

# Poster Presentation

# Organic Chemistry 2019 Green Chemistry 2019



International Conference on Organic and Inorganic Chemistry 8<sup>th</sup> World Congress on Green Chemistry and Technology February 18-19, 2019 | Paris, France



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#### Copper-catalyzed intra-molecular $\alpha$ -c-h amination via ring-opening cyclization strategy to quinazolin-4-ones: Development and application in rutaecarpine synthesis

#### Srilaxmi M Patel

Indian Institute of Technology, India

A copper catalysed intramolecular  $\alpha$ -C–H amination has been developed for the synthesis of quinazolin-4(3H)one derivatives from commercially available isatoic anhydride besides primary and secondary benzyl amines via Ring-Opening Cyclization (ROC) Strategy. This method shows good functional group tolerance and allows access to a range of 2-aryl, 2-alkyl and spiro quinazolinone derivatives and also 2-methyl and 2-aryl quinazolin-4(1H)-one derivative by C–C and N–C bond cleavage in the progress of ROC strategy. It is the first general method to construct the potentially useful 2-methyl

quinazolin-4(3H)-one by copper-catalyzed intramolecular C–H amination. And also, this ROC strategy has been successfully applied to the synthesis of quinazolinone alkaloid rutaecarpine.

#### **Speaker Biography**

Srilaxmi M Patel was born in 1988 in Ameenpur, India. She obtained her BSc degree from SLDC, Osmania University (OU), India in 2008 and MSc (Organic Chemistry) degree from the MNR PG College, Osmania University (OU) in 2010, Later she worked as a Lecturer in NTR Degree College for Women's (June 2011 to July 2013) Mahaboob Nagar, India. Then she joined the IIT Hyderabad in August 2013 as a junior research scholar.

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# An unprecedented exocyclic n-acyliminium ion (nai) cyclization: Access to fully substituted oxazoles and furocoumarins

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-acyliminium ions (NAIs) are well recognized as potent or Nhighly reactive intermediates in C-C and C-heteroatom bond forming reactions, and extensively explored for the synthesis of diverse natural-products and bioactive molecules due to their highly electrophilic nature. Chemists have developed N-acyl iminium ion based biomimetic approaches for the synthesis of various alkaloids inspired by nature's design principles. The development of a direct route to access NAI precursors and their further transformations toward diverse scaffolds in single pot is a daunting challenge. The reason is the formation of NAI ion species prerequisite is a good leaving group at the  $\alpha$ -position to the nitrogen atom. In order to bring leaving groups at desired position in substrates involves multistep syntheses and which are highly difficult to operate in single pot. These challenges led us to examine a direct synthetic route to access NAI precursors and their further efficient transformations through a cascade process.

Herein, we report a novel super-acid-promoted tandem cyclization strategy to synthesize diversified fully substituted Oxazoles and Furocoumarins from readily available starting materials via insituly generated exocyclic NAI precursor in one pot. The key step in this transformation involves insitu generation of N-acyliminium ion (NAI) precursor under catalyst and solvent-free conditions, and their further transformations promoted by superacid in the same pot. We have also presented the experimental evidence for the involvement of proto-solvated novel exocyclic N-acyliminium ion. Further, we have examined the photophysical properties of some of the synthesized Furocoumarins and Pyrid-oxazole derivatives.

The important features of the present protocol are transition-metal free, robust,  $H_2O$  as sole byproduct, and cleaner reaction profile, and practical method for the synthesis of diverse fused Oxazole's and Furocoumarins.

#### **Speaker Biography**

Venkata Nagarjuna Babu obtained his bachelor's degree (B.Sc.), in 2009 and master's degree (M.Sc.) in Organic Chemistry from Osmania University, Hyderabad, Telangana, in 2011. Then he worked as a Lecturer on contract basis in Narendra Degree & PG College, Armoor, Telangana in 2012 to 2013. After securing CSIR-UGC-JRF (2013), he joined the research group of Dr. Sharada's Catalysis and Chemical Biology Lab in the Department of Chemistry as a Doctoral Fellow at Indian Institute of Technology Hyderabad (IITH), in Jan-2014. He has publications on the topic of organo-iodine reagents promoted C-H functionalization, acid catalysed cyclization's and catalyst-free & solvent-free sustainable organic transformations.

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# E-Poster

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#### Deconstruction of lignocellulosic biomass to bio-oils with zieglar-natta catalyst in ethanol and water

Naijia Hao

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Lignocellulosic biomass (grape seeds) was deconstructed in both hydrothermal and supercritical ethanol media with Zieglar-Natta catalyst components (TiCl<sub>4</sub>/MgCl<sub>2</sub>) to produce the bio-oils. The use of catalyst in the deconstruction in supercritical ethanol achieved the highest bio-oil yield of 49.2% at 300 °C with a residence time of 30 min, which was 37.4% higher than the bio-oil yield obtained from the same condition. Both the hydrothermal and supercritical ethanol deconstruction reactions with the highest catalyst loading (TiCl<sub>4</sub>/MgCl<sub>2</sub>=4mmol/4mmol) produced the bio-oils with a higher heating value (HHV) of 35 MJ/Kg which was comparable of the HHV of petroleum based liquid fuels. Most significantly, gas chromatography-mass spectrometry (GC-MS) analysis of the bio-oils showed that the major products in bio-oils from the hydrothermal deconstruction were acids while majority products in bio-oils form the supercritical ethanol deconstruction were esters. 31P Nuclear magnetic resonance (NMR) data suggested that both non-catalytic and catalytic hydrothermal/supercritical ethanol deconstruction reactions significantly reduced the C5 substituted phenolic OH in bio-oils.

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## Recent trends of research on green chemistry and technology and its implication to environment awareness and management

#### Banabehari Mishra

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Green chemistry or sustainable chemistry is more resourceefficient, focused on the designing of products and processes that minimize the use and generation of hazardous substances and become environment friendly. Recent Trends -Attempts are being made not only to quantify the greenness of a chemical process but also to factors in other variables such as chemical yield, the price of reaction components, safety in handling chemicals, energy profile and ease of product workup and purification in one quantitative study.

The manufacture of Green Solvents, development of synthetic products, carbon dioxide as blowing agent, production of Hydrazine, production of organic carpet tile backings, Transesterification of fats, manufacture of Bio-succinic acid, addressing alternatives to Toxic chemicals and production of other environment friendly lab chemicals are some of the growing fields of research which are to be discussed in detail in the Congress subject to the time limit.

In addition to it, the broad spectrum and scope of Education on Green Chemistry and Global awareness programmes on reduction of environmental pollution and degradation through Green Chemistry shall be a major point of discussion. Our club plans to organise awareness programmes in different parts of our country on "The Role of Green Chemistry Technology in the Context of Global Environment Pollution and Climate Change" among public and students from our limited resource and request to our Govt. to include a chapter on Green Chemistry in the syllabus/ courses of studies of the Master Degree in Science(Chemistry) to develop the interest in higher study and research among them.

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# Accepted Abstracts

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#### **Petrochemicals - Trends and challenges**

**Dorothee Arns** Petrochemicals Europe, Belgium

The intervention will focus on the following elements: How the European Petrochemicals industry contributes in a sustainable way to the economic and societal wellbeing of Europe. How chemical markets evolve. Why a lower oil price does not change the situation for the European Petrochemicals industry. The competitiveness challenge for the European Petrochemicals industry: Feedstock price, electricity price, regulatory challenge, investment leakage. Debrief on the European Commission's cumulative costs assessment of its legislation on the European Petrochemicals industry. The performance of the European Petrochemicals industry in reducing GHG emissions.

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#### Gold versus silver towards domino processes and diversity

Veronique Michelet University Cote d'Azur, France

Over the past few years, significant research has been directed toward the development of new methodologies for synthetic efficiency and atom economy processes in the presence of gold and silver catalysts. We have been engaged in a wide project dedicated to the development of catalytic methodologies for the synthesis of original and functionalized carbo- and heterocycles. Our interest has been focused on the cyclization and/or functionalization of alkynes including enynes, alkynyl silyl enolethers and o-alkynyl benzaldehydes. We also got interested in cycloisomerization reactions of allenols and developed sustainable catalytic systems. Despite significant progress in the development of enantioselective gold(I) catalysis, challenges still remain largely as a result of the high substrate-dependency and the linear geometry the chiral gold(I) complexes.This presentation will show an overview of the latest results implying achiral and chiral gold and silver complexes.

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#### A new artificial imine reductase based on dalbapeptides metal interaction

Isabella Rimoldi University of Milan, Italy

H omogeneous catalysis by transition metals containing chiral bidentate ligands has been often considered a valid strategy to obtain high productivity, stereoselectivity and atom economy by many academic and industrial researchers interested in the synthesis of optically pure compounds. The same attraction has been reserved to enzymatic catalysis based on the fact that biocatalysis has many benefits to offer in the context of green chemistry. Considering the ability of macromolecules to selectively discriminate substrates and the number of chemical transformations catalyzed by transition metals, which have not been observed to occur enzymatically, in the last decade several research groups reasoned that a hybrid catalyst may combine some of the most attractive features of metal and enzymatic catalysts. In this contest, the use of a dalbapeptides, such as vancomycin, teicoplanin, ristocetin etc, could be an interesting alternative to the well-known biotin/(strept)avidin system. Dalbapeptides are known for their strong antibacterial activity due to their interaction with the dimer D-Ala-D-Ala in the terminal chain of bacterial cell wall peptidoglycan with a dissociation constant KD = ~10-17 M and they have recently been investigated for their capability to interact with different transition metals such as copper. By exploiting these features of the class of glycopeptides, new hybrid iridium systems were prepared and evaluated as catalysts in asymmetric transfer hydrogenation of different cyclic imine substrates chosen for their important applications in medicinal chemistry.

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#### Computer analysis of the adsorption process on metal-organic frameworks

Miroslaw Kwiatkowski

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In recent years, with the increasing use of adsorption processes, both in technology, environmental protection and everyday life, better new adsorbents have been sought, and one of the most promising materials that can be used in these processes are MOF organometallic materials. The work presents original results of MOF Basosiv M050 metalorganic frameworks material structure and adsorption processes occurring on its surface. The studies were conducted based on adsorption isotherms of N<sub>2</sub>, CO<sub>2</sub>, and CH<sub>4</sub> analysed separately as well as on the basis of analysis of two and three isotherms simultaneously, using a unique LBET method. The results presented in this article confirmed the high usability of LBET method in the study of adsorption processes occurring on the surface of Basosiv M050 material, as well as in the analysis of its structure. As it has been shown, the application of the LBET method enables precise determination of the structure of the studied material and mechanisms of adsorption processes taking place in its structure, which in turn ensures the possibility of optimal selection of its preparation and effective use in a given adsorption process.

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#### Investigation of the anticancer activity of electron-deficient organometallic complexes

Maria Azmanova University of Bradford, United Kingdom

Ran attractive alternative to platinum-based anticancer drugs since the latter have major disadvantages such as high toxicity, low selectivity and chemoresistance. We have recently developed strong interest in electron-deficient ruthenium and osmium complexes and investigated their anticancer properties. The design of such molecules, with possibilities of altering their activity by introducing different ligands, is of a great importance, as well as unveiling their

mechanisms of action. Their cytotoxicity towards human colon HCT116  $p^{53+/+}$  and HCT116  $p^{53-/-}$  cancer cell lines has been investigated, including the effects these precious metal complexes have on different genes involved in DNA damage responses, cell cycle arrest, and apoptosis. Their mechanism of action has been explored further by cell cycle analysis and investigation of the oxidative stress they induce in cells.

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#### Biomaterials as targeted tool for medical applications

Amany A Mostafa National Research Centre, Egypt

ver the past decades, biomaterials play an important role in the field of medicine and health care. The use of synthetic biomaterials has extensive progress due to chronic diseases, malfunction, traumatic accendients and surgical reconstruction. Many research works have been focused on biomaterials in the field of tissue engineering, drug delivery besides imaging as a diagnostic tool. Targeted delivery of drug incorporated nanoparticles as well as 3D scaffolds will enhance the efficacy of the anticancer or other organ-targeted drugs but also reduce the unwanted toxicity of the drug. Our team developed some promising nanobiomaterials and nanohybrids for the improvement of physical, mechanical and cell-biomaterial interactions beside controlling the targetting drug release. Different techniques have been used to prepare nanobiomaterials that help in improving the human life. New formula

incorporated these nanoparticles with an antiinflammatory drug is used for the nonsurgical treatment of preapical lesion arisng trauma or bacterial infection as an innovative tool. Kinetic approach has been used to asses the in vitro bioactivity of differnt nanocomposites formulae used in bone regeneration. Other work aimed to the use of cationic bPEI capped AuNPs for intracellular siRNA delivery that targeted c-Myc gene in human hepatocellular carcinoma cells. Material for imaging such as quatum dots stabilized with magnetic nanopaticles or carbon dots are also benifiial. A multidisciplenary team has been involved in these work activities. Herein, I will present and discuss different laboratoy's research advancement for medical applications.

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#### Impact of crop residue burning practices on air quality, related health issues and best alternatives

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Large quantities of crop residues are left in the agricultural fields globally after harvesting of different crops. The proper disposal of crop residues before the next crop takes time and requires huge manpower as well as investment. Burning of crop residue in open fields has been banned in many countries but still, farmers use to burn the crop residue in open field and find it a rapid, effortless and cost-effective method to clear their fields for next crop. But these practices increase the concentration of air pollutants (like PM<sub>10</sub>, PM<sub>25</sub>, SO<sub>2</sub>, NO<sub>2</sub>,

PAHs) and create serious health issues. Various studies have reported increased levels of fine particles and toxic gases in atmosphere during crop residue burning episodes. Many studies have revealed that children and elderly people are more prone. This discussion covers the emissions of toxic pollutants during crop residue burning, related health issues and possible alternatives to crop residue burning practices.

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#### Functional polymers and nanocomposites: Applications in organic devices and sensors

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The architecture of coordination or conjugated polymers containing functionalized building blocks and metal nanoparticles have emerged appealing attention because of their excellent response towards various technological applications. However, the synthesis of such materials with reproducible properties is always a challenge for the researchers. The ordering and alignments of polymers chains or the uniform distribution of nano-fillers and homogeneous composite formation and the morphology control are some of the crucial requirements for various applications and enhancement of device performance. We have recently developed facile interfacial technique for the controlled morphology and ordering of the polymer chains. For the first time interfacial technique is used for the formation of uniform polymer nanocomposites and demonstrated for organic electronics and sensing applications.

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#### Furfural as platform chemical - Recent advances

Christophe Len PSL University, France

With an increasingly severe outlook for depleting oil-based resources, wood-based biomass and especially plant waste rich in lignocellulosic feedstocks, appear to be the main alternative to produce many kinds of platform molecules such as furan derivatives. However, recent researches have shown that other kinds of carbohydrates as alginate derivatives could also be exploited as feedstocks for furfural production. As a molecule platform chemical, furfural permits to produce a large range of chemicals having different properties and utilities as solvents, plastics, fuel additives. One important valorisation route of furfural is the liquid phase catalytic hydrogenation. Whereas molecular hydrogen is mostly used in industrial

hydrogenation processes, recent studies also showed that alcohols can be used as reductants from which hydrides can be transferred catalytically to furfural. These two strategies: hydrogenation and transfer hydrogenation were developed in batch as well as in continuous flow to produce value-added chemicals such as 2-methylfuran. Our works explore the catalytic behaviour in batch and continuous flow of mono- and bimetallic metal catalysts (Cu, Pd, Pt, Ni) supported on various types of materials (microporous, mesoporous). Methodology, recycling, metal leaching will be discussed.

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# The reactions of cyclohexan-1,3 and 1,4-diones for the synthesis of heterocyclic compounds with antitumor activities

Rafat M Mohareb Cairo University, Egypt

s typical reactive cyclohexan-1,4-dione and cyclohexan-A1,4-dione were recently used for the synthesis of different heterocyclic compounds. On the other hand, its one or two carbonyl groups could take part in substitution and cyclization reactions through the tautomerized enolate form. Thus the cascade reactions of addition, elimination and substitution could be achieved in many reactions involving dimedone. The reactions of cyclohexane-1,3-dione and cyclohexan-1,4-dione with aldehydes have been extensively studied in the past years, from which several types of compounds have been produced according to the reaction conditions. The normal Knoevenagel condensation of the title compounds with aldehydes have been conducted with numerous methods including promotion via amines surfactants, zeolites, ionic liquids. The use of environmentally benign methods like in aqueous medium or in the absence of vents and the usage of ultrasound or microwave heating have also been developed in recent years. The reactions usually proceed further through Michael addition reaction of the second molecule of dimedone to yield tetraketones as main products. On the other hand, tetraketones could be easily converted to 9-substituted 1,8-dioxo-xanthenes by dehydration step. In our continued interest in the design of new multicomponent reactions and the application in the synthesis of heterocyclic compounds, we found some unprecedented reaction patterns in the reaction of the aryl hydrazodimedone derivatives with elemental sulfur and cyanomethylene reagents to produce thiophene derivatives. These were capable for further heterocyclization reactions to produce potential antitumor agents. Also due o the lower reactivity of cyclohexan-1,4-dione our goals were to increase its reactivity through building of active centers through the molecule.

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#### **Environment and development: Biomass for future**

Abdeen Mustafa Omer Energy Research Institute (ERI), UK

People are relying upon oil for primary energy and this will continue for a few more decades. Other conventional sources may be more enduring but are not without serious disadvantages. The renewable energy resources are particularly suited for the provision of rural power supplies and a major advantage is that equipment such as flat plate solar driers, wind machines, etc., can be constructed using local resources. Without the advantage results from the feasibility of local maintenance and the general encouragement such local manufacture gives to the build-up of small-scale rural based industry. This communication comprises a comprehensive review of energy sources, the environment and sustainable development. It includes the renewable energy technologies, energy efficiency systems, energy conservation scenarios,

energy savings in greenhouses environment and other mitigation measures necessary to reduce climate change. This study gives some examples of small-scale energy converters, nevertheless it should be noted that small conventional, i.e., engines are currently the major source of power in rural areas and will continue to be so for a long time to come. There is a need for some further development to suit local conditions, to minimise spares holdings, to maximise the interchangeability of the engine parts, and of the engine applications. Emphasis should be placed on full local manufacture. It is concluded that renewable environmentally friendly energy must be encouraged, promoted, implemented and demonstrated by a full-scale plant (device) especially for use in remote rural areas.

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#### Supported polyoxometalates: Tailoring and sustainable glycerol valorization

Anjali Patel

The Maharaja Sayajirao University of Baroda, India

Polyoxometalates (POMs) comprise a class of inorganic complexes of unrivaled versatility and structural variation, with applications in many fields of science. Modification of parent POMs are likely to help in development of new generation of catalysts with enhance properties of acidity, redox properties and stability. In the present talk, the designing of heterogeneous catalysts based on parent as well as lacunary silicotungstate and mesoporous supports as well as zeolites will be discussed.

Glycerol is formed as by-product (~10 wt.%) during the biodiesel production leading to an increase of crude glycerol in the market. The high manufacturing cost of biodiesel raises the need to study the uses of glycerol as a renewable feedstock for synthesis of value added fine chemicals. Amongst all, cyclization of glycerol via acetalization as well as carboxylation of glycerol are the most important reactions as the formed products have direct applications as fragrances, in cosmetics, food and beverage additives, pharmaceuticals, in detergents, in lacquer industries and as ignition accelerators and antiknock additives in combustion engines and in port wine productions. The present talk describes the new prospects for conversion of glycerol into value added products by choosing viable reaction conditions with parent as well as lacunary silicotungstates anchored to mesoporous as well as zeolites, as catalysts. The unique catalytic activity of all the catalysts is due to the combination of well defined order, channel framework, homogeneous dispersion of the active sites, as well as strong acidity. All these characteristics also make them promising environmentally benign heterogeneous catalysts.

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## The main chemical, rare earth and trace elements and minerals formation of mountain soil as an indicator of source and treatment pedogenetic in the palestinian mountain soil

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University of Forschungszentrum Julich, Germany

he purpose of this study was to explore the pedogenesis processes and to examine the source (parent material) of Mediterranean mountain soil; especially Terra Rossa, Rendzina and other associated soils through chemical (major, trace and Rare Earth Elements (REEs)), grain size and mineralogical compositions. Forty soil samples were collected form 13 pedons from different areas in Palestine that represent different soil types, lithology, elevation and precipitation along a climatic transect to demonstrate variability between south, north sections and west east transects. The north section around Nablus consists of: western and eastern transect. The western one in turn consists of Qusin pedon which was Terra Rossa, and Bait Eba pedon which was Rendzina. While the eastern one in turn consists of Tubas pedon which was Rendzina, and Tayaseer pedon which was Terra Rossa. The south section, which was Bethlehem and Jerusalem mountains, consists of: western and eastern transect, the western one in turn consists of Battir1, Battir2 and AlQbu, which is Karstic, pedons which were Terra Rossa, while Ishwa and Ishwa (the road) pedons which were Rendzina soil. In other hand, the eastern one in turn consists of Tego'a east and Tego'a west pedons which were Terra Rossa, While Beit Sahour and Bayth Ta'amar pedons which were Rendzina. Two dust samples from Al-Quds University and

seven rock samples from different pedons were collected also. From grain size, chemical compositions (major, trace and REEs), and mineralogical compositions results, dust was found to be the dominant parent material in studied soils. Leaching was dependent on rainfall amount and bedrock and soil permeability. Ca, Sr and U elements leached more than these trace elements Fe, K, Mg, Na, Al, Ba, Co, Cr, Cu, Mn, Ni, Rb, Sb, V, Zn and Zr and REEs. Some Terra Rossa samples were alike Typical Terra Rossa but with relatively high calcite content but mineralogical and chemical characteristics were like Pale Rendzina as in Qusin pedon. On the other hand, Brown Rendzina resembles Typical Terra Rossa as in Beit Sahour and Bayth Ta'amar pedons. The east transects samples leached less than the western, but the difference in leaching was low. Battir 2 profile has two soil layers deep layer, layers were composed of one on top of the other Dust samples were polluted with these trace elements Al, Cu, Pb, Sb and Zn, and this may be due to industrial or construction sources. Vanadium element found to be affected by rain and this is like Aluminum which considered to be well retained in soil. A baseline of grain size, major and trace elements, REEs and minerals was added to soil science in Palestine in general and Mediterranean virgin mountain soil (Terra Rossa and Rendzina). e: m.zaid@fz-juelich.de



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# AuPd/3DOM CeO<sub>2</sub> catalysts with good chlorine-resistant performance and catalytic stability in trichloroethylene combustion

**Zhang Xing** Beijing University of Technology, China

Chlorinated volatile organic compounds (CVOCs) are harmful to the atmosphere and human health. Catalytic oxidation is a good promising method for the removal of CVOCs and the development of high-performance catalysts is the key issue. In this work, the high-efficiency three dimensionally ordered macro-porous (3DOM) CeO<sub>2</sub>-supported AuPd alloys (xAuPdy/3DOM CeO<sub>2</sub>; x = 0.46-2.85 wt.%, y = 1.85-1.89) catalysts were prepared using the polymethyl methacrylate templating and polyvinyl alcohol protected reduction methods. Physicochemical properties of the samples were characterized by means of various techniques, and their catalytic activities for trichloroethylene (TCE) combustion (reaction condition: 750 ppm TCE + 20 vol% O<sub>2</sub> + N<sub>2</sub> (balance) and space velocity was 20,000 mL/(g h)) were evaluated. It is found that the catalysts possessed a good-quality 3DOM structure and the noble metal nanoparticles (NPs) with a size of 3–4 nm were uniformly dispersed on the surface of 3DOM  $CeO_2$ . The 2.85AuPd1.87/3DOM  $CeO_2$  sample showed the highest catalytic activity with a T90% (the temperature required for achieving a conversion of 90%) of 415°C and this sample also possessed excellent catalytic stability and moisture-resistant ability. Based on the characterization results and activity data, we conclude that the excellent catalytic performance of 2.85AuPd1.87/3DOM  $CeO_2$  was associated with its high adsorbed oxygen species concentration, good low-temperature reducibility, and strong interaction between AuPd nanoparticles and 3DOM  $CeO_3$ .

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# Study on *Mentha Pulegium* L. from M'rirt (Morocco): Antibacterial and antifungal activities of a pulegone-rich essential oil

Amalich Smail University Moulay Ismail, Morocco

Pennyroyal or *Mentha Pulegium L*. is a species from Lamiaceae family which is extremely rich in aromatic essence.

This species is used for various purposes. In the present work, we have carried out a study on chemical composition and evaluation of antimicrobial activity and antifungal activity of its essential oil. To achieve this aim, essential oil was first extracted by hydrodistillation from bloomy tops of *Mentha pulegium L*. harvested in the wild during the month of July 2014 in M'rirt. This extraction yielded about  $5.2 \pm 0.25\%$  of essential oils (EOs). Then, EO was analyzed by gas chromatography coupled with mass spectrometry (GC-MS).

Results of this analysis showed that it contains two major compounds: the first one is "pulegone" and the second is "piperitenone". Both, these molecules represent 98.01% of the whole identified compounds. Antibacterial activity of this EO was assessed against four bacterial strains by disc-diffusion method on agar medium and macrodilution method in liquid medium. Results showed that EO of *Mentha pulegium L*. has a very significant antibacterial activity in a liquid medium towards *Escherichla Coli* and *Staphylococcus Aureus* with respectively 1.4  $\mu$ l/ml and 2.8 $\mu$ l/ml as minimal inhibitory concentrations. Evaluation of antifungal activity revealed that this essential oil is able inhibit mycelial growth as well as sporulation of the three fungal species tested (*Aspergillus Sp., Penicillium Sp.* and *Rhizopus Sp.*) at low concentrations. In conclusion, essential oil of pennyroyal was very active. Indeed, it was endowed with a relatively interesting antibacterial activity and an excellent inhibitory potency on mycelial growth and sporulation of the tested fungi. Inhibitory effect of this essential oil suggests prospects of application in the field of foodstuffs conservation.

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#### Heterocycles: Benign and sustainable synthetic methodologies

Fayez Eissa Aswan University, Egypt

New heterocycles that can interact with biological organisms as active leads shaped an ever-increasing competition for proficient synthetic structures aiming to establish various drug-like structures. Heterocycles were commonly established through conventional and non-eco-friendly procedures and it made their production environmentally non-proficient and multifaceted process. Developing simple, benign and sustainable synthetic methodologies for heterocycles will be described. Grinding Chemistry, microwave-assisted synthesis, solar-assisted synthesis, and others were feasible benign, simple, and rapid methodologies for synthesis instead of risky conventional procedures. The appointed green methodologies presented excellent conversions with optimum yields, energy proficient, and more economically and ecologically constructive pathways to valuable organic compounds.

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#### Mathematical modelling of metal ion chromium (Cr) bio-sorption by biomass

Assnaoui Hassan University Moly Ismail, Morocco

**B**io-sorption is an innovative low-cost and effective procedure for the removal of heavy metal ions from wastewater. It primarily depends on the diffusion of metal ions through a porous structure of biomass (Ulva lactuca) and the resistance effects arisen as the result of electrostatic repulsive interactions between ions within the sorbent. The intra-particle diffusion of metal ion Cr from aqueous solution by biomass was investigated in order to develop a mathematical model that would describe the phenomenon of different ions transport through porous algae matrices. FTIR analysis of algal biomass revealed the presence of amino, carboxyl, hydroxyl and carbonyl groups, which are responsible of metal ions biosorption. The results obtained have shown a particle diffusion coefficient Dint=0.1363(mgg-1.min-1/2), R<sup>2</sup>=0.99, and partition coefficients greater than 0.95, showing that the bio-sorption process is very fast at the beginning and mainly indicated by the diffusion of the ions through the porous algae structure. However, over a period the bio-sorption slows down due to the increase of the resistance to the further transport of metal ions through the Algae. A mathematical model based on the second Fick's law determined the profile of heavy metal ion concentration in the algae and the effectiveness of sorption and optimize the bio-sorption of heavy metal ions by means of connecting the model parameters with the Algae performances.

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#### Greener protocols for synthesis of biological and pharmaceutical compounds

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**B**-amino alcohols and its derivatives are the versatile intermediates for synthesis of biologically active natural compounds. For ring opening of epoxides, several groups have been used various type of catalyst like Lewis acids, metal salts, lanthanide halides, triflates, boranes, heterogeneous catalysis, ionic liquids and alumina. But we have synthesized these derivatives by synthesis of new type of epoxides by using this below mentioned synthetic route where ACC juice has been used. Again, we are interested to synthesize bisheterocyclic and pyran annulated heterocyclic scaffolds which have also biological and pharmaceutical applications, synthesised using waste material.

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#### Fenton reaction in porous media

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Emplacement of meso zero-valent iron particles (mZVI) in porous media to degrade organic pollutants (Phenol as model pollutant) in continuous column studies is first of its kind. Columns with different configurations varying in ZVI distribution and location of  $H_2O_2$  were investigated for factors influencing sustainable phenol removal. The performance of columns were in the ascending order of C > A > B > D where columns A and B had full-length ZVI distribution, C and D had half-length ZVI distribution, with  $H_2O_2$  injection at initial conditions in A and C and at intermittent points in B and D. Distribution of mZVI particles in column C contributed 61-84% more interaction between  $Fe^{2+}$  ions and  $H_2O_2$ , promoted good radical generation

and continuous corrosion, invigorated effective Fe<sup>2+</sup>-Fe<sup>3+</sup> cycling, retained active iron surface area and circumvented precipitation and secondary sludge production. The breakthrough curves showed that mZVI particles extended the active corrosion stage by 5 to 8 times and resulted in 3 to 7 times increment in mg phenol removed/mg mZVI along with 80% to 99.8% utilization of mZVI. Additional sand-only columns proved that Fenton's oxidation in in situ porous media can be improvised by 14% to 34% without incumbent addition of ZVI particles.

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#### Compassionate conservation: Biodiversity enhancement on green roofs

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Green roofs may provide opportunities to enhance biodiversity in urban areas. Island biogeography theory (IBT) predicts that diversity decreases with both increasing horizontal distance from green areas and vertical distances (building height) and increases with increasing plot size. Habitat heterogeneity on green roofs may also influence species richness and species richness may also act as a barrier against invasive species. We address these questions with a number of experimental studies: (1) effects of identical arrays of plants on roofs of varying horizontal and vertical distances on arthropod diversity; (2) assessing plant species richness as a function of plot size; (3) effects of inorganic substrate and organic heterogeneities on species richness; (4) effects of plant species richness on invasive plant colonization; (5) bird species, plant species and arthropod species colonizing green roof habitats.

Our studies yielded the following results: (1) arthropod diversity

decreased with increasing distance from green areas and increasing vertical distance supporting Island Biogeography Theory (IBT). Roof plots and adjacent yards had low community overlap suggesting that green roof habitats are unique habitats in urban areas; (2) diversity increased with increasing plot size, also supporting IBT; (3) increased fine-scale heterogeneity did not increase plant or arthropod richness. Fine-scale heterogeneity may result in small populations which increases the probability of local species extinctions; (4) increased plant species richness served as a barrier against invasive plants; (5) Birds utilize these green roof habitats; (6) Storm water drainage refers to reducing storm water. This result is consistent with many other studies demonstrated a lack of successful invisibility when species richness is high. Overall, our studies suggest that green roofs can contribute to higher diversity in highly urban systems.

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#### Formation of functionalized graphene by submerged liquid plasma process

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R ecently, graphene has been emerged as a smart material specifically in the field of materials chemistry due to its remarkable mechanical flexibility, optical transparency, electrical and thermal conductivity. Functionalization of graphene is an important route to increase its dispersibility and stability in aqueous and/or organic solvents. Graphene oxide (GO) and reduced graphene oxides (r-GO) have been extensively studied by various research groups, but the major short come are (i) increase of oxygen in graphene domain increases the number of sp<sup>3</sup> carbon, (ii) high content of sp<sup>3</sup> carbon restricts electron mobility and leads to poor electrical properties, (iii) presence of sp<sup>3</sup> carbon reduces the conductivity and amplifying disorderness in graphene domain. Similarly, studies have been done on the formation of chemically modified graphene with organic moieties such as polyaniline, amino acids etc., by  $\pi - \pi$ stacking and/or van der Waals interactions. The strength of graphene hybrids or composite are highly vulnerable and their long-term association with graphene is thus highly questionable.

In addition, large-scale synthesis of functionalized graphene should use a sustainable, economical, and eco-friendly process. In this study we have successfully demonstrated the formation of highly dispersive nitrogen functionalized graphene (N-FG) and nitrogen functionalized r-GO by submerged liquid plasma (SLP) process at ambient condition. Advantages of the SLP process include a simple setup, minimal surface damage due to fast moving electrons, no required further purification, possible large-scale synthesis, low operating cost and eco-friendliness. N-FG shows greater stability and electrical conductivity due to the presence of pyridinic and pyrrolic nitrogen. Raman spectrum confirms only marginal increase in dis-orderness when compared to the graphene and displayed remarkable dispersibility in both aqueous and organic solvents. Furthermore, fluorescence property of N-FG confirms the presence of -NH and -N=C- at the graphene sites, as supported by UV-Vis spectrometry and X-ray photoelectron spectroscopy studies. e: jsn@iitm.ac.in



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## The endophytic fungus *Trametes hirsuta* as a novel alternative source of podophyllotoxin and related aryl tetralin lignans

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The aryl tetralin lignans are synthesized by Podophyllum sps. and are in great demand worldwide due to their use in synthesis of topoisomerase inhibitors. However, the sustained production of these aryl tetralin lignans requires large-scale harvesting from the natural environments, which has resulted in the plant-endangered status. In view of the difficulties in their total chemical synthesis, cultivation and failure of metabolic engineering approaches, there is a need to search for alternative sources of production of aryl tetralin lignans. We unequivocally established the methodology for isolation, identification, and characterization of a novel fungal endophyte (Trametes hirsuta) that produces aryl tetralin lignans consistently as shown by HPLC, LC–MS, LC/MS–MS and 1H NMR. The lignans produced by the microorganism are biologically active, and exhibit potent antioxidant, anticancer and radioprotective properties. This strategy promises to improve the production of these therapeutically important compounds at lower costs.

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# Estimation of lead levels in soil for some areas at East Gezira regions and khartoum-Sudan (A comparative study between the rural areas and urban areas)

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Lead is a chemical element with an atomic number 82 and Symbol Pb, and nowadays recognized as a heavy-metal poisonous, it affects every system of the body. Acute exposure to high level of Lead can result in death or significant damage to the brain or other organs. The study aimed to determine the concentration of Lead in Soil of some areas in Khartoum and East of Gezira (Baanat, Rufa'a, and Tamboul) Specifically. Also, to make a comparison between the rural areas and the urban areas. Eighteen samples of soil were collected from the bus stations, batteries repairing Market in Souk Sha'bi and specific distances away from them. The analysis work was done by Atomic Absorption Spectrometer method. Lead concentration in samples of soil in this study was ranged 0.78 ppm (Baanaat) – 10.58 ppm (Batteries Market Souk Sha'bi). A positive correlation was found between Urbanization and lead mean concentration 1.22 ppm in Khartoum and 0.40 ppm in East of Gezira. A positive correlation was also found between the concentrations of lead as being nearer to the centre of each of the bus station and Batteries repairing market and the Main road. So, this study recommended that all Lead-related industries and markets should be far enough from human living to avoid environmental lead pollution.

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