

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Panobinostat is a drug developed by Novartis for the treatment of various cancers (Figure 1). It is a hydroxamic acid and acts as a non-selective histone deacetylase inhibitor (pan-HDAC inhibitor). Panobinostat inhibits multiple histone deacetylase enzymes, a mechanism leading to apoptosis of malignant cells via multiple pathways.

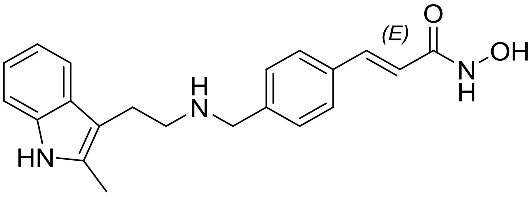

Figure 1: Panobinostat

On 23 February 2015 it received FDA accelerated approval for use in patients with multiple myeloma who had received at least 2 previous treatments, including bortezomib and an immunomodulatory agent after clinical trials.

We describe the synthesis of API of panobinostat and the effort made for new and different approaches to reach the most efficient way to produce it using suitable starting material.

The details about the synthesis approach will be further discussed in the conference.

References

[1] Revill, P; Mealy, N; Serradell, N; Bolos, J; Rosa, E.; Drugs of the Future., 2007, 32, 315.

Efficient new method for One-Pot synthesis of 2-aryl-4,5-dicyanoimidazoles catalyzed by Ceric ammonium nitrate (CAN)/HNO_3 under mild conditions

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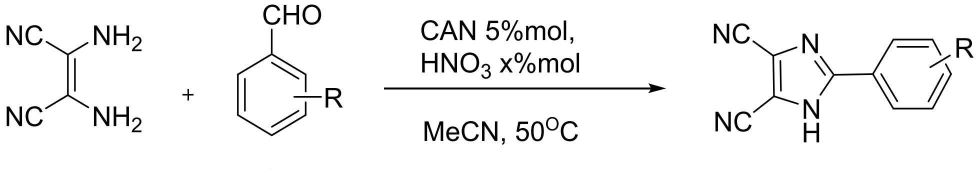
Imidazole derivatives including 4,5-dicyanoimidazoles exhibit a wide range of pharmacological activities and have broad applications in medicinal [1]. The spectral and photophysical characteristics this compounds attracted high interest for the synthesis as new promising acceptor moiety [2].

According to importance of this compounds, up to now, four methods have reported for the synthesis of these compounds, all of which are pathway for their synthesis of Schiff-base. However, the most of these methods have some limitations such as refluxing for 4 days, use of expensive and toxic catalysts or reagents, low yields, long reaction times and tedious workup procedure [3].

In view of these points and as a part of our interest researches on the development of new methods for the facile synthesis of 4,5-dicyanoimidazoles, we reported the condensation reaction of 2,3-diaminomaleonitrileand aromatic aldehydes and following thatoxidative cyclization reaction in the presence of catalytic amount of Cerium(IV) Ammonium nitrate (CAN) and HNO_3 in acetonitrile (Scheme **1**). Some of the major advantages of this practical procedure are use of available catalyst, high yields, short reaction timescompared with previous reports, and simplicity of the reaction and workup.



1 **2** **3a-k**

Figure 1. Scheme of the reaction.

References

[1] A. Katritzky, Imidazoles and their benzo derivatives: (iii) synthesis and applications. 1st edn. Pergamon Press, New York, 457 (1984).

[2] P. Apent, P. G. Rasmussen, J. Am. Chem. Soc. 113 (1991) 6178.

[3] (a) G. A. Feldwick, L. R. Hatton, EP0269238, (1988);(b) R. W. Begland, D. R. Hartter, F. N. Jones, D. J. Sam, W. A. Sheppard, O. W. Webster, F. J. Weigert, J. Org. Chem. 39 (1974) 2341.

Synthesis of pyrazole derivatives containing carbothiohydrazide skeleton via mild approach

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Many pyrazole derivatives are acknowledged to possess a wide range of bioactivities. The pyrazole motif makes up the core structureof numerous biologically active compounds [1]. Much attention was paid to pyrazole as a potential antimicrobial agent after the discovery of the natural pyrazole C-glycoside, pyrazofurin which demonstrated a broad spectrum of antimicrobial activity [2].

Pyrazole derivatives containing carbothiohydrazide skeleton are not only useful fragments of antibiotics, but are also used as intermediates and synthons for the production of several organic compounds [3].

This research involved the syntheses of chalcones 1, the cyclization of these chalcones by thiocarbonohydrazide 2 and synthesis of pyrazoline derivatives 3 (Scheme 1). In our studies, we found that ethanol was the solvent most appropriate for these reactions, giving the best results. Under catalysts scanning, the yield of products 3 increased.

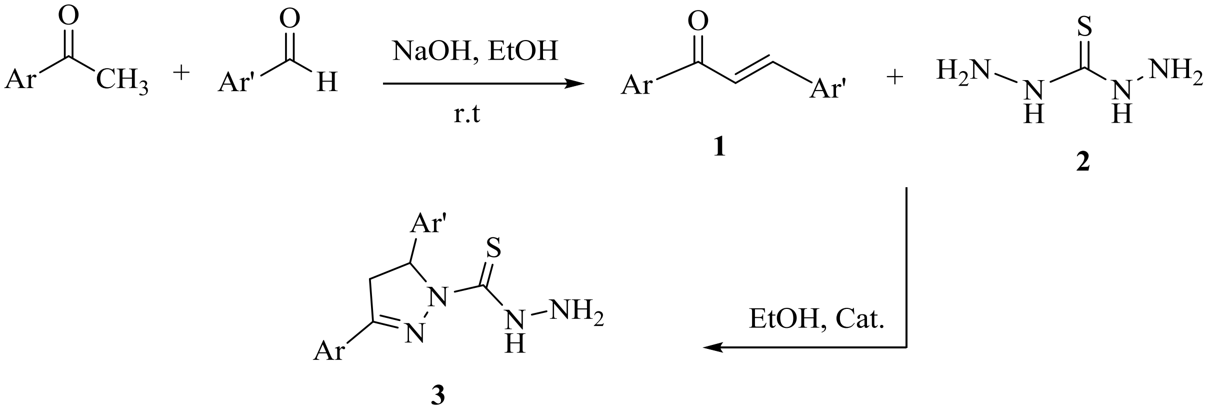

Figure 1. Synthetic pathway of pyrazole-1-carbothiohydrazides 3

References

[1] H. A. Park, K. Lee, S. -J. Park, B. Ahn, J. -C. Lee, H. Y. Cho, K.-I. Lee. Bioorg. Med. Chem. Lett. 15 (2005) 3307.
[2] R. N. Comber, R. J. Gray, J. A. Secrist. Carbohydr. Res. 216 (1992) 441.
[3] A. Budakoti, A. R. Bhat, F. Athar, A. Azam. Eur. J. Med. Chem. 43 (2008) 1749.

Synthesis and Characterization of Flexible Silica Nanoporous Aerogel as High Efficient Thermal Insulator

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Silica aerogel is a highly porous material with pore diameters in the range of 2–50 nm [1, 2]. The nanoporous structure of the silica aerogels having a high porosity above 90%, makes the aerogels a highly thermal insulating materials with a super-low thermal conductivity as low as 0.013 W.m^{-1}.K^{-1} [3]. However, because of their nanoporous nature and high porosity, silica aerogels generally have poor mechanical stability (e.g., low strength and high brittleness). The low flexural and collapse strength of the aerogels greatly limit their applications for thermal insulation applications. Many researches are done to improve the mechanical properties of silica aerogels which among them introducing reinforced fibers into the silica aerogels and synthesizing the fiber-reinforced aerogels is one of the most effective methods for improving the mechanical properties of the aerogel [4].

In this study, we synthesized flexible silica aerogels with low density and thermal conductivity. Silica aerogel was synthesized from tetraethoxysilane (TEOS) using sol-gel method in the presence of fibers. The obtained alcohogel was dried via solvent exchange method at ambient pressure without using highly expensive supercritical drying method. Obtained aerogels have high degree of flexibility and low thermal conductivity (0.0.18 W.m^{-1}.K^{-1}). The porosity of synthesized aerogel was obtained around 89.5% which is a high porosity among aerogels. Also the thermal property of synthesized aerogel was studied by thermal gravimetry analysis (TGA).

References

[1] A. C. Pierre, in Aerogels Handbook, M.A. Aegerter, Ed. Springer (2011) 3.
[2] E. Rezaei, J. Moghaddas, Advanced Materials Letters 7 (2016) 296.
[3] R. Baetens, B. P. Jelle, A. Gustavsen, Energy and Buildings 43 (2011) 761.

Surface Functionality Effect on the Relaxivity of Superparamagnetic Iron Oxide Nanoparticles as Negative MRI Contrast Agent

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Nowadays, magnetic resonance imaging (MRI) thanks to its ability in providing non-invasive and three-dimensional examination of biological events is one of the most powerful diagnostic tolls in modern clinical medicine [1]. The MRI mechanism is based on the excitation and relaxation of hydrogen nuclei that are abundant in water and lipids of tissue. Differences in intrinsic longitudinal (T_1) and transverse (T_2) relaxation times of different parts of the tissues induce changes of MR signal intensity, which in turn result in imaging contrast [2]. However, it is often the case that the diseased and healthy tissues are similar in composition and MRI technology alone will not always differentiate the two. In these cases, a contrast agent is necessary to distinguish the normal and diseased tissue. Among different contrast agents, superparamagnetic iron oxide nanoparticles by enhancing the proton relaxation times in the tissue microenvironment are used as T_2 (negative) contrast agents. However, because of aggregation of bare nanoparticles and quick sequesteration by RES system, a main challenge in using iron oxide nanoparticles as MRI contrast agent is their surface modification by a hydrophilic and biocompatible layer [3, 4].

In the present study, superparamagnetic iron oxide nanoparticles were synthesized in polyol media by monodisperse particle size distribution. Then the surface of nanoparticles was covalently modified with three different functionalities including amine, carboxylic acid, and PEG. The synthesized nanoparticles were characterized with different methods including FT-IR, TEM, PCS, and relaxometry. In order to investigate the effect of pH and surface charge on the relaxivity of nanoparticles, the r_1 and r_2 relaxivity of nanoparticles were examined in different pHs at 20 and 60MHz magnetic fields. The results showed that amine-functionalized nanoparticles agglomerate at basic or neutral media, while they are completely stable for a long time at acidic media because of induced charges on the surface of nanoparticles. Carboxylic-functionalized nanoparticles showed a reverse effect i.e. they agglomerate in acidic media, while they are stable at neutral or basic media. PEG-coated nanoparticles are completely stable in all studied basic or acidic media which can be attributed to the neutral and hydrophilic nature of PEG. Another main achievement is that by agglomeration and increasing the particle size, the r_2/r_1 ratio increases which is a main factor in evaluating the magnetic nanoparticles efficiency as T_2 contrast agent.

References

[1] P.A. Rink, Magnetic resonance in medicine, Wiley (2003) 5.
[2] C.F.G.C. Geraldes, S. Laurent, Contrast Media and Molecular Imaging 4 (2009) 1.
[3] P. Eghbali, H. Fattahi, S. Laurent, R.N. Muller, Y. Moseai Oskouei, Journal of the Iranian Chemical Society 13 (2016) 87.

Determination and Quantification of TPC, Toxic and Non-Toxic Heavy Metals in Herbals

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Knowledge about organic and inorganic compounds in slim teas has always been in a center of attention since the consumption of these beverages has increased for the past years. Therefore, on the one hand, the goal of the present study was to develop an accurate method of the multi-element analysis of black tea by inductively coupled plasma optical emission spectrometry (ICP-OES) with three various extraction methods. Ten different samples of slim teas, including imported and local were analyzed to survey total concentrations of Al, Cd, Cu, Fe, Pb and Zn. Results indicated high level of Fe and Zn in a descending order. On the other hand determination of total phenolic content (TPC) in ten different samples of black tea were conducted by using two distinct extraction procedures, MeOH at 50% (v/v) and water extraction.

TPC were measured by using photometric Folin-Ciocalteu assay. Total phenolic content were expressed in mg Gallic acid equivalents (GAE) per gram of the sample.

Eventually, phenolic compounds compared to water, are more soluble in organic solvents with less polarity. Also according to the results, there were some variations in the TPC on account of types of black tea.

References

[1] Md. Harunur Rashid, Zeenath Fardous, M. Alamgir Zaman Chowdhury, Md. Khorshed Alam, Md. Latiful Bari, Mohammed Moniruzzaman,Siew Hua Gan(2016).Determination of heavy metals in the soils of tea plantations and in fresh and processed tea leaves: an evaluation of six digestion methods. Biological trace element research.

[2] TFu L1, Xu BT, Gan RY, Zhang Y, Xu XR, Xia EQ, Li HB.total Phenolic Contents and Antioxidant Capacities of Herbal and Tea Infusions. Int J Mol Sci. 2011.12(4):2112-24.

[3] Xin Li, Zhaowei Zhang, Peiwu Li, Qi Zhang, Wen Zhang, Xiaoxia Din(2013)Determination for major chemical contaminants in tea (Camellia sinensis) matrices: A review.Food Research International 53(2):649-658.

Electronic Structure and Force Field Parameterization of Graphene Monoxide Nanosheet

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The chemical modification of graphene leads to a non-toxic, 2-dimensional graphene-like nanomaterial named graphene monoxide, GMO. In GMO, two oxygen atoms are bridged between two carbon atoms to form a double epoxy structure. There are growing reports on the theoretical, computational and experimental studies on GMO nanosheet as a promising nanomaterial for pharmaceutical, nanoelectronic and catalytic applications. Knowing the electronic structure of GMO as an individual nano-particle and its interactions with other molecules are of essential requirements for designing novel applications for it, as modern pharmaceuticals or smart drug delivery systems. Here we have used the ab initio method for studying the electronic structure of GMO and obtaining the CHARMM force field parameters [1] used in classical molecular simulations. The geometrical and electronic structure of GMO nanosheet was optimized by using the HF theory, at the B3LYP level of theory using the HF-6-31C* basis set implemented in G09 suits of computer codes [2]. The Leonard-Jonez parameters were choosed by homology method from the existing the CHARMM force field parameters for oxygen and carbon atoms.

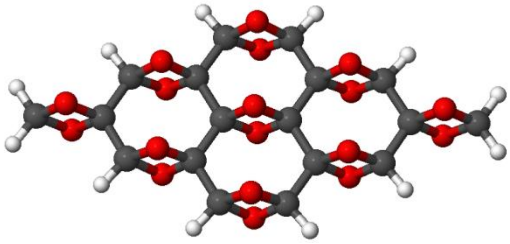

Figure 1. The structure of parameterized GMO nanosheet

References

[1] K. Vanommeslaeghe, E. Hatcher, C. Acharya, S. Kundu, S. Zhong, J. Shim, E. Darian, O. Guvench, P. Lopes, I. Vorobyov and A. D Mackerell Jr. Drug Design 31 (2010) 671

[2] M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman and et al. Gaussian 09, Revision E.01, Gaussian, Inc., Wallingford CT, 2009.

Synthesis of aNew Hydrophilic Copper Complex Supported on γ-Fe_2O_3

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Compared to the use of organic solvents, catalytic reactions in aqueous systems have many advantages including low cost, low toxicity and safety.Water, a readily available and non-toxic solvent, has attracted much attention due to its features as improving reactivity and selectivity, simplifying workup procedure and so on. The well-defined hydrophilic catalysts might be an effective tool to promote organic transformations in aqueous media. It is noted that hydrophilic organic ligands could increase the hydrophilicity of the resulting catalysts. More importantly, hydrophilic catalysts can be easily separated from the organic products by supporting the catalyst on solid materials [1].

Consequently there has been a growing demand for the design of heterogeneous hydrophilic catalysts that could promote organic reactions in water. Different solid materials have been used as solid supports for the preparation of heterogeneous catalysts. Within these materials, nanoparticles have attracted a great deal of attention as solid materials for supporting different catalysts. However, nanometer-sized particles are easily dispersible in solution by forming stable suspensions. Therefore, their separation needs a tedious recovery procedure *via* expensive ultracentrifugation, which caused the inevitable loss of solid catalysts.To further address the issues of recyclability and reusability, magnetic nanoparticles have emerged as excellent supports amenable to simple magnetic separation. The magnetic nature of MNPs allows a convenient method for removing and recycling MNPssupported catalysts by applying an appropriate magnetic field, this kind of separationis not time-consuming and prevents the loss of solid catalyst in the process. It also enhances products purity and optimizes operational costs. In addition, the MNPs supported catalysts show high dispersion and reactivity with a high degree of chemical stability [2].

In continue of our recent work on the development of new heterogeneous catalysts, herein,a new hydrophilic copper complex supported on magnetic iron oxide is synthesized and characterized by different methods.

References

[1] J. Xie, J.Bao, H. Li, D. Ton, J. Lang. Journal of Royal Society of Chemistry4 (2014) 54007.
[2] G. Zhang,X. Han,Y. Luan,Y. Wang, X.Wen, L.Xu, C. Ding, J. Gao.Journal of Royal Society of Chemistry3 (2013) 19255.

Hydrophobic Cu(II) Complex as a New Catalyst for The Synthesis of α-Amino Phosphonates

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α-Aminophosphonates are structurally and biologically analogous to amino acids, hence their synthesis has attracted much interest. The reaction of phosphites with aldehydesand aminesusing Lewis and Brønsted acid catalysts is the convenient and the most preferred method for the synthesis of α-aminophosphonates. Various catalysts have been developed to realize this organic synthesis [1].However, their practical approach is limited since the water formed during the course of the reaction adsorbed on the surface of the catalyst.The adsorbed water poisons the surface of the catalyst and produces a more hydrophilic environment, resulting in reduced catalytic activity. In fact, hydrophobic-hydrophilic balance on the surface of the catalyst has considerable effect on the progress of the reaction. Thus, the development of a new synthetic method using a reusable hydrophobic catalyst would be an attractive goal for the synthesis of these important scaffolds[2].

In continuing of recent research on the introducing new magnetically recyclable heterogeneous catalysts, herein we synthesized hydrophobic Cu(II) complex supported on γ-Fe_2O_3 (hydrophobic Cu-Fe_2O_3). The newly synthesized catalyst was characterized by different methods such as TEM, SEM, TGA, CHN and ICP analysis. The catalytic activity of hydrophobic Cu-Fe_2O_3 was also studied in the synthesis of α-aminophosphonates.

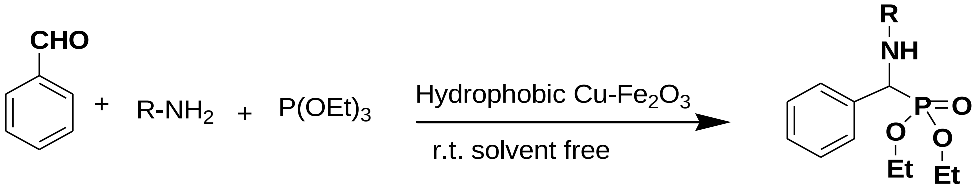

Figure 1. α-aminophosphonate synthesis catalyzed by hydrophobic Cu-Fe_2O_3

References

[1] M. Wu, R. Liu,D. Wan.Journal of Heteroatom Chemistry 24(2013) 110.
[2] A. Mobaraki, B. Movassagh, B. Karimi.Journal of ACS Combinatorial Science472(2014)123.

Green Synthesis of Silver Nanoparticles Using *Orobanche Cernua* Extract

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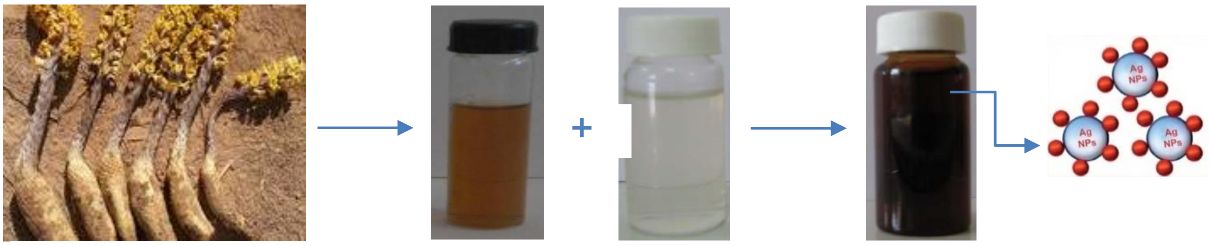
In recent years, nanotechnology is emerging as a revolutionizing field of research with multiple disciplines of science like physics, chemistry, materials science and biology. In conventional, various chemical and physical methods are utilized for the synthesis of nanomaterials, but due to the fact of usage of a large amount of hazardous chemicals, it becomes a mandate to find an alternative eco-friendly methodology. In search of green chemistry approach, the usage of plants and microbes were of the prime target, which were considered safe, simple, nontoxic, biocompatible and environment friendly [1].

Noble metal nanoparticles, such as gold (Au) and silver (Ag), have gained the attention of many scientific due to applications in medicine, biology, and the environment. Plant extracts are rich bioreducing agents (e.g: Secondary metabolites, enzymes and proteins) that can reduce silver ions to silver nanoparticles [2].

In this study, Biosynthesis of silver nanoparticles using plant extracts of *Orobanchecernua*was accomplished(Figure 1). This plant which lacks leaves and chlorophyll is parasite to roots of the crops [3]. Optimization of experimental conditions such as the concentration of both silver nitrate and herbal extract, temperature and pH were investigated. Furthermore, optimum conditions for the synthesis of silver nanoparticles was characterized with different techniquessuch as UV–vis spectroscopy, FT-IR spectroscopy and X-ray diffraction (XRD).

UV–vis spectroscopy was indicative the Surface plasmon resonance of nanoparticles. FT-IR spectroscopy was investigated for identification and study of functional groups that are involved nanoparticles and XRD was indicative the crystalline nature and structure of the nanoparticles.



Plant (*orobanche cernua*) Aqueous extract $AgNO_3$ solution Color change of the solution

Figure 1.Schematic diagram of the green synthesis of silver nanoparticles using aqueous extract of Orobanche cernua

References

[1] K.B. Narayanan, N. Sakthivel. Journal of Hazardous Materials 189 (2011) 519.
[2] R.R.R. Kannan, W.A. Stirk, J. Van StadenK. South African Journal of Botany 86 (2013) 1.
[3] Z-y. Qu, Y-w. Zhang, C-l. Yao, Y-p. Jin, et al. Biochemical Systematics and Ecology 60 (2015) 199.

Extraction and Determination of Fatty Acid Compositions of *Ziziphus spina-christi (L.)*

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Primary metabolitessuch as carbohydrates, amino acids, fatty acids, chlorophylls and etc. were found in all plants. Unlike primary compounds, secondary metabolites are present in some plants only. Secondary metabolites are not directly involved in thenormal growth, development or reproduction of an organism [1]. Fatty acids, especially unsaturated fatty acids, are important as nutritional substances and metabolites in living organisms. Many kinds of fatty acids play an important role in the regulation of a variety of physiological and biological functions There is currently scientist interest in studying polyunsaturated fatty acid sources due to correlation between these fatty acids (omega-3 and omega-9) and the prevention of cardiovascular disease and the reduction of LDL cholesterol levels among other benefits [2].

Zizyphus spina-christi L. (Rhamnaceae) is a plant that grows into a tree with thorny branches and is used as a hedge to form defensive fences for cattle. The fruit have a sweet edible pulp, the leaves are applied locally to sores, and the roots are used to cure and prevent skin diseases [3]. In this study, The plant material was collected from Fars province, Iran, in April 2016. The seeds were separated from the fruit. The seeds was split and core removed and the extract was obtained by n-hexane as solvent, using a Soxhlet apparatus for 12h. The lipids were esterified with 2% methanolic NaOH - 25% BF_3/methanol reagent. The fatty acid methyl esters were extracted with hexane/saturated NaCl and analyzed by Gas chromatography–Mass spectroscopy (GC- MS). 19 fatty acids were detected in fruit seed.

References

[1] D-K. Lee, M.H. Yoon, Y.P. Kang, et al. Food Chemistry 141 (2013) 3931.
[2] P.B.F. Biondo, V.J. Santos, P.F.Montanher, et al. Analytical Methods 7 (2015) 9773.
[3] B. Adzu, S. Amos, C. Wambebe, K. Gamaniel. Fitoterapia 72 (2001) 344.

Total Phenolic Content, Flavonoid Concentration and Antioxidant Activity of *Orobanche Cernua* Extracts

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Free radicals such as reactive oxygen species are formed naturally in the living things cells that have important roles in cell signalling, also in environment some toxins may contain free radicals or stimulate the cells to produce free radicals. High amount of this compounds are hazardous to the cells and damage all major its components. Plant extracts and essential oils can be used as potentially useful sources of antimicrobial and antioxidant compounds. The antioxidant activities of plants are mainly attributed to their phenolic and flavonoid compounds [1].

In this study, in vitro antioxidant activity, total phenolic content and concentration of flavonoids of five different extracts, from the whole herb of *Orobanche cernua* were determined using spectrophotometric methods [2].*Orobanche cernua* is aparasite loss chlorophyll and leaves, from *Orobanchaceae* family. *Orobanchaceae* comprises about 170 species, mostly distributed in the temperate and semi-arid regions of the world. The genus *Orobanche* has 39 species in Iran of which nine taxa are endemic to Flora Iranica area [3].

The plant material was collected on April 2016 in Birjand area, in Iran. The aerial part and rootstock of plant were air- dried at ambient temperature in the shade and subjected to extraction by maceration method with water, ethanol, n-buthanol, ethylacetat and acetone.

Total phenol and flavonoid content of the *O. cernua* extracts was determined by Folin-Ciocalteu and aluminum chloride methods, respectively. Antioxidant activity of extracts were expressed as percentage of DPPH radicals inhibition and IC50 values (μg/ml). Figure 1, below, shows the mechanism by which DPPH• accepts hydrogen from an antioxidant. Acetonic exstract of *O. cernua* showed the highest phenolic and flavonoid concentration and strong antioxidant activity.

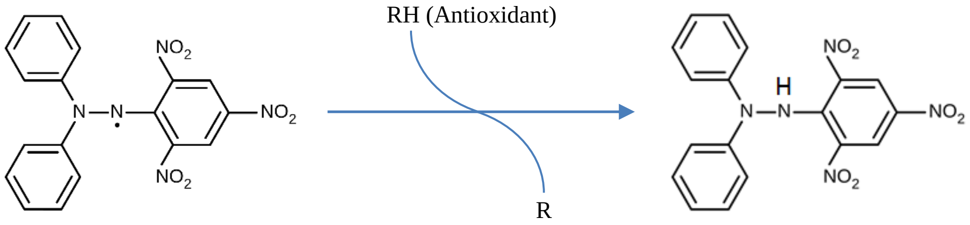

Figure 1.DPPH• free radical conversion to DPPH by Antioxidant compound.

References

[1] M. Valko, D. Leibfritz, J. Moncol, M.T.D. Cronin, M. Mazur, J. Telser. The International Journal of Biochemistry & Cell Biology 39 (2007) 44.

[2] M.A. Ebrahimzadeh, S.M. Nabavi, S.F. Nabavi, F. Bahramian, A.R. Bekhradnia. Pakistan Journal of Pharmaceutical Sciences 23 (2010) 29.

[3] Z-y. Qu, Y-w.Zhang, C-l.Yao, Y-p.Jin, et al. Biochemical Systematics and Ecology 60 (2015) 199.

Phytochemical and Physicochemical Studies of *Ziziphus spina-christi (L.)*

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Ziziphus spina-christi (L.) (ZSC) commonly known as Christ's thorn or Jerusalem-thorn in English and Sidr in Arabic belongs to family Rhamnaceae. It is a deciduous tree, native to the warm-temperate and subtropical regions, including south and east of Asia and Middle East [1].

In this study, *Ziziphus spina-christi* was collected on April 2016 from shiraz (Fars Province, Iran) and subjected to extraction by maceration method with water, methanol, ethanol and acetone. The phytochemical screening in four crude extracts showed the presence of Steroids, Alkaloids, Tannins, Coumarins, Proteins, Flavonoids, Terpeniods, Phenols and Carbohydrates. Also, total Phenolic, total Flavonoids and Tannins contents were determined in four different extracts with spectrophotometer [2]. In addition, determination of mineral elements amount like K, Fe, Ca, Mn, Mg, Na, Zn and Cu were investigated. Among the four selected solvents, methanol was the best for total Flavonoids and total Phenolic contents extraction. The total ash value was found to be 3.97% w/w indicating the considerable presence of inorganic radicals [3].

References

[1] F. Alhakmani1, S. Alam Khan, A. Ahmad. Asian Pacific Journal of Tropical Biomedicine 4 (2014) 656.
[2] C. Quettier-Deleu, B. Gressier, J. Vasseur, et al. Journal of Ethnopharmacology 72 (2000) 35.
[3] A. Jindal, H. Vashist, A. Gupta, et al. Pharmaceutical Technology 7 (2012) 24.

Microwave-assisted Synthesis of Xanthones Promoted by Sulfonic Acid-Functionalized Graphene Oxide Catalysts

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Xanthones and thioxanthones derivatives are interesting compounds, because of their well-known properties in the fields of medicinal and biological activities (anticancer, antioxidant, antimicrobial, antiviral, antiinflammatory, antiallergy, antihypertensive, antithrombotic and anti-Alzheimer activity, depending on their diverse structures). Therefore, their syntheses have attracted a large number of organic chemists[1].

Xanthones are usually synthesized using benzophenones or diaryl ethers as starting materials under harsh reaction conditions and often in the presence of strong acids or toxic metals as catalysts, but generally providing the desired products in low yields. Improvements have been achieved applying microwave irradiation especially in theterms of higher yields and shorter reaction times [2].

In this study, a new method for the chemical synthesis of xanthones is described. The title compounds have been synthesized in good yields under microwave irradiation from substituted 2-hydroxybenzoic acids and resorcinol in the presence of GO/SO_3H as the catalyst.In preliminary experiments, the model reaction was carried out in refluxing solvents and solvent free conditions using solid acids.After 24 h, the yields of products were low (<20%) with large amounts of starting materials remaining increasing reaction time and temperature did not affect the yield of the product. To improve the yield and optimize the reaction conditions, the same reaction was carried out under microwave irradiation. In this condition products were obtained in good to excellent yields (80-95%).The pure product was identified by ^{1}H NMR, ^{13}C NMR and FT-IR spectroscopy (Figure 1).

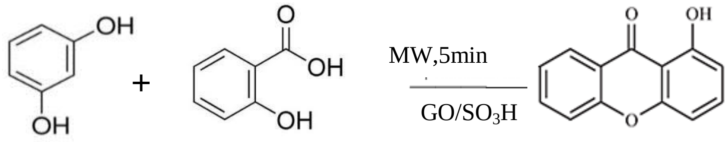

Figure 1. Synthesis of 1-hydroxy xanthone in the presence of GO/SO_3H

References

[1] X. Zhang, L. Yang,Y. Wu, J. Du, Y. Mao,X. Wang, S. Luan, Y. Lei, X. Li, H. Sun, Q. You. Journal of Tetrahedron Letters 55 (2014) 4883.
[2] S. Genovese, S. Fiorito,M.C. Specchiulli, V.A. Taddeo, F. Epifano.Journal ofTetrahedron Letters 56 (2015) 847.

Efficient Approach for the Synthesis of Eptifibatide as Antiplatelet Drug

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Over the years, peptides have been evolved as promising therapeutic agents in the treatment of cancer, diabetes, and cardiovascular diseases, and application of peptides in a variety of other therapeutic areas is growing rapidly.

Eptifibatide is an antiplatelet drug of the glycoprotein IIb/IIIa inhibitor class (Figure **1**). It is a cyclic heptapeptide which belongs to the class of the arginin-glycin-aspartat (RGD) mimetics and reversibly binds to platelets. Eptifibatide has a short half-life. The drug is the third inhibitor of GP IIb/IIIa that has found broad acceptance and has been approved by FDA in 1998.

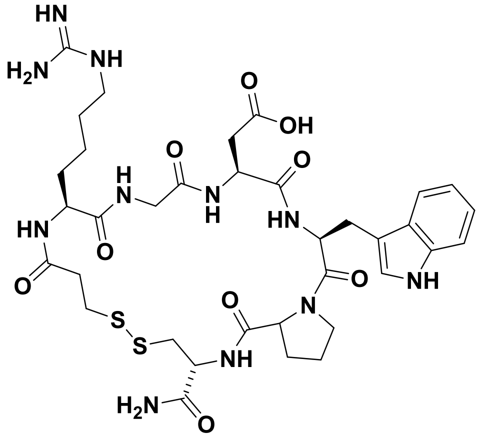

Figure 1. Eptifibatide

Herein, we wish to report the new approach for the synthesis of an API antiplatelet drug using Solid Phase Peptide Synthesis (SPPS) and suitable coupling reagents. The structure of compounds was confirmed based on the HR-MS (ESI) data. The details about synthetic approach and structure of product will be further discussed in the conference.

References

[1] Ciborowski, M.; Tomasiak, M.; *Acta poloniae pharmaceutica*., 2008, *66*, 235-42
[2] Scarborough, R.M.; Gretler, D.D.; *J. Med. Chem.*, 2000, *43*, 3453–3473.

Synthesis a New series of Quinazolines

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Quinazolines are a classof fused heterocyclic compounds that are of considerable interest because of the diverse range of their biological properties [1]. Many substituted quinazoline derivatives possess a wide range of bioactivities such as antimalarial, anticancer, antimicrobial, antifungal, antiviral, antiprotozoan, anti-inflammatory, diuretic, muscle relaxant, antitubercular,antidepressant, anticonvulsant, acaricidal, weedicide, and many other biological activities. Quinazoline compounds are also used in preparation of various functional materials for synthetic chemistry and also present in various drugs molecules [2].

In this work we reported the synthesis of new quinazoline derivatives from (Z)-2-amino-N'-phenylbenzimidamideand ninhydrin in ethanol as a solventat ambient temperature for 30 min. The product was identified by IR, ^{1}H- NMR, ^{13}C-NMR data.

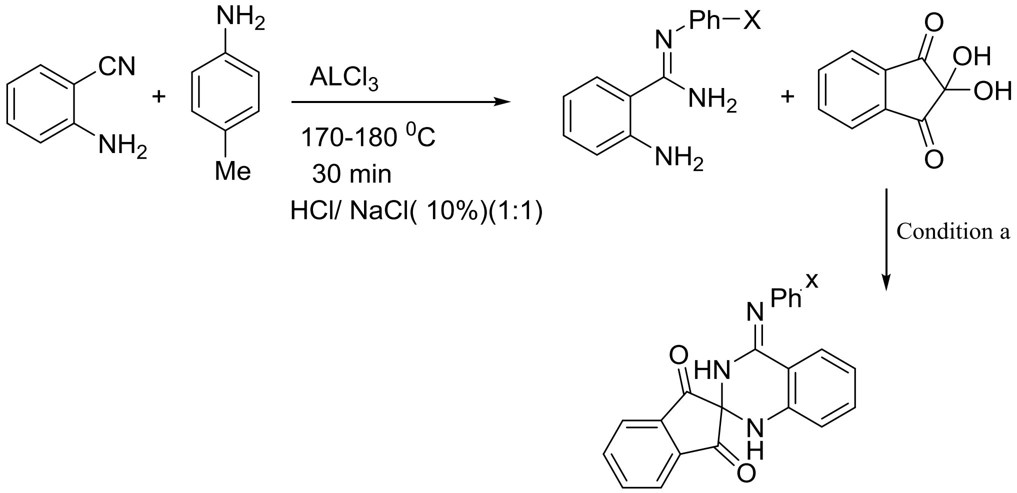

Figure 1. Scheme of the reaction.

References

[1] D. J. Connolly, D. Cusack, T. P. O' Sullivan, and P. J. Guiry, "Synthesis of quinazolinones and quinazolines," Tetrahedron, vol. 61, no. 43, pp. 10153‑10202, 2005.

[2] Abida, P. Nayyar, and M. Arpanarana, "An updated review: newer quinazoline derivatives under clinical trial," International Journal of Pharmaceutical & Biological Archive, vol. 2, no. 6, pp. 1651‑1657, 2011.

[3] S. B. Mhaske and N. P. Argade, "The chemistry of recently isolated naturally occurring quinazolinone alkaloids," Tetrahedron,vol. 62, no. 42, pp. 9787–9826, 2006.

Synthesis of new oxadiazole derivatives with potential anti cancer effect

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Many diaryl and triaryl heterocycles with different central ring such as, pyrrole, oxadiazole,triazole and imidazole as anticancer agents are reported in several scientific sources [1,2]. 1,2,4-oxadiazole derivatives got many attentions during last decade due to their various biological activities such as anticancer activity [3].

Therefore in the present study an approach for the synthesis of some derivatives of triaryl-4,5-dihydro-1,2,4- oxadiazole and their reactions was innovatived. triaryl-4,5-dihydro-1,2,4- oxadiazole derivatives were prepared from reaction ofdifferent imines and 4-substitutedbenzohydroxyiminoyl chlorides. In this study the derivatives of triaryl-4,5-dihydro-1,2,4- oxadiazole were synthesized.. The structures of the foregoing products were confirmed by NMR, IR and Mass spectroscopy methods.Then the scope of the reaction was taken into account.

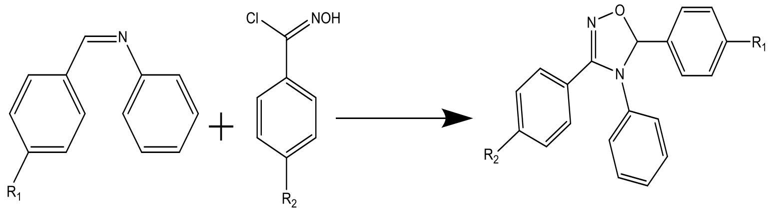

Figure 1.scheme of the reaction

References:

[1] Odlo K. et al. Bioorg.Med. Chem. 2008, 16, 4829.

[2] Schobert R. et al. J.Med.Chem.,2010, 53, 6595.

[3] Joo YH, Kim JK, Kang S-H, Noh MS, Ha J-Y, Choi JK, Lim KM, Chung S (2004) ,79,4752

One-Pot , multi-component synthesis of various 5-amino-4-carbonitrilepyrazole derivatives with green conditions

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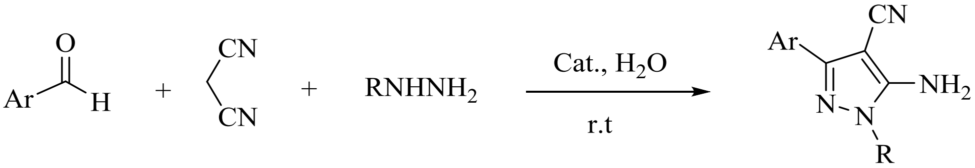
Pyrazole and derivatives are key substructures in a large variety of compounds with important biological activities and pharmacological properties [1].

Multi-component reactions (MCRs) have emerged as an attractive and powerful strategy for organic synthesis compared to multistep reactions due to the creation of several new bonds in a One-Pot reaction, low number of reaction and purification steps, selectivity, synthetic convergence, high atomeconomy, simplicity, and synthetic efficiency [2].In fact, development of MCRs can lead to new efficient syntheticmethodologies to afford many small organic compounds in the field of modern organic, bioorganic, and medicinal chemistry [3].

We have developed a highly efficient and green One-Pot methodology for the synthesis of a wide range of 5-amino pyrazole-4-carbonitrile derivatives, which are often encountered in biologically and pharmacologically actives compounds. The present methodology requires low catalyst loading as a mild Lewis acid catalyst. The most important advantages of this method include the use of cost-effective and mild transition metal catalyst, aqueous conditions, excellent yields, clean and simple work-up procedure, and avoidance of using hazardous organic solvents that makes this method an instrumental alternative to the previous methodologies for the scale-up of these One-Pot three-component reactions.



References

[1] (a) S.R. Donohue, C. Halldin, V.W. Pike. Tetrahedron Lett.49 (2008) 2789 (b) G. Szabo, J. Fischer, A. Kis-Varga,K. Gyires. J. Med.Chem. 51 (2008) 142.

[2] (a) B. Ganem, Acc. Chem. Res. 42 (2009) 42 463e472; (b) A. Domling, I. Ugi,Angew. Chem., Int. Ed. 39 (2000) 3169.

[3] M. G. Dekamin,Z. Mokhtari,Tetrahedron, 68 (2012) 922.

Use of $CaCO_3@Fe_3O_4$ nanoparticles as an efficient and eco-friendly nanocatalyst for facile synthesis of perimidine derivatives

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Perimidines are tricyclic heterocycles containing a dihydropyrimidine ringortho and peri-fused to the naphthalene structure. These heterocyclic systems,which have been shown to be interesting candidates for biological studies, arewidely applied in industry, agriculture, and medicine [1].

Magnetic porous hollow nano-sphere is a new class of structured nanomaterials for drug delivery, magnetic resonance imaging, hyperthermia cancer treatment, and bioseparation[2].Magnetically $Fe_3O_4/CaCO_3$recoverable nanoparticles represent an economical, practical and environmentally benign means for catalyst recovery [3]. The nano-catalyst was characterized by IR, EDX, scanning electron microscopy (SEM) and TEM. The some novel compounds were identified by spectroscopic and spectrometric analyses.This environmentally benign and clean synthetic procedure has several advantages, including the availability, safety, and reusability of the catalyst, high yields, short reaction times, and easy and rapid isolation of the product.

Encouraged by this result and the development and generality of a simple method for synthesizing of heterocyclic compound, One-Pot reaction of 1,8-diaminonaphthalene 1 with a variety of aromatic aldehydes 2 by using of $Fe_3O_4@CaCO_3$ nanoparticles as highly efficient catalyst in ethanol at room temperature was performed (Figure1).

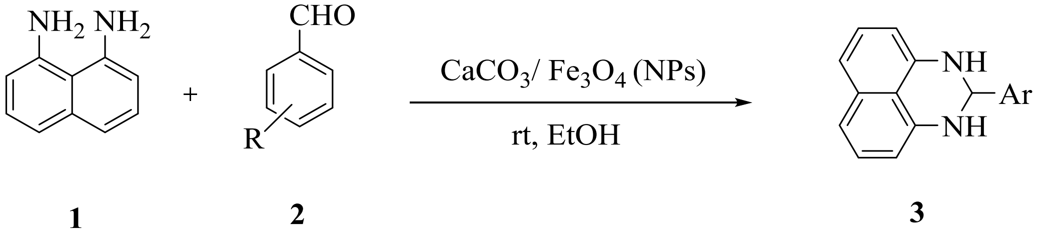

Figure 1. Synthetic method of perimidines3

References

[1] A.F. Pozharskii, V.V. Dalnikovskaya, Russ. Chem. Rev. 50(1981)816.

[2] (a) H. H. Yang, S. Q. Zhang, X. L. Chen, Z. X. Zhuang, J. G. Xu, and X. R. Wang, Anal. Chem. 76 (2004) 1316; (b) L. Levy, Y. Sahoo, K. S. Kim, E. J. Bergey, P. N. Prasad, Chem. Mater. 14 (2002) 3715.

[3] T. -J. Yoon, W. Lee, Y. -S. Oh, J. -K Lee New J. Chem. 27(2003), 227

Synthesis and characterization of new imprinted polymer nanocomposites as colon-specific drug delivery vehicles

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Molecularly imprinted polymers (MIP) exhibiting high selectivity and Special performance in identifying the target molecule are now seeing a fast growing research. In this paper, we synthesized the new types of nancomposite non-covalent molecularly imprinted polymers (MIPs) and non-imprinted polymers (NIPs) which are used in the field of drug release and by optimizing them can be enhanced effectiveness. The aim of this work was to investigate this new types of nanocomposite as controlled release devices forin biological fluids, especially gastrointestinal. Two types of nanocomposites were synthesized (MIP and NIP) by HF. Through corrosive nature of this type of acid, silica nanoparticles in the polymeric matrix be omitted and amount the holes created for template molecules trapped were increased. The releasing of drug was carried out in cellophane membrane dialysis bags and the in vitro release profiles were established separately in enzyme-free simulated fluids (SGF, pH 1 and SIF, pH 7.4).

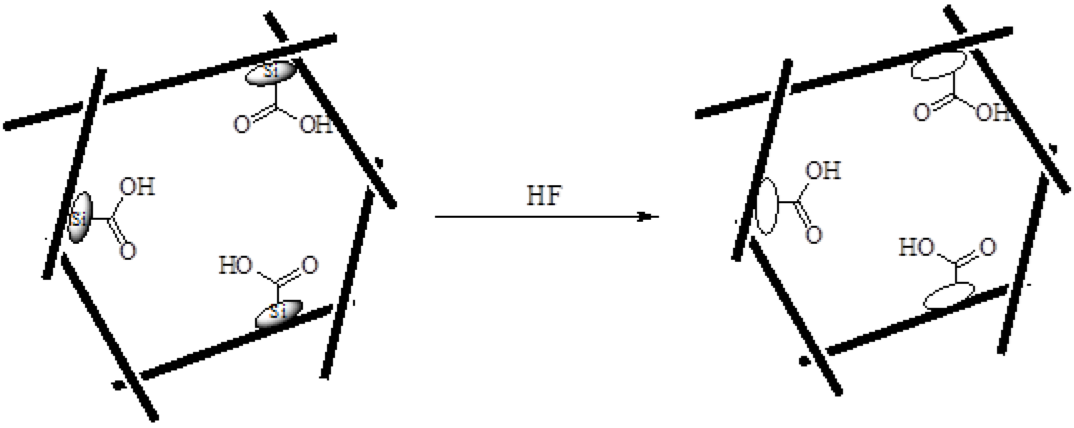

Figure 1. Formation of nanoporouses MIP by using of HF

References
[1] Mahkam M.,Poorgholy N.; Nature and Science (2011) 9, 163-168.
[2] Yan H., Ho Row K.; International Journal of Molecular Sciences (2006) 7, 155-178.

Impressive Catalytic Capacity to Synthesis of Benzamide Derivatives in the Presence of Cu(II)–EDTA Complex Supported on Magnetic Nanoparticles

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The direct amidation of alcohols and amines using supported heterogeneous catalysts has been rarely studied [1]. In the area of magnetic catalysts, no attempt has been focused on the direct amidation from alcohols and amines in the presence of supported heterogeneous catalysts on the magnetic nanoparticles. In continuation of our interest in using magnetic nanoparticles [2] as a catalyst support in the oxidative amidation of aromatic aldehydes with amine hydrochloride salts [3], herein, we demonstrate the application ofFe$_3$O$_4$@EDTA–Cu(II) for the amide synthesis via alcohol dehydrogenation in One-Pot direct oxidative amidation. The Fe$_3$O$_4$ nanoparticles were functionalized by EDTA and the Cu–EDTA complex was stable under oxidation conditions with high efficiency in solvent. This atom-economical and cost effective transformation can be used as the most favorable replacement for the synthesis of amides.

Superparamagnetic Fe$_3$O$_4$@EDTA–Cu(II) nanoparticles were readily prepared and identified as an effective catalyst for the tandem transformation of benzyl alcohols and amine hydrochloride salts into the corresponding amides with *tert*-butyl hydroperoxide (TBHP) as an oxidant. After completion ofthe reaction, the catalyst can be removed from the reaction vessel by assistance ofan external magnet and reused at least six times without significant loss of its activity.

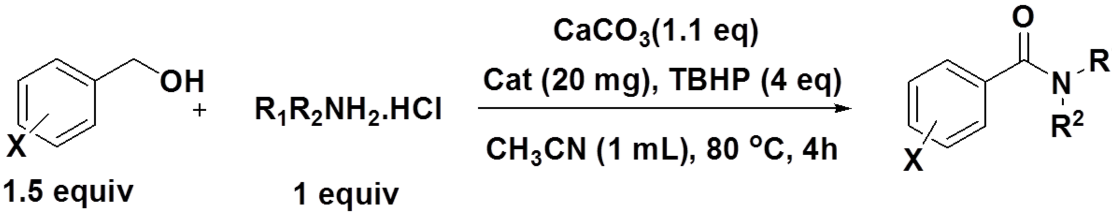

Figure 1.scheme of the reaction

References

[1] Y. Wang, D. Zhu, L. Tang, S.Wang, Z. Wang, Angew. Chem. Int. Ed. 50 (2011) 8917.
[2] a) K. Azizi, A. Heydari, RSC Adv. 4 (2014) 8812; b) K. Azizi, A. Heydari, RSC Adv. 4 (2014) 6508.
[3] D. Saberi, A. Heydari, Appl. Organomet. Chem. 28 (2014) 101.

In Situ-Generated (Hypo) iodite Ions-Catalyzed Oxidative Amidation of Unactivated Methylarens

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Iodine is most stable with an oxidation state -1; however, it forms stable polycoordinate, multivalent compounds.Current researches focus on its use in carbon-carbon and carbon-heteroatom bond forming reactions.[1] Zhang et al. demonstrated that 1-(4′-diacetoxyiodo benzene)-3-methylimidazolium tetrafluoroborate [dibmim][BF_4] catalyze the selective oxidation of alcohols to carbonyl compounds.[2] Zhdankin and co-worker presented that 2-Iodylphenol ethers can selectively oxidize sulfides to sulfoxides and alcohols to the respective aldehydes or ketones.[3]

Herein, we demonstrate that the direct oxidative amidation of unactivated methylarenes with hydrochloric salts of amines in the presence of in situ-generated (Hypo) iodite with TBHP for the first time. Various secondary and tertiary amides were synthesized in good to excellent yields in One-Pot manner under our conditions.

Hypervalent iodine-catalyzed oxidative amidation of methylarens to the corresponding amides by using an environmentally available oxidant (*tert*-butyl hydroperoxide, 70% aqueous solution) is discussed. This oxidizing agent presented a high degree of selectivity for the oxidation of toluene to amide without oxidation to carboxylic acid. This reaction involves the metal-free oxidation, mild reaction condition and *tert*-butyl alcohol as the only by-product.

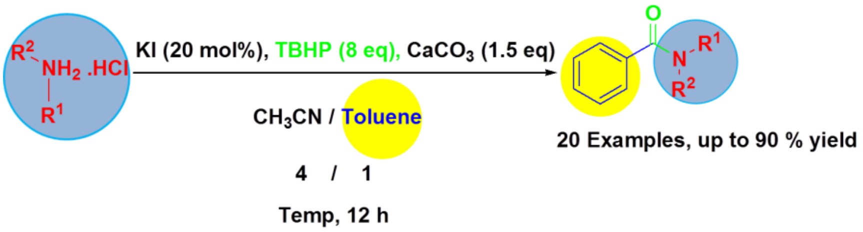

Figure 1.scheme of the reaction

References

[1] T. Dohi, A. Maruyama, Y. Minamitsuji, N. Takenaga, Y. Kita, Chem. Commun. 12 (2007) 1224.
[2] W. Qian, E. Jin, W. Bao, Y. Zhang, Angew. Chem. Int. Ed. 44 (2005) 952.
[3] A. Y. Koposov, R. R. Karimov, I. M. Geraskin, V. N. Nemykin, V. V. Zhdankin, J. Org. Chem. 71 (2006) 8452.

L-arginine-functionalized magnetic nanoparticles as a recyclable organocatalyst for synthesis of chromenes

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A practical, convenient, and cheap methodology is developed for the synthesis of a series of chromene derivatives via cyclocondensation of α- or β-naphthol, malononitrile and aromatic aldehydes, in the presence of L-arginine-immobilized magnetic nanoparticles, under ultrasound irradiation, in high yields. This catalyst can be easily separated from the reaction by an external magnet and recycled four times without its activity loss. This methodology has shown shorter reaction times when compared with conventional thermal heating.Chromenes constitute one of the major classes of naturally occurring compounds. The basic structural skeleton of these compounds is an ordinary characteristic of polyphenols(1) found in tea, fruits, vegetables and red wine. Fused chromenes exhibit antimicrobial,(2) mutagenicitical, antiviral, antiproliferative, antitumoral properties and be employed as cosmetics and pigments. These compounds can be used as potential biodegradable agrochemicals.(3)

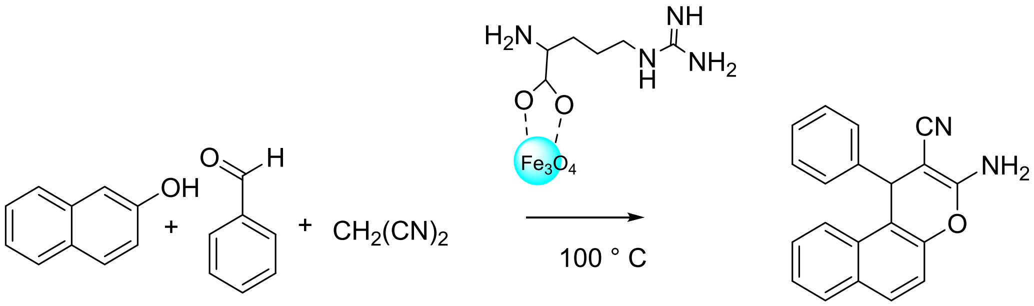

Figure 1. Synthesis of chromenes using Fe_3O_4@L-arginine MNPs

References

[1] J. Jankun, S. H. Selman, R. Swiercz and E. SkrzypczakJankun, Nature, 1997, 387, 56.
[2] M. M. Khafagy, A. H. F. A. El-Wahas, F. A. Eid and A. M. ElAgrody, Farmaco, 2002, 57, 715.
[3] M. R. Naimi-Jamal, S. Mashkouri and A. Sharifi, Mol. Diversity, 2010, 14, 473.

A green synthesis of α-aminophosphonates in glycerol

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A simple and efficient method is described using glycerol as a solvent in the catalyst-free synthesis of α-aminophosphonates in high purity. Products are prepared by the Kabachnik–Fields reaction from amines, phosphites, and carbonyl compounds. The method does not require a toxic catalyst.α-Aminophosphonic acids and their derivatives exhibit a widerange of biological properties,(1) and are able to function as α-aminocarboxylic acid surrogates.(2)α-Aminophosphonate esters haveattracted attention because not only are they biologically attractivepeptide mimics of α-amino acids, but they also exhibit intriguing biological activities.(3)Glycerol can be considered as‘organic water’ since, like water, it is abundant, biodegradable,inexpensive, nontoxic, highly polar, immiscible with hydrocarbons,is able to form strong hydrogen-bond networks, and can dissolve awide range of organic and inorganic compounds, including transitionmetal catalysts.(4)In addition, compared to water, it has the advantage of a higherboiling point, lower vapor pressure, and is able to dissolve organiccompounds usually immiscible with water.(5)

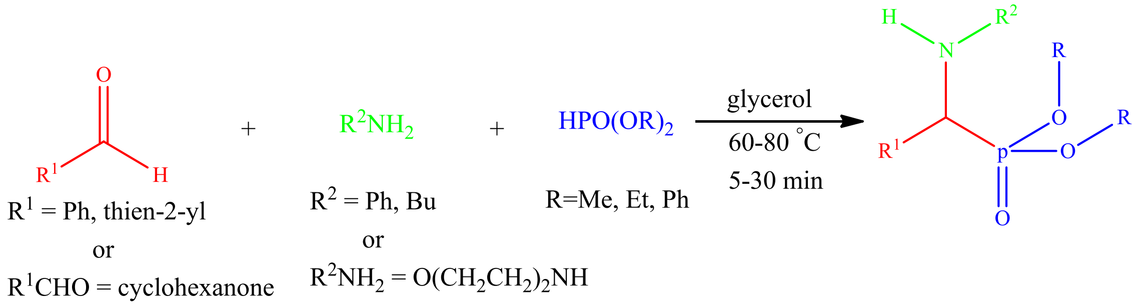

Figure 1..NoncatalyzedKabachnik–Fields reaction in glycerol.

References

[1] Atherton, F. R.; Hassall, C. H.; Lambert, R. W. J. Med. Chem. 1986, 29, 29.
[2] Baldwin, C.; Williams, J. M. J. Tetrahedron: Asymmetry 1995, 6, 679.
[3] Shang, Z. Q.; Chen, R. Y.; Huang, Y. Heteroat. Chem. 2007, 18, 230.

Nano-$TiCl_4$ /gama-Al_2O_3: an Efficient Heterogeneous Solid Acid Catalyst for Rapid and Solventless Synthesis of Azo dyes based on 2-Naphthol at Room Temperature

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At the beginning of the new century, synthesis of organic compounds using grinding technique under solvent-free conditions has received much attention, as it provides manipulative simplicity, easier workup, and higher yields which match with the green chemistry protocol [1]. On the other side, more attention has been directed toward the application of solid acids in organic synthesis because such reagents not only simplify purification processes but also help prevent release of reaction residues into the environment [2].The reactions that are affected by the nano catalysts immobilized on the inert porous solid supports, have received significantposition in organic synthesis.The individual features of supported Lewis acids such as their ease of handling, enhance reaction rates, greater selectivity, and recoverability of catalysts make the use of supported Lewis acids attractive [3].In this work we wish to report diazotization of aromatic prime amines with $NaNO_2$, $TiCl_4$/*gama*-Al_2O_3 nano particle at room temperature and diazo coupling with 2-naphthol has developed a mild and convenient method for the synthesis of azo dyes under solvent-free conditions at room temperatureFigure 1.

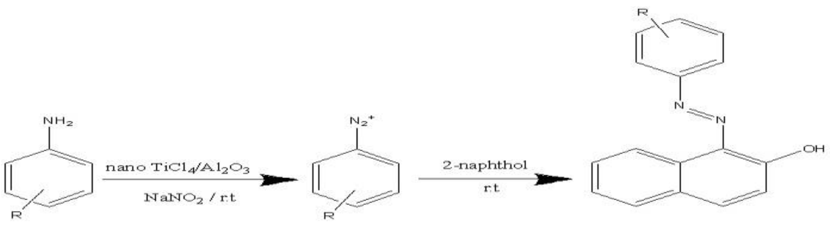

Figure 1.scheme of the reaction

References

[1] A. Bamoniri, B.F. Mirjalili, N. Moshtael-Arani. Journal of Green Chemistry Letters and Reviews 7 (2014) 393.
[2] A. Bamoniri, B. F. Mirjalili, S. Pooladsanj, F. Teymouri.Iranian Journal of Organic Chemistry 3 (2011) 573.

[3] B. F. Mirjalili, A. Bamoniri, A. Akbari.Current Chemistry Letters 1 (2012) 109.

Water-Soluble Porphyrins as Novel Sensitizers for Photodynamic Therapy

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Photodynamic therapy (PDT) is a successful treatment method for various types of cancer, that leads to the selective destruction of tumor by cytotoxic singlet oxygen generated via visible laser light activation of photosensitizer [1, 2]. porphyrins are have been widely used clinically in PDT for cancer treatments because of their capability to generate singlet oxygen efficiently and their tendency to accumulate in tumor tissue, However, porphyrin structure is unsuitable for biomedical application [3]. Novel water-soluble 5,10,15,20-tetrakis(4-N-carbonylacrylic aminophenyl)porphyrin was designed and synthesized for the first time as the tetrasodium salts by via reaction of tetrakis(4-aminophenyl)porphyrin(NH_2-TPP) with maleic anhydride. 4-Nitrobenzaldehyde was employed in order to synthesize tetrakis(4-nitrophenyl)porphyrin (NO_2-TPP) and then it was converted to NH_2-TPP by $SnC1_2$. The structure of the porphyrin was thoroughly studied by a variety of techniques such as NMR, FT-IR and UV-visible spectrophotometer. In this work, the efficiency of porphyrin as photodynamic therapy (PDT) systems was investigated. The production of reactive singlet oxygen, cytotoxity and phototoxicity of it was assessed. The study showed that the singlet oxygen production ability of porphyrin can be well controlled by irradiation. We tested on A453 cells to compare effectiveness. This photosentesizer exhibited cell viability over 97% and good photocytotoxity, indicating it is promising photodynamic photosentesizer for cancer therapy.

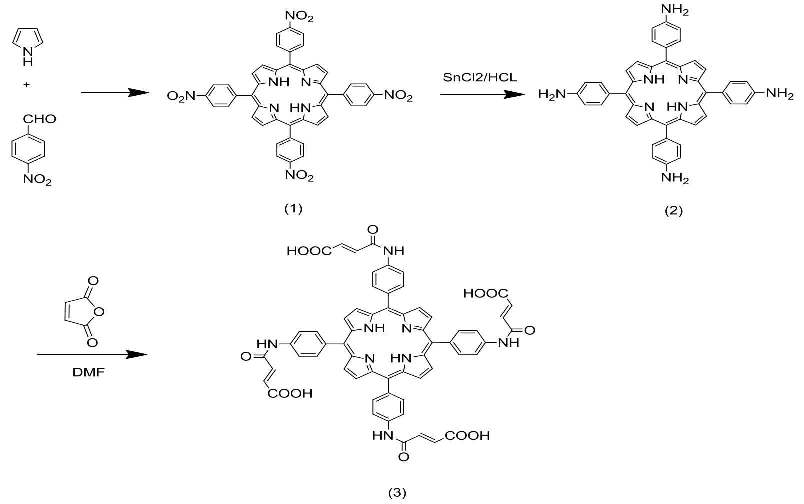

Figure 1. Scheme of the reaction

References

[1] M. Kempa, et al. Spectrochimica Acta Part A, 146 (2015) 249.

[2] K. Haedicke, et al. Acta Biomaterialia, 14 (2015) 197.

[3] J. Luo, et al. Inorganic Chemistry, 53 (2014) 4184.

Synthesis of pyranocoumarins derivative by three-component coupling reaction of aryl glyoxals, malononitrile, and 4‑hydroxycoumarin catalysed by ZrO_2 nanoparticles

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Multicomponent reactions (MCRs) represent a very useful tool at the interface of the fields of organic synthesis and chemical biology due to their superior atom economy, convergent nature, and straightforward experimental procedures. In addition, they are valuable in the pharmaceutical industry for the construction of low molecular weight compounds[1].

Pyrano-fused coumarins (pyranocoumarins) are natural products that exhibit important biological properties, such as antifungal, insecticidal, anticancer, anti-HIV, anti-inflammatory, and antibacterial activities[2].

Recently, the application of nanoparticles (NPs) as catalysts has attracted worldwide attention because of their high catalytic activity and improved selectivity [3]. The surface of metal oxides, such as TiO_2, Al_2O_3, ZnO, CuO and MgO, exhibits both Lewis acid and Lewis base character [4]. They are excellent adsorbents for a wide variety of organic compounds and increase the reactivity of the reactants.

here we report the results of our studies on the reaction between 4‑hydroxycoumarin1 ,aryl glyoxals2 and malononitrile3 in the presence of ZrO_2 nanoparticles as an efficient, and environmentally benign catalyst under solvent-free conditions to produces pyranocoumarins derivative4 in fairly good yield.

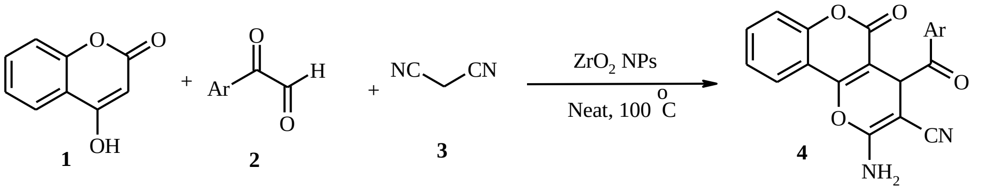

Figure 1.scheme of the reaction

References

[1] B.M. Trost, Science 254 (1991) 1471.
[2] D. C. Mungra, M. P. Patel, D. P. Rajani and R. G. Patel, Eur. J. Med. Chem. 46(2011) 4192.
[3] S. Wang , Z. Wang , Z. Zha, Dalton Trans 9363(2009).

The role of Amyloid Fbrils and Peroxidase Inhibition in Alzheimer's Disease

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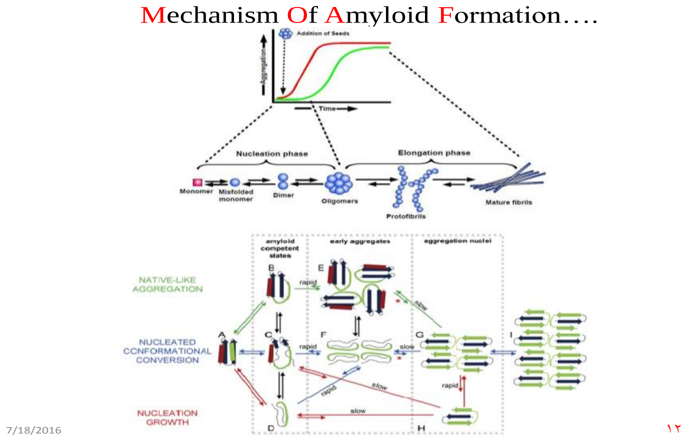
Neurodegenerative diseases are characterized by amyloid deposition. Thioflavin T (ThT) is one of the molecules considered for detection of amyloid deposits; however, its lipophilicity is too low to cross the blood brain barrier. Therefore, there is a strong motivation to develop suitable compounds for in vitro fibril quantification as well as for in vivo amyloid imaging. Moreover, oxidative stress (particularly, uncontrolled peroxidase activity) has frequently been reported to play a critical role in the onset/progression of some neurodegenerative disorders. In this study, we describe the synthesis of some benzothiazole, benzofuranone and curcumin-based 5-halophenyl/5-aryl pyrano pyrimidine derivatives compounds and examine their peroxidase inhibitory properties. Furthermore, to establish the potential binding of synthesized compounds to amyloid aggregates, their in vitro binding to some nondisease related amyloidogenic proteins were characterized.



Mechanism Of Amyloid Formation….

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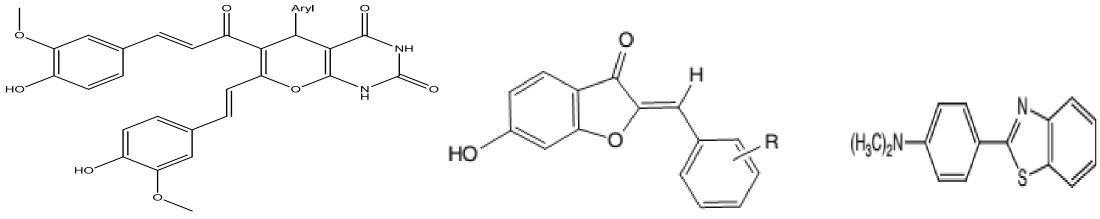

Figure 1.scheme of the reaction

References:

[1] Atamna H. Heme binding to amyloid-beta peptide: mechanistic role in Alzheimer’s disease. J Alzheimers Dis 10 (2006) 255– 266.

Theoretical study on the coupling of imidazole derivatives and haloalkanes: investigation of structures, effects of substituents and Gibbs free energy of reactions

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N-Arylazoles which are produced from coupling aryl halides and imidazoles are important building blocks in numerous agrochemicals, pharmaceuticals, biological active compounds, and *N*-heterocyclic carbene chemistry (1-2). In this work density functional theory has been used for investigation of the structure and formation of some *N*-arylazole compounds. For this purpose the geometries of all *N*-arylazoles were optimized with B3LYP method combined with SVP basis set. Vibrational frequency analyses, was calculated at the same level of theory, indicated that optimized structures are located at the stationary points corresponding to local minima without any imaginary frequency. The solvation energy (ΔG_{solv}) was calculated with the CPCM model by using DMF as a solvent. After that the Gibbs free energy in solution was calculated by using equation $\Delta G_{gas} + \Delta G_{solv} = \Delta G_{(aq)}$.We considered substitution effect including H, F, Me and CF_3 groups on imidazole and 1,4-diboromo and 1,4-dichloroarylhalids for synthesis of *N*-arylazole compounds (see Figure 1). Our calculations show that the $\Delta G_{(aq)}$amounts for all N-Arylazole compounds is exothermic and those with H and CF_3groups as R′ substituents have maximum and minimum amount of $\Delta G_{(aq)}$, respectively. About aryl halids, it should be noted that the best obtained results is for 1,4-diboromo compound.

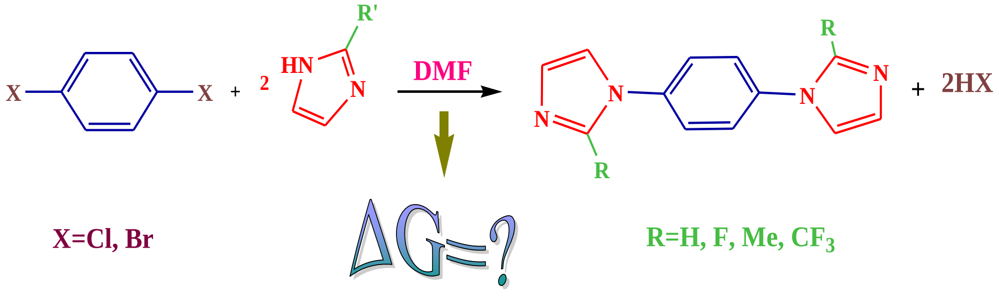

Figure1. Synthesis of *N*-arylazolesbycoupling of imidazole derivatives and haloalkanes

References

[1] T. Wiglenda, I. Ott, B. Kircher,P. Schumacher, D. Schuster, T. Langer and R. Gust, J. Med. Chem.,2005,48, 6516.
[2] Z. Jin, Nat. Prod. Rep.,2005, 22, 196.

Triethyl ammonium trinitro methanide[TEATNM] as a novel ionic liquid catalyst for the synthesis of 2-amino-4-aryl-6-(arylamino)pyridine-3,5-dicarbonitriles via anomeric based oxidation

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The pyridine ring plays a main role in numerous biological processes, most remarkably in the oxidation/reduction cofactors such as: NADPH, NADH, NADH and NAD$^+$; the vitamin niacin is required for its biosynthesis.[1] 3,5-Dicyanopyridines have been applied as intermediates in the synthesis of pyrido[2,3-*d*]pyrimidines as antihistaminic agents, pyridothieno- and pyridodithienotriazines endowed with antihistaminic and cytotoxic activity and acyclo-3-deazapyrimidine *S*-nucleosides that are active toward HIV.[2] Triethylammoniumtrinitromethanide [TEATNM] as a novel ionic liquid catalyzed the synthesis of 2-amino-4-aryl-6-(arylamino) pyridine-3,5-dicarbonitrile derivatives *via* the One-Pot three-component condensation reaction between various aromatic aldehyde, malononitrile and aniline derivatives at 50 °C under solvent-free conditions. The synthesized ionic liquid catalyst was fully characterized by using FT-IR, ^{1}H NMR, ^{13}CNMR, Mass and thermal gravimetric (TG) analysis. The major advantages of the described methodology are ease of separation, good yields and short reaction times.The scope and limitations of the described methodology will be discussed.

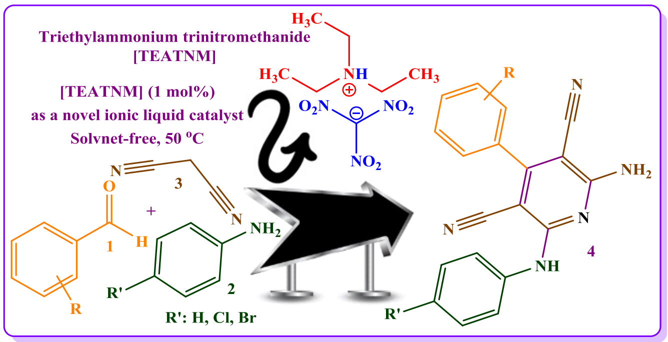

Figure 1. Synthesis of 2-amino-4-aryl-6-(arylamino)pyridine-3,5-dicarbonitrile derivatives catalyzed by triethylammoniumtrinitromethanide [TEATNM] as a novel ionic liquid

References

[1] (a) J. M. Berg, J. L. Tymoczko and L. Stryer, *Biochemistry*, W. H. Freeman and Company, New York, 2002; (b) G. Hamasaka, H. Tsuji and Y. Uozumi, *Synlett*, 2015, *26*, 2037.

[2] (a) J. M. Quintela, C. Peinador, L. M. Botana, M. Estèvez and R. Riguera, *Bioorg. Med. Chem.*, 1997, *5*, 1543; (b) J. M. Quintela, C. Peinador, M. C. Veiga, L. M. Botana, A. Alfonso and R. Riguera, *Eur. J. Med. Chem.*, 1998, *33*, 887; (c) A. M. E. Attia and A. E. H. A. A. Ismail, *Tetrahedron*, 2003, *59*, 1749.

Synthesis of 7-Aroyl-8-methyl-10-phenyl-10H-benzo[h]pyrazolo [3,4-b]quinoline-5,6-diones by One-Pot ,three component reaction

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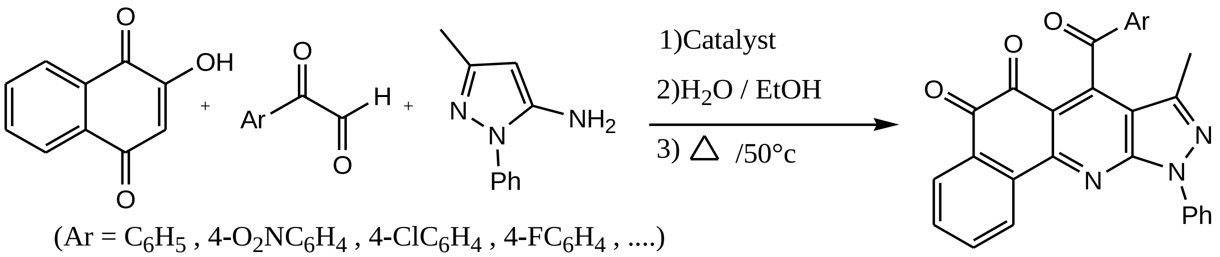
One-Pot ,three-component reaction of arylglyoxals , lawsone and 5-amino-3-methyl-1-phenyl pyrazole in water/EtOH (3:1) at 50$^{\circ c}$Using nanosilver and amino acidsas catalysts gave the corresponding7-aroyl-8-methyl-10-phenyl-10H-benzo[h]pyrozolo[3,4-b]quinolone-5,6-dionesin high yields.

The synthesized pyrazolo [3,4-b] quinoline-5,6-diones derivative may have a biological and pharmaceutical activities [1-3] as a class of o-quinone derivatives.



(Ar = C_6H_5 , 4-$O_2NC_6H_4$, 4-ClC_6H_4 , 4-FC_6H_4 , ...)

Figure 1.scheme of the reaction

The structure of new products were confirmed by their (^{1}H-NMR , ^{13}C-NMR , FT-IR) spectral data and microanalyses.

References

[1] S.Rajesh, B.DeviBala, S. Perumal and J. Carlos Men endez. Green Chem., 2011, 13, 3248.
[2] B. T. Walton, C.-H. Ho, C. Y. Ma, E. G. O'Neill and G. L. Kao,Science, 1983, 222, 422–423.
[3] T. M. Fong and S. B. Heymsfield, Int. J. Obes., 2009, 33,947–955.

Mechanochemical acceleration of Eschenmoser sulfide contraction reaction

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The Eschenmoser sulfide contraction is a common method for the synthesis of enaminones. Typically, thioamide and α-halocarbonyl compounds are coupled in these kinds of reactions [1]. The Eschenmoser coupling reaction commonly requires a base and a long reaction time [2]. Different natural products for example vitamin B12-derivatives, fuligocandin-, mersicarpine and diplodialid macrolactone-were synthesized with the help of sulfide contraction steps [2,3].

Figure. The Eschenmoser coupling reaction

The idea that using mechanical force can affect the reaction and complete it in a shorter time was interesting. We planned to apply mechanical force and consider the effects of planetary mixer and beads. We accelerated the reaction and provided condition to do the reaction without solvent. The scope and limitations of the described procedure will be presented.

References

[1] S. Cunha, A. T. Gomes, Tetrahedron Lett., 2012, 53, 6710.
[2] (a) N.D. Koduri, RSC Adv., 2013, 3, 181; (b) J. Mulzer, B. List, J. W. Bats, J. Am. Chem. Soc., 1997, 119, 5512; (c) B. Pettersson, V. Hasimbegovic, J. Bergman, J. Org. Chem., 2011, 76, 1554.
[3] (a) R. Nakajima, T. Ogino, S. Yokoshima, T. Fukuyama, J. Am. Chem. Soc., 2010, 132, 1236; (b) R. E. Ireland, F. R. Brown, J. Org. Chem., 1980, 45, 1868.

Preparation and effect of juglone on the antibacterial activity of the polycaprolactone nanofibers

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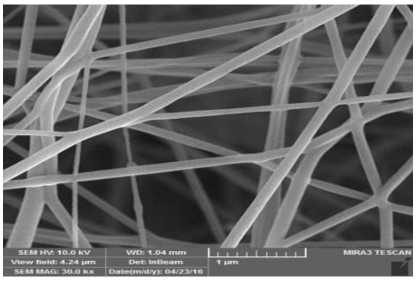
Human beings are often infected by microorganisms such as bacteria, molds, yeasts, and viruses in the living environment [1]. Nanofibers have excellent filtration properties, and due to the variety of polymers that can be used to fabricate nanofibers, and the versatility of being able to add functional molecules and chemical groups to the nanofibers, make nanofibers applicable to sanitation and purification of air which we breathe [2, 3]. In this work, polycaprolactone (PCL) -juglone nanofibers were manufactured by *electrospinning*. PCL polymers were synthesized using a ring-opening polymerization (ROP) method. PCL and juglone were dissolved in dimethyl sulfoxide (DMSO), and then thin-layered on a glass plate or electrospun followed by coagulation in sodium hydroxide solution. The above polymers were characterized by Fourier transform infrared spectroscopy (FT-IR). The morphology of the PCL-juglone nanofibers was characterized by scanning electron microscopy (Fig. 1). Antibacterial tests indicated that the prepared nanofibers have a bactericidal effect. The PCL-juglone nanofibers produced a reduction against Escherichia coli, Salmonella enteritidis, Staphylococcus aureus, and Streptococcus agalactiae.

Figure. 1 Scanning electron microscopy of the PCL-juglone nanofibers



References

[1] A.R. Shahverdi, A.Fakhimi Pharm, H.R. Shahverdi, S. Minaian, Nanomedicine: Nanotechnology, Biology, and Medicine 3 (2007) 168.

[2] S. Sundarrajan, K. Luck Tan, S. Huat Lim, S. Ramakrishna. Procedia Engineering 75 (2014) 159.

[3] L.-R. Yao, X.-M. Song, G.-Y. Zhang, S.-Q. Xu, Y.-Q. Jiang, D.-H. Cheng, Y.-H. Lu. Journal of Nanomaterials (2016), Article ID 4515769, 10 pages.

Chemical Composition And Antibacterial Activity Of Essential Oil Of Flowers Of *Nepeta binaludensis* From Khorasan

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Difference in the essential oil and solvent extract composition of *Nepeta* species influenced by ecological conditions and type of the organ in which essential oil are produced and/or accumulated have also been reported. this study was designed to examine the chemical composition and antimicrobial activity of the essential oils of flowers of *Nepeta binaludensis* Jamzad. in flowering stage which grows wild in binaloud mountainous. The composition of the essential oil hydrodistilled from the flowers of *N. binaludensis*, was analyzed by gas chromatography-mass spectrometry (GC-MS). Identification of the components was based on GC retention indices computer maching with wiley GC-MS library, and by comparison of the fragmentation patterns of the mass spectra with those reported in the literature([1]). Then for evaluation of antibacterial effects of the essential oil, disc diffusion method through the measurement of the inhibitory zone diameter and micro broth dilution for determining the minimum inhibitory concentration (MIC), and minimum bactericidal concentration (MBC), on several standard bacteria, were used. Essential oil yield of dried plants obtained by hydrodistillation was 0.92 (w/w %). Twenty-seven components were identified, representing 98.2% of the total oil composition. The major components in flowers oil were, 1,8-cineole (52.0%), 4aβ,7a,7aa-Nepetalactone (17.5%), β-Pinene (4.5%), and δ-3-Carene (4.4%). Amongst them monoterpenes and oxygenated monoterpenes were predominant.

Also essential oil inhibited growth of all studied bacteria. Among them, zone of growth inhibition was larger in *Sh. dysenteriae*, which is in consistent with the results of micro-broth dilution method.This research results showed that *N. binaludensis* essential oil has a moderate effect on the studied bacteria. Its effect on gram negative bacteria was more than gram positive bacteria.

References

[1] Adams, R.P. Identification of Essential Oil Components by Gas Chromatography / Mass Spectrometry, 4th Ed. Allured Publishing Co. Carol Stream, Illinois, 2007.

Synthesis, characterization and solvatochromism of 7-hydroxy-2-(2-hydroxy-5-(phenyldiazenyl) benzylidene) amino)-4-phenyl-4H-chromene-3-carbonitrile

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2-Amino-4H-chromenes are of particular utility as they belong to privileged medicinal scaffolds serving for generation of ligands with a broad spectrum of potent biological activities that include anti-microbial, anti-tumor, anti-cancer, anti-viral,antimalarial, anti-proliferative, and anti-alzheimer’s [1]. Also, the azo dyes are one of the major groups of synthetic organic dyes with broad range of biological activities [2, 3]. The new chromene-based azomethine dyes were synthesized *via* two-component coupling of 2-amino-7-hydroxy-4H-chromene with 2-hydroxy-5-(aryldiazenyl)benzaldehyde and characterized by elemental analyses, mass, NMR, IR, UV–Vis spectroscopy and X-ray diffraction analysis. Easily available and easy work-up are the key features of the present method. The pyran, chromene moiety and aromatic rings in the azomethine linkage are flattened. Intramolecular hydrogen bonding is possible between hydroxyl group and the imine nitrogen atom.

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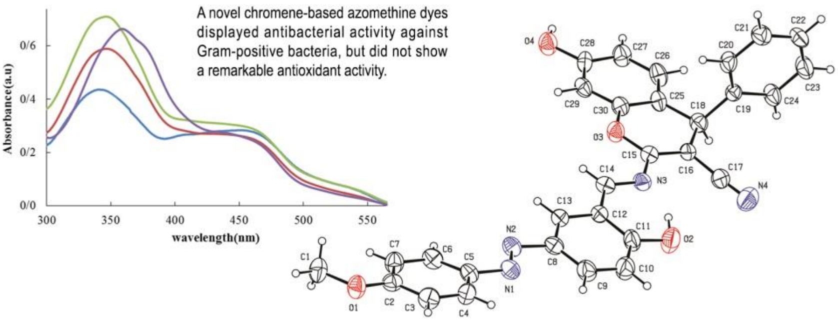

A novel chromene-based azomethine dyes displayed antibacterial activity against Gram-positive bacteria, but did not show a remarkable antioxidant activity.

References

[1] A. Gaspar, M.J. Matos, J. Garrido, E. Uriarte, F. Borges, Chem. Rev. 114 (2014) 4960−4992.

[2] A. Kakanejadifard, F. Azarbani, A. Zabardasti, S. Kakanejadifard, M. Ghasemian, F. Esnaashari, S. Omidie, S. Shirali, M. Rafieefar, Dyes Pigm. 97 (2013) 215–21.

[3] M. Ghasemian, A. Kakanejadifard, F. Azarbani, A. Zabardasti, S Shirali, Z. Saki, S. Kakanejadifard, Spectrochim. Acta A. 138 (2015) 643–7.

Synthesis, solvatochromism, and theoretical study of 4-(2-hydroxy-5-(phenyldiazenyl)benzylideneamino)benzenesulfonamide

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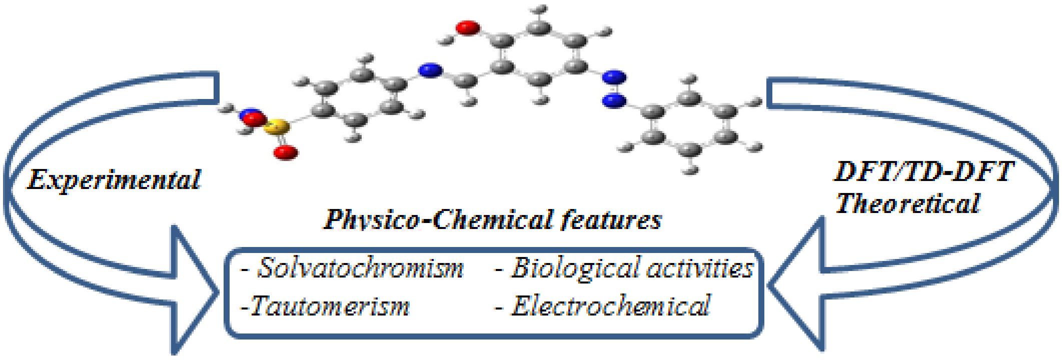
The azo dyes are the largest class of industrial synthesized organic dyes due to their various applications, such as dyeing textile fiber, laser, liquid crystalline displays, electro-optical devices and ink-jet printers [1]. They are also known to have a broad range of antibacterial, antifungal, antitumor and antioxidant activities [2-4].The sulfanilamide azo-dyes were designed and characterized by elemental analysis, mass, IR, UV–Vis and NMR spectroscopy. The UV–Vis spectra of dyes derivatives were determined in different acidities for evaluating factors affected intramolecular hydrogen bonding, enol–keto tautomerism, dipole moment and solvatochromism behavior. The solvatochromism behaviors of dyes were evaluated in solvents with different polarities also their cyclic voltammetry were carried out in DMSO as a solvent. The optimum molecular geometries, molecular electrostatic potential, Nucleus-Independent Chemical Shift, frontier molecular orbitals, infrared and electronic absorption spectra of products were investigated with theoretical methods. Results of theoretical calculations have good agreement with the experimental values.



References

[1] Y.D. Kim, J.H. Cho, C.R. Park, J.H. Choi, C. Yoon, J.P. Kim, Dyes Pigm 89(2011)1-8.
[2] M. Ghasemian, A. Kakanejadifard, F. Azarbani, A. Zabardasti, S. Kakanejadifard, Spectrochim. Acta A 124 (2014) 153–158.
[3] M. Ghasemian, A. Kakanejadifard, F. Azarbani, A. Zabardasti, S. Kakanejadifard, J Mol Liquids 195 (2014) 35-39.
[4] M. Ghasemian, A. Kakanejadifard, F. Azarbani, A. Zabardasti, S Shirali, Z. Saki, S. Kakanejadifard, Spectrochim. Acta A. 138 (2015) 643–7.

Design of biodegradable and pH sensitive antimicrobial nanocomposite as dual drug delivery system for cancer therapy

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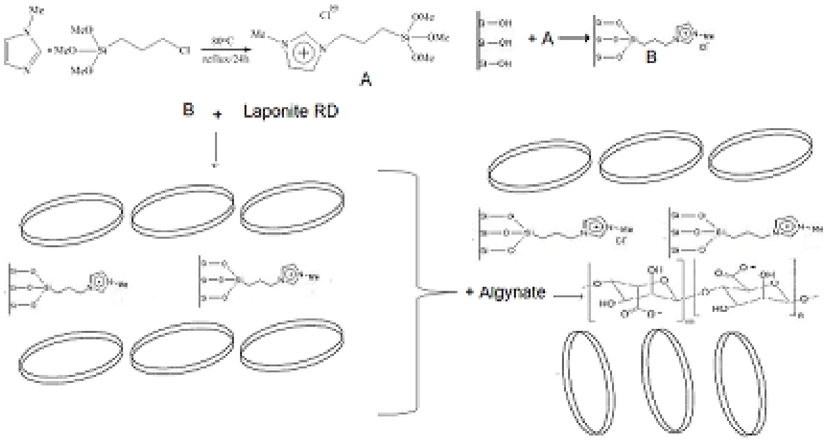
During the past few decades, many researchers have made considerable efforts to develop drug delivery systems(DDSs) . To date, several dual-drug delivery systems using polymer micelles, hydrogel, hydrogel/polymer micelle composite, alginate beads and other materials have been reported [1]. Recently, a new class of materials represented by bionanocomposites has proven to be the promising option in improving mechanical and barrier properties of biopolymers. The most common class of materials used as nanoparticles are layered clay minerals such as montmorillonite (MMT), hectorite, sapnotite, and laponite[2]. Laponite (LA) is a plate-like synthetic hectorite-type clay with the empirical chemical formula $Na^{0.7+}[Si_8Mg_{5.5}Li_{0.3}O_{20}(OH)_4]^{-0.7}$ [3].

In this study, a novel antibacterial polymer/clay nanocomposite with average particle size of 20-40 nm with modified laponite and alginate was synthesized by an ion exchange process. The structure of the obtained nanocomposites was characterized by XRD, FT-IR, TG-DTA and SEM. This multifunctional nanocomposite was used for dual drug delivery of anticancer drug methotrexate (MTX) and an antibacterial agent ciprofloxacin (CIP) with encapsulation efficiency of more than 90% for both drugs.



References

[1] T. Okuda, K. Tominaga, S. Kidoaki, Journal of Controlled Release 143 (2010) 258–264

[2] N.Pradhan, M. Das, Y. Panditrao, P.Nayak, International Journal of Research in Pharmaceutical and Biomedical Sciences 3 (2012) 1513-1522.

[3] W. Xia, J. Chang, J. Lin, J,Zhu,, European Journal of Pharmaceutics and Biopharmaceutics 69 (2008) 546–552

Synthesis of Magnetic Molecularly Imprinted Nanoparticles based on Grafting Polymerization

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Imipramine, trimipramine and desipramine are active ingredients of psychiatric drugs widely used in the treatment of depressive disorders. These tricyclic antidepressants are used primarily in the clinical treatment of mood disorders such as major depressive disorder, dysthymia, and bipolar disorder, especially of the treatment-resistant variants. However, their overdose is fatal to the central nervous system and may result in drowsiness, convulsions, respiratory disorders, ophthalmoplegia and finally coma. Hence, their determination in pharmaceutical formulations, urine and blood serum is of tremendous importance [1].

In more recent years, magnetic nanoparticles (MNPs) have been studied for biomedical and biotechnological applications. For many of these applications, surface modification of MNPs is a key challenge and can be accomplished by molecularly imprinted polymer (MIP) [2]. MIPs are artificial polymers which are formed in the presence of a target molecule that finally is removed by the proper solvents; therefore, the obtained specific cavities are complement to the target molecule in shape, size and functional groups [3].

The conventional method for the preparation of MIPs is bulk polymerization, which is traditional and exhibit high selectivity. There are some defects for this polymerization method such as: imperfect removal of template molecules, slow mass transfer of template molecules from the polymer backbone, heterogeneous distribution of the binding sites, poor site accessibility and small binding capacity in some cases. Therefore, surface polymerization has been suggested for the improving of accessibility to the target molecules, more suitable mass transfer and complete removal of templates. In this regard, the surface grafting MIPs have been developed on the different surfaces [3]

In this work, we performed the combination of imprinting polymers and MNPs for selective and effective recognition of imipramine from different samples. The MNPs were modified by vinyl groups and then the modified surface was employed for grafting of copolymerized methacrylic acid and ethylene glycol dimethacrylate which imprinted by imipramine.

References

[1] B.J. Sanghavi, A.K. Srivastava, Analyst, 138 (2013) 1395.
[2] X. Wang, L. Wang, X. He, Y. Zhang, L. Chen, Talanta 78 (2009) 327.
[3] A. Mehdinia, T. Baradaran Kayyal, A. Jabbari, M. O. Aziz-Zanjani, E. Ziaei, Journal of Chromatography A, 1283 (2013) 82.

Azobenzene based nanocomposites exibiting sharp light sensetivity and controlled drug release

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Light-responsive materials are a very attractive possibility, since optical triggering has many advantages over both chemical and electrical stimulation. Light is a clean, fast, and environmentally friendly energy source, which can be projected onto a specific position of the target system with great accuracy in a wireless, noninvasive fashion. These useful features have inspired the development of many photoswitching systems whose temporal response range is limited only by the kinetics of the chromophore that acts as a molecular switch. Azobenzenes are well known photochromic dyes capable of trans-cis isomerization. The photochromic reactions of these compounds in the interlayer space of Na-montmorillonite have been extensively investigated and the photochromic behavior has been found to be different from that observed in solutions or other solid matrixes [1, 2].

In this work, we synthesized a series of imidazolium ionic liquids based on variable alkyl chain length modified azobenzene derivatives. Then, these ILs intercalate into the interlayer space of montmorillonite due to its high surface area and high cation exchange capacity. The intercalation conducted by the conventional ion exchange method. The successful preparation of nanocomposite was confirmed by powder X-ray diffraction, EDX and thermal gravimetric analysis (TGA). Also, investigated of photochemical behaviors of organo modified montmorillonites (OMMT) showed that the cationic azo dyes isomerized effectively in the interlayer space of montmorillonite. p-Aminobenzoic acid as a model drug was entrapted in these light sensitive OMMTs and release profiles were established separately in darkness and under Uv irradiation (365nm) simulated human skin physiology conditions (pH~5.5).

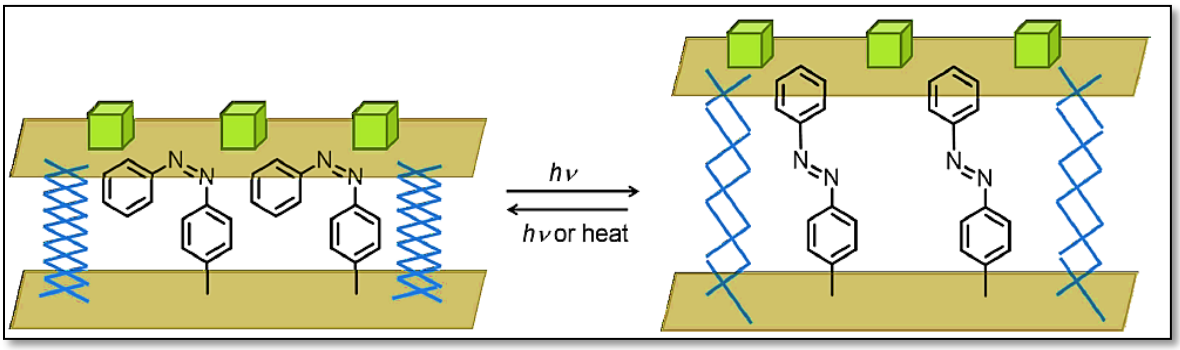

Figure 1. Light-activated azo based nanocomposites.

References

[1] T.Okada, , S.Hideki and O.Makoto, *Appl. Clay Sc.*, 40, (2008),187-192.
[2] H. Xu, Y.Yuan, W. He, *J. of Wu. Uni. of Tech.-Mater. Sci. Ed.*, 22, (2007), 466-9.

Preparation of a new smart stimulus-responsive nanohybrid system based on mesoporous nanosilica as a drug delivery system

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A smart nano-carrier for controlled release was developed through a facile route. The nano-carrier consisted of two main parts: the mesoporous silica nanoparticles (MCM-41) and a polymeric shell as a smart gatekeepers. In the first step, MCM-41 was synthesized via template assisted sol-gel process. In the second step, polymerizable functional groups were attached onto pore entrances. In the third step, polymeric gatekeepers were introduced onto pore entrances via precipitation polymerization of functionlized MCM-41 with monomers. Different methods and analysis were employed to approve the successful attachment of polymers. Additionally, the release studies of an anti-cancer drug were performed in different media. The release profiles show that the release rates are completely pH-dependent and it proceeds with a decrease in pH. It is concluded that in the higher pH the gatekeepers are in their close state, but they switch to the open state as a consequence of repulsive forces between positively charged polymer chains appear in acidic media. The results suggest that this smart nano-carrier can be considered as an appropriate candidate to deliver therapeutics to cancerous tissues[1,2].

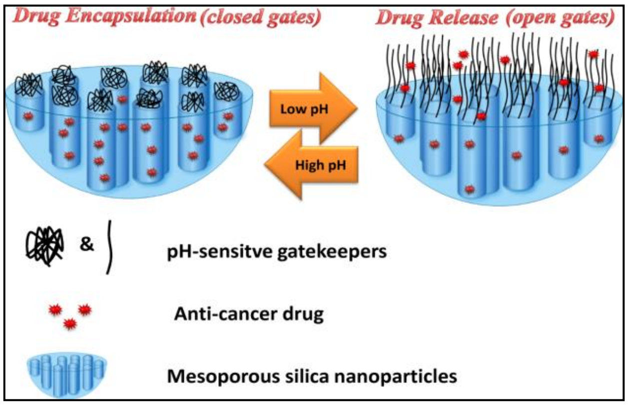

Figure 1. The prepared pH-sensitive nanohybrid system as a drug carrier.

References

[1] I. I. Slowing, J. L. Vivero-Escoto, C-W Wu, V. S. Y. Lin, Advanced Drug Delivery Reviews 60 (2008) 1278.
[2] N. Vadia, S. Rajput, European Journal of Pharmaceutical Sciences 45 (2012) 8.

Synthesis of graphene oxide and preparation of Graphene oxide-polyamide nanocomposite-based stir bar coating applying solvent exchange method

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Graphene and graphene oxide (GO) has remarkable properties, such as huge surface area good chemical stability, and graphitized basal plane structure, which allow it to have strong π–π interactions with the aromatic moieties that exist in many molecules[1,2]. Therefore it can be considered as an efficient sorbent in sample preparation purposes. In this study a new simple method based on solvent exchange method was developed to prepare GO/polyamide nanocomposite (GO/PA) coated stir bar. Polyamide was applied as nanocomposite bulk polymer due to its polar nature and feasibility of coating methods of nanocomposite on stir bar substrate. The morphology and surface characteristic of PA and GO/PA coated stir bars were investigated using scanning electron microscopy (SEM). The stir bar coated by GO/PA nanocomposite was used as an extraction device for stir bar sorptive extraction[3] (SBSE) of organophosphorous pesticides in aqueous samples followed by gas chromatography-flame ionization detector (GC-FID) detection. The effect of GO doping level on the extraction capability of the coating was investigated. Important factors influencing the extraction and desorption processes including extraction time, salt content, sample volume, pH desorption solvent, its volume and desorption time were studied and optimized using response surface methodology (RSM) applying central composite design (CCD).

References

[1] Q. Su, S. Pang, V. Alijani, C. Li, X. Feng, K. Mullen, ,Adv. Mater. 21 (2009) 3191.
[2] K. Loh, Q. Bao, P.K. Ang, J. Yang, The chemistry of graphene, J. Mater. Chem. 20 (2010) 2277–2289.
[3] E. Baltussen, P. Sandra, F. David and C. Cramers, J. Microcolumn Sep., 11 (1999) 737.

Preparation and application of a carbon nanotube -polyamide nanocomposite using solvent exchange method as a novel stir bar coating

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A novel method for simple, fast and reproducible preparation of a reinforced polyamide (PA)-based stir bar was presented. The carbon nanotube/polyamide stir bar was prepared by dispersion of an appropriate amount of oxidized multiwalled carbon nanotubes (MWCNTs) in a solution of PA in formic acid (FA) followed by dipping the stainless steel substrate of stir bar into the prepared solution. Finally, dipping the CNT/PA coated substrate into water causes the diffusion of formic acid into water and remaining CNT/ PA forms a homogenous layer on the stainless steel substrate. The surface characteristics of PA and CNT/PA coated stir bars were investigated using scanning electron microscopy (SEM). The prepared CNT/PA nanocomposite-based stir bar was used as an extraction device for stir bar sorptive extraction [1-3] (SBSE) of naproxen (NAP) from biological samples followed by fluorimetric detection. The effect of CNT doping level on the extraction capability of the prepared coating was investigated. Important parameters influencing the extraction and desorption processes including extraction time, salt content, pH, desorption solvent, its volume and desorption time were optimized using response surface methodology (RSM).

References

[1] E. Baltussen, P. Sandra, F. David and C. Cramers, J. Microcolumn Sep., 1999, 11, 737.
[2] E. P´erez-Carrera, V. M. L. Len, A. G. Parra and E. Gonzalez- Mazo, J. Chromatogr. A, 2007, 1170, 82.
[3] P. Serodio and J. M. F. Nogueira, Anal. Chim. Acta, 2004, 517, 21.

Synthesis of 2-(alkylamino)-2-oxo-1-arylethyl benzoate derivatives from alkyl isocyanides, benzaldehydes and water

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Due to unique properties of the isocyanides group, which may function both as an electrophile and as a nucleophile coupled with the now easy availability of a wide range of isocyanides have turned these compounds into indispensable building blocks for organic synthesis[1]. The diversity of transformations, which isocyanides can undergo, includes various isocyanides-based multicomponent reactions, the Ugi and Passerini reactions,[2] other (Lewis acid-catalyzed) cocyclizations utilizing isocyanides as one carbon donor as well as their transition-metal catalyzed insertions, oligo- and polymerizations[3]. Isocyanides are also well-known to participate in different types of radical processes to provide various heterocycles. In some reactions aldehydes are one of the important species in isocyanide multicomponent reactions. Synthesis of oxa-1- azaspiro [4, 5] dec-1-ene derivatives and phenylacetamide derivatives from reaction of aldehyde and isocyanide are reported. In the literature there are several examples of biological and therapeutic properties such as spasm, synergistic, antitumour, antimicrobial, anti-proliferative, antioxidant, anti-inflammatory, anti-HIV, antineoplastic and antiviral activities. Some of the 2-(alkylamino)-2-oxo-1-arylethyl benzoate derivatives have been widely used as monomer or comonomer in polymeric reaction.

We now describe a convenient synthetic procedure for the preparation of the 2-(alkylamino)-2-oxo-1-arylethyl benzoate derivatives via reaction of aromatic aldehydes, isocyanides and water in dichloromethane at room temperature is described. These simple reaction conditions allow the preparation of 2-(alkylamino)-2-oxo-1-arylethyl benzoates in good yields and at very short time reaction.

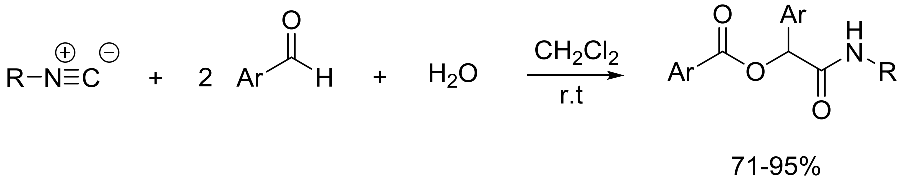

Figure 1.scheme of the reaction

References

[1] M. Suginome, Y. Ito, In *Science of Synthesis* 19 (2004) 445.
[2] A. Dömling, I. Ugi, *Angew. Chem.* 112 (2000), 3300.
[3] N. Chatani, T. Hanafusa, *J. Org. Chem.* 56 (1991) 2166. b) E. Kroke, S. Willms, M. Weidenbruch, W. Saak, S. Pohl, H. Marsmann, *Tetrahedron Lett.* 37 (1996) 3675.

N-methyl imidazole as an efficient catalyst for Knoevenagel condensation

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Carbon-carbon bond formation reaction is one of the most important reaction in organic synthesis[1]. Knoevenagel condensation is one of the most useful and widely employed reactions for carbon-carbon bond formation in organic synthesis[2]. Generally, Knoevenagel reactions are carried out by the condensation of active methylene compounds with aldehydes using some catalysts such as some bases, their salts, Lewis acids and ionic liquids in the presence or solvent free synthesis. Also the condensation products are the key intermediates for the synthesis of natural and therapeutic drugs, polymer, cosmetics and perfumes[3].

However, many of those procedures require the use of long reaction time, harsh reaction conditions and have difficulties in the reuse of catalysts, which prompt chemical researchers to further develop more efficient, cheap, operationally simple Knoevenagel protocols. Herein, we report the synthesis of arylmethylidenes from aromatic aldehydes and active compounds catalyzed by catalytic amount of N-methyl imidazole as an efficient catalyst in 50/50 ratio of Ethanol/ H_2O. The reactions go to completion within 3 min and give products in excellent yields at room temperature. The effect of reaction time, amount of catalyst, solvent, different aromatic aldehydes and acidic methylene reagents (malononitril and diethylmalonate) was investigated in this condensation.

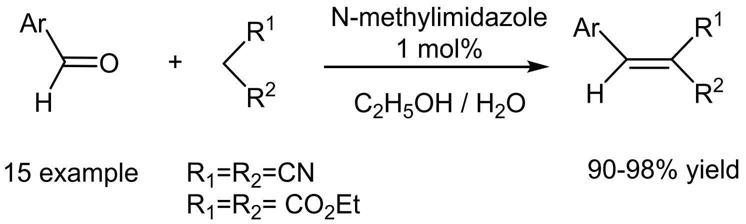

Figure 1.scheme of the reaction

References

[1] G. Jones, Organic Reaction, 15 (1967) 204.
[2] E. Knoevenagel, Berichte, 31 (1898) 2585.
[3] L. F. Tietze, Pure. Appl. Chem., 76 (2004) 1967.

One-Pot four-component synthesis of pyrrolo [1,2-*a*]isoquinolines under solvent free condition

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The isoquinoline skeleton is found in a large number of naturally occurring[1] and synthetic biologically active heterocyclic compounds such as pyrroloisoquinoline ring systems. pyrroloisoquinolins are *N*-bridgehead heterocyclic compounds which are found as a major structural of alkaloids that have. Pharmacological effects including sedative, hypotensive, neuromuscular blocking, CNS activities, cell differentiation inhibition, cytotoxicity and anticancer activity[2]. The synthesis and properties of the pyrrolo[2,1-*a*]isoquinolines were reviewed in 1997 by Mikhailovskii and Shklyaev[3], but the synthesis and characterization of these compounds is still of current interest, the proof being the important number of very recently reported papers.

Herein, we describe the synthesis of a simple, efficient and solvent-free synthesis of pyrrolo[1,2-a]isoquinolines were described by One-Pot four component reactions of malononitrile, aromatic aldehydes and isoquinoline in the presence of isocyanides as domino Knoevenagel-nucleophilic cycloaddition. The structure of the compounds was assigned by IR, NMR and mass spectroscopy.

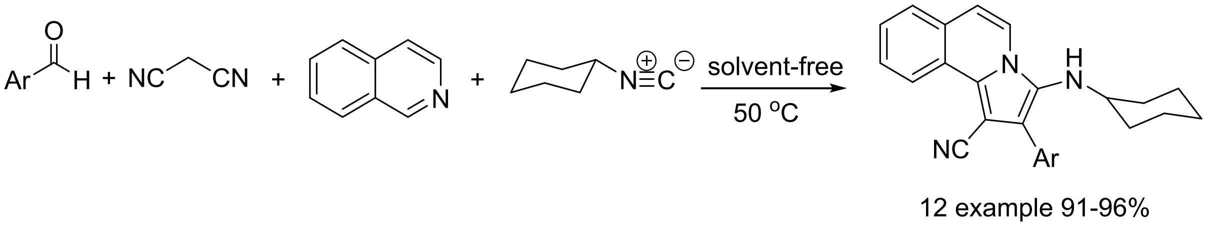

Figure 1.scheme of the reaction

References

[1] J. Michael, P. *Nat. Prod. Rep.* 25 (2008**)**, 166.
[2] S. Coulton, R. Novelli, R. A. Porter, M. Thompson, R. W. Ward, *Chem. Abstr.* 132 (2000) 151686.
[3] G. Mikhailovskii, V.S. Shklyaev, *Chem. Heterocycl. Compd.* 33 (1997) 243.