5th Global Chemistry Congress

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Posters

Aleksandr Kozhushkevich et al., Mod Chem Appl 2017, 5:3(Suppl)
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Optimization of automated pressurized liquid extraction and cleanup of PBDE in animal feed

Aleksandr Kozhushkevich, A A Komarov, V V Ovcharenko, A A Shelepchikov, A V Sorokin and **A M Kalantaenko**
VGNKI Institute, Russia

Introduction: Polybrominated diphenyl ethers (PBDEs) are massively used as flame retardants. They are chemically and biologically persistent, lipophilic, and able to bio-accumulate in fatty tissues and biomagnify throughout food chains. Similarly to dioxins, PBDEs may be transferred from animal feed to lipid-containing food such as milk and eggs. Therefore, there is a need for developing efficient methods of PBDE determination in animal feed matrices. With animal feed matrices, an automated Power Prep system (FMS Inc., USA) has previously been used for PBDE clean-up following manual column extraction and shaking with concentrated sulfuric acid. Our goal was to optimize PBDE extraction and clean-up from a typical feed matrix (fish meal) using a more advanced Total-Rapid-Prep system (FMS, USA) which includes a pressurized liquid extraction module (PLE), multi-column sample cleanup module (Power-Prep) and evaporation/solvent exchange module (SuperVap).

Materials & Method: About 10 g of feed were mixed with diatomaceous earth, and then spiked with 100 µl mixtures of mass-labeled PBDE congeners and 100 µl mass-labeled PBDE internal standard solutions to monitor recoveries. Extraction was performed on PLE with n-hexane at 1200C and 15 MPa (two static cycles of 20 min each, the purge time 120 s). The extracts were evaporated on SuperVap to 10 ml and subjected to automated cleanup on silica and alumina columns. Elution parameters were optimized (Fig. 1). Elution by 40 ml 20% DCM/Hex followed by 120 ml 50% DCM/Hex gave the best recovery values for all congeners including di-brominated BDE-15 (Fig. 2). The purified extracts were concentrated on SuperVap and analysed on a TSQ 8000 Evo GC-MS/MS (Thermo, USA).

Results & Discussion: Compared to the semi-automated method, we obtained better recoveries for di- to tetra-brominated congeners (Fig. 2) in a fully automated setup which saves time and solvents.

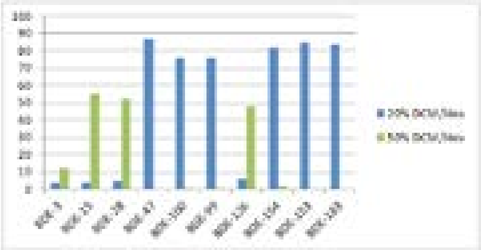

Figure 1: PBDE recoveries after single-run elution with either 20% DCM/Hex or 50% DCM/Hex solvent systems.

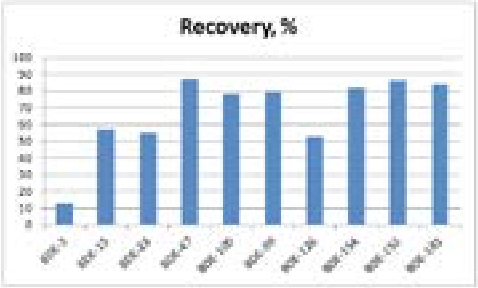

Figure 2: PBDE recoveries after consecutive elution with 20% DCM/Hex and 50% DCM/Hex solvent systems.

Biography

Aleksandr Kozhushkevich is a Senior Scientist at All-Russian State Center for Quality and Standardization of Veterinary Drugs and Feed (VGNKI), Department of POPs Control in Feedstock and Feeds. He has many years of experience in the analysis of persistent organic pollutants in food and feed.

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Anna K Przybył et al., Mod Chem Appl 2017, 5:3(Suppl)
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Synthesis, spectroscopic and structural analysis with electron density distribution of (-)-cytisine and its derivatives

Anna K Przybył, Agata Owczarzak, Dominika Gołowin and **Maciej Kubicki**
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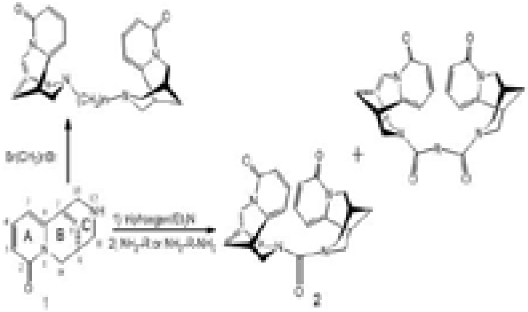
Statement of the Problem: (-)-Cytisine (1, Scheme 1) is an alkaloid, naturally occurring in plants of the Leguminosae family. It interacts with nAChRs and has been applied in investigation of the central nervous system. Moreover, cytisine derivatives have been tested for their use in the treatment of Alzheimer's and Parkinson's diseases. This alkaloid has been found to moderately increase the concentration of dopamine alleviating the symptoms of nicotine deprivation. Therefore, cytisine and its derivative (varenicline) have been employed in nicotine withdrawal therapy. Some N-derivatives of (-)-cytisine show analgesic, antidepressant, anti-inflammatory, hypoglycemic and hypertension reducing properties.

Methodology & Theoretical Orientation: (-)-Cytisine was isolated from the seeds of *Laburnum anagyroides*. The modifications were made with alkane dibromide or BTC/amines/diamines. The products were separated by flash chromatography. Structural data were collected using Rigaku diffractometers: Supernova with Atlas detector and Excalibur E. The NMR spectra were measured on NMR Bruker Advance II 600 MHz.

Findings: Biological activity of (-)-cytisine is related to the presence of pyridone ring A and piperidine ring C. Such structure also permits obtaining a number of derivatives with biological activity even greater than that of cytisine itself. It has been found that modifications of the molecular structure change the pharmacological properties including the affinity to certain nAChR subtypes. We decided to use the high-resolution X-ray diffraction method which allows for experimental determination of the details of the electron density distribution in molecular crystals and brings the details of e.g. electrostatic potential and dipole moments that are the features underlying the biological action.

Conclusion & Significance: (-)-Cytisine is an excellent substrate in syntheses of the adducts in which other molecules can be bonded to cytisine through N-12 of piperidine ring C (Scheme 1). The hybrid compounds of this type often show much better therapeutic properties than the parent ones. Additionally basing on the relation of the electronic/energetic features with the biological activity, it should be in future possible to design more potent compounds and even to build the pharmacophore model.



Biography

Anna K Przybył completed her Graduation in Chemistry at Adam Mickiewicz University in Poznań, Poland. In 2000, she received her PhD degree from the same institution under the supervision of Prof. Waleria Wysocka. She was a Post-doctoral fellow at National Institutes of Health, NIDDK, Laboratory of Medicinal Chemistry, Bethesda, MD, USA (2001–2003), under the supervision of Dr. Kenner C Rice. In 2015, she obtained her Habilitation degree. She is currently an Associate Professor at Adam Mickiewicz University, Poznań. Her scientific interests include natural products, especially alkaloids, modern organic synthesis and medicinal chemistry. Her research focuses on modification of quinolizidine alkaloids, in particular transformations into conjugated systems, enantiomer separation and structure analysis.

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Aysha Mezoughi et al., Mod Chem Appl 2017, 5:3(Suppl)
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Synthesis of potential lytic transglycosylase inhibitors

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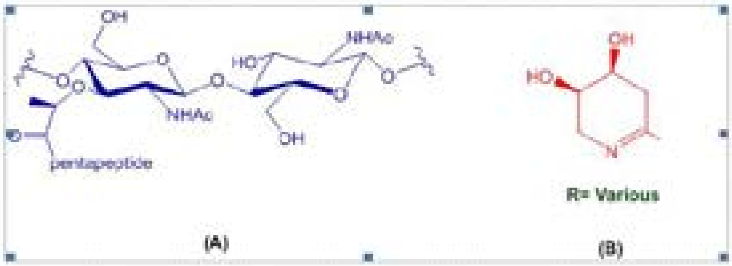
Lytic transglycosylases are bacterial enzymes that are responsible for creating space within the cell wall to insert new material during cell growth and division as well as making pores to allow transport of DNA and proteins across the cell wall. Due to these important roles, lytic transglycosylases may present an attractive new target for the development of broad-spectrum antibiotics. Different inhibitors have been synthesized using mimics for the intermediate species in the reaction catalysed by lytic transglycosylases. Herein we aimed to synthesis and evaluate a series of amidine derivatives as inhibitors of soluble lytic transglycosylases.



Biography

Aysha Mezoughi has an experience in organic synthesis, protein synthesis and purification and enzyme kinetics. She is working in chemical biolog, her project is based on antibiotic resistance. Her experience is based on her education, teaching and research in the university. Her qualifications are: MSc in organic chemistry, school of chemistr, Tripoli university (2005), lecturer in organic chemistry, school of chemistry, Tripoli university (2005-2013), PhD student at Cardiff university(2014-present), she has published five papers, three in organic chemistry journals and two in biochemistry journals

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Eman Alghamdi et al., Mod Chem Appl 2017, 5:3(Suppl)
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Development of rationally-designed polymers for α-tocopherol extraction and purification using solid phase extraction

Eman Alghamdi[1] and **Elena Piletska**[2]
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[2]University of Leicester, UK

α-tocopherol is a valuable compound in terms of its therapeutic and industrial applications. There is an increasing focus on the natural sources of this compound, such as wheat germ, sunflower oil, vegetable oil and vegetables, because its bioactivity is observed only if it is extracted from natural resources that have not been synthesized. Since α-tocopherol is one of the minor components in the edible oil, it is essential to pay attention to the selectivity, efficiency and precision of the extraction method. The aim of this research is to develop rationally-designed polymers (RDPs) for the extraction and purification of α-tocopherol from sunflower oil as a natural source. RDPs were prepared based on the molecular imprinting principles, and then used as an adsorbent in the solid phase extraction (SPE) in order to extract and purify α-tocopherol. RDPs were synthesized using meth-acrylic acid (MAA) as a functional monomer and ethylene glycol dimethacrylate (EGDMA) as a crosslinking agent using a thermo-polymerization procedure. RDP demonstrated the recoveries of tocopherol from model solution of 94%. UV spectroscopy was used for the optimization of the solid phase extraction of α-tocopherol from the model samples. 60% ethanol was found that the best washing solution and better eluting solution was 5% acetic acid with methanol. GC separation was applied to detect and quantify the α-tocopherol in the natural sample (sunflower oil).

Biography

Eman Alghamdi completed her Master degree in Natural Products Chemistry in 2008 and became an Administrator in Department of Chemistry at King Abdul Aziz University up to 2012. After that, she has become a full-time PhD student at University of Leicester. Currently, she is pursuing her third-year research in the lab of biotechnology group under supervision of Dr. Piletska and Prof. Piletsky. She is interested in Optimization of the protocols for purification, separation and quantification of natural and synthetic compounds from different natural sources.

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Notes:

Entesar Al-Hetlani et al., Mod Chem Appl 2017, 5:3(Suppl)
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Detachable photocatalysts of anatase TiO2 nanoparticles: Annulling surface charge for immediate photocatalyst separation

Entesar Al-Hetlani, Mohamed O Amin and **Metwally Madkour**
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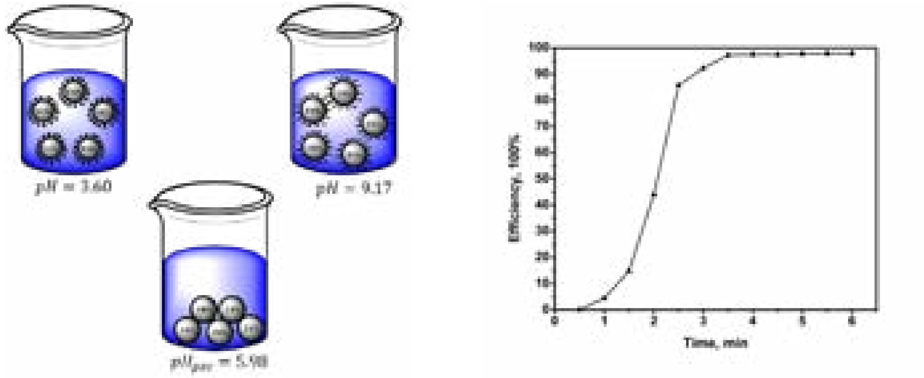
TiO^2 photocatalysis is commonly utilized in diverse applications such as environmental waste management, biomedical and energy fields. The present study demonstrates the effect of temperature on the characteristics of TiO2 nanoparticles using XRD, XPS, DLS, UV-Vis, N2 sorpometry and TEM techniques. The optimum surface area of the photocatalyst was obtained when it was prepared at 60°C. Additionally, the TEM images showed semi-spherical morphology. Afterwards, rapid photo-degradation of rhodamine 6G dye (R6G) with efficiency of 92.5% at pH=9.17 was accomplished using the optimized nanoparticles. The main focus of this study is to establish a new avenue that can be used to separate the photocatalyst from the reaction medium after the photo-degradation experiment is completed. In this study, the photocatalyst was completely detached from the reaction medium in 3 minutes without utilization of coagulant agents or magnetic nanoparticles. This was lucratively accomplished by adjusting the pH of the medium to match the isoelectric point (pHPZC) of the photocatalyst and annulling its surface charge, hence rapid sedimentation was observed, Figure 1. This new method has proven to be simple, rapid, and applicable to all types of photocatalysts on the industrial scale.



Biography

Entesar Al-Hetlani is Lecturer at Kuwait University and currently pursuing her PhD in Chemistry at University of Hull, UK. Her research interest includes “Forensic analytical chemistry, organic and inorganic monolith columns, chemiluminescence and electro chemiluminescence, and synthesis of magnetic nanoparticles.

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Magnetic paper based ELISA

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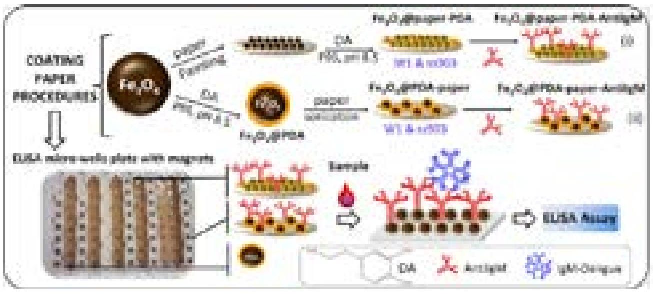
In recent years, magnetic beads and nanoparticles (mainly magnetite) are reported, patented and commercialized as new platforms to improve ELISA (enzyme linked immunosorbent assay) performances. However, most of these technologies can be costly and impractical for the diagnosis of certain endemic and epidemic diseases in underdeveloped countries, where a considerable amount of patient samples must be studied. On the other hand, the most important application of paper (cellulose material) support of sensors by the scientific community has been the development of new paper-based analytical devices such as paper based ELISA assays. However, their sensitivity is currently more than ten times lower than that of traditional ELISA. This contribution reports a novel magnetic paper–based ELISA using core–shell magnetite@polydopamine nanoparticles supported on a Whatman paper-like new solid immunoassay platform specifically for IgM-dengue antibodies recognition as the proof-of-concept target for antibodies isotype IgM detection. Affordable procedures to deposit magnetite nanoparticles on cellulose paper sheets (Whatman type-1 and ss903) and to conjugate such nanoparticles with antihuman-IgM antibodies using polydopamine as linker are reported. Structural features, magnetic behavior, coating homogeneity, and the nanoparticles/linked antibodies ratio were determined. Additionally, magnetic paper – based ELISA for IgM-dengue antibodies detection provides a system with improved analytical response (two orders more sensitive with a 700 times lower limit of detection (LOD) than traditional ELISA or using magnetic beads without depositing), appropriate accuracy for real sample detection, low cost, easy manufacturing, and effortless and easy handling. Finally, a novel transducer based on quantum dots contained in polymeric capsules is proposed to be coupled in the magnetic paper–based ELISA for enhancing analytical response.



Biography

Greter Ortega completed her Bachelor of Science in Chemistry and Master of Science in Chemistry at University of Havana, Cuba in 2012 and 2015, respectively. At present, she is a graduate teaching Assistant in Department of Inorganic Chemistry, Faculty of Chemistry, University of Havana and a PhD student at Center for Applied Science and Advanced Technology of IPN, Legaria Unit, Mexico. She has published two research articles and participated in 10 international scientific meetings held in Cuba, Mexico and Spain and has done research on the synthesis, functionalization and the use of the novel properties of metal, magnetic and semiconductor nanoparticles to design nanostructured biosensors.

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Herlys Viltres Cobas et al., Mod Chem Appl 2017, 5:3(Suppl)
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Adsorption study in aqueous medium of arsenite by goethite nanorods

Herlys Viltres Cobas[1], **Oscar F Odio Chacon**[2], **Susel Del Sol Fernandez**[1], **Raul Borja Urby**[3] and **Edilso Reguera Ruiz**[1]
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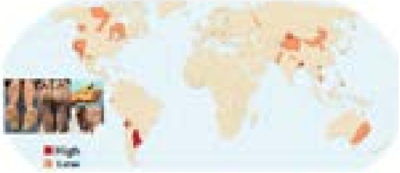
Arsenic is one of the most widespread inorganic pollutants worldwide and represents a significant potential risk to human health and the biosphere. It is well known that arsenic is highly toxic and carcinogenic; at present, there are reports of diverse countries with arsenic concentrations in drinking water higher than those proposed by the World Health Organization (10 µg/L). Nanomaterials and nanotechnologies inspire new possible solutions to major environmental issues nowadays. It has been reported that adsorption strategies using iron oxyhydroxide as goethite are very efficient for the removal of arsenic in drinking waters; the adsorption mechanism is not yet clear. In order to shed light on this subject, we attempt to study the interactions between arsenic species and α-FeOOH nanorods in aqueous medium. Goethite nanorods were prepared using a precipitation method with FeCl3 as metal source and KOH aqueous solution as precipitating agent. As-synthesized nanorods were put in contact with As2O3 solutions at room temperature at pH 4 and 7. Goethite particles were characterized by DRX, TEM, FT-IR and XPS. Results showed that goethite nanoparticles had 30 nm wide and 410 mm long, and a narrow size distribution. The presence of arsenic on particles surface was confirmed, which is more remarkable when pH=7 condition is employed. On the other hand, when As (III) species interact with the nanoparticle surface, oxidation to As (V) occurs, which produces the surface reduction. Besides, after adsorption experiment, it was evidenced from FTIR and XPS that once arsenic species interact with the nanoparticles, they form doubly protonated monodentate and simply protonated monodentate complex of As(III) at pH=4 and 7, respectively, and bidentate complex of As(V) after As(III) oxidation, in both conditions. The developed methodology could be implemented in the water treatment industries, reducing the costs of the processes and making them more environmental friendly.



Biography

Herlys Viltres Cobas has expertise in the synthesis and characterization of nanomaterials. She has completed her Master's degree at Center for Research in Applied Science and Advanced Technology (CICATA), Legaria Unit, National Polytechnic Institute, Mexico City, Mexico. Currently, she is a PhD student at CICATA, Legaria Unit. She worked on the synthesis and characterization of iron oxide nanoparticles (magnetite, hematite and goethite) to remove arsenic from the aqueous medium.

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Hye Soon Kang et al., Mod Chem Appl 2017, 5:3(Suppl)
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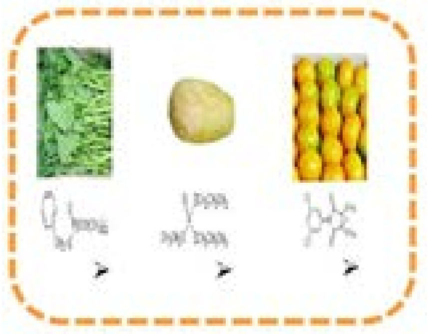
Simultaneous analysis of multi residue pesticides method in agricultural commodities by gas chromatography-mass spectrometry

Hye Soon Kang, Hyung-Il Kim, EunJung Jang, YongWoo Shin, Miok Kim, KiMi No, Yukyung Lee, Ji-Yong Yang, JiHey Min, Jun-Ho Jeon, Chul-Joo Lim and **Sun-Ok Choi**
Gyeongin Regional Office of Food and Drug Safety – MFDS, South Korea

Ministry of food and drug safety makes an effort in monitoring the contaminated pesticides in commercial agricultural products. The monitoring of pesticides in food is nowadays a major objective in order to get extensive evaluation of food quality and to avoid possible risks to human health. Gas chromatography-mass spectrometry (GC-MS/MS) is rapidly becoming an accepted technique in pesticides for regulatory monitoring purpose. An analytical method for the simultaneous target analysis of 344 pesticides in agricultural products by GC-MS/MS has been developed. We developed an accurate, simple, rapid and simultaneous analytical method of 344 pesticides in agricultural products. The monitoring analysis was aimed to establish for determination of an analytical method for 344 pesticides by GC-MS/MS. Recovery, precision, accuracy, linearity, and limit of quantitation (LOQ) in the analytical method were validated in different matrices. The recoveries obtained at fortified levels of 0.01~0.5 mg/kg were 60~130% for pesticides, with relative standard deviations (RSDs) of ≤30%. The proposed method has possibility to be applied successfully in Korean Food Standards Codex for the residue determination of 344 pesticides in agricultural products. The proposed method was applied successfully for the residue determination of 344 pesticides in agricultural commodities.



Biography

Hye Soon Kang is an Assistant Director at Gyeongin Regional Food and Drug Safety of Ministry of Food and Drug Safety in Korea.

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Jun Zhang, Mod Chem Appl 2017, 5:3(Suppl)
DOI: 10.4172/2329-6798-C1-006

Fluorescent derivatives of the amyloid ligand Congo red for the detection of Aβ and Tau aggregates

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Statement of the Problem: Alzheimer's disease (AD) is the most common neurodegenerative disorder of the brain and a leading cause of dementia. Aβ plaques consisting of Aβ peptides and Neurofibrillary Tangles (NFTs) consisting of hyperphosphorylated Tau has been recognized as the main two pathological hallmarks of AD. Investigation of Congo red led to the discovery of bis-styrylbenzenes as a class of compounds with strong Aβ plaque binding properties.

Methodology & Theoretical Orientation: Starting from the amyloid ligand X-34, Aβ-fibril and Tau fibril binding affinities and specificities for the four fluorescent derivatives of X-34 were determined by means of fluorescence titrations with Aβ1-42 and Tau fibrils, respectively and a fluorescence assay using human AD brain sections.

Findings: The five ligands can bind to Aβ1-42 and Tau fibrils with augmented intensities, respectively, but with very weak fluorescence changes in the presence of Aβ1-42 oligomer and monomer. Benzene and naphthalene derivatives upon binding to Aβ1-42 fibrils showed significantly increased quantum yields (QY). The thiophene derivative in buffer displayed high QY compared with the other probes, while quinoxaline and benzo[c][1,2,5]thiadiazole derivatives showed very low QY in the absence/presence of Aβ1-42 fibrils. The two pathological hallmarks, Aβ plaques and NFTs, could be readily identified due to bright fluorescence especially quinoxaline derivative, specifically stain Aβ plaques.

Conclusion & Significance: The central benzene motif of X-34 can be replaced with other heterocyclic moieties without reducing the ligands' selectivity. However, the quinoxaline derivative can selectively detect Aβ plaques and not NFTs. We foresee that these ligands will be useful candidate markers for monitoring the formation and progression of a variety of disease-associated protein aggregates.

Biography

Jun Zhang has his expertise in designing and synthesizing small fluorescent ligands for the identification of protein aggregates, the common pathological hallmark of many neurodegenerative diseases such as Alzheimer's and Parkinson's disease (AD and PD). These novel ligands will expand the tool box of fluorescent ligands for *in vitro* monitoring of amyloid fibril formation and *in vivo* monitoring of progression and deposition of various disease-associate proteins.

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Notes:

Manojkumar K Rathod, Mod Chem Appl 2017, 5:3(Suppl)
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An efficient synthesis of annulated novel pyrimido[4,5-d]pyrimidine derivatives: DFT, docking, SAR and antimicrobial evaluation

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A simple green synthetic approach was developed to synthesize medicinally important heterocyclic novel pyrimido[4,5-d] pyrimidine(PP) derivatives by using heterogeneous solid acid catalyst, through single reaction chamber. This green process offer high yields within short reaction time. *In silico* proficiency of Lipinski's, DFT, docking and SAR study have been carried out in order to get target drug like novel PP molecules with desired activity through multidisciplinary green approach. Computer aided drug designing (CADD), molsoft and Osiris tool were used to predict PP structural parameters of Lipinski rule which meant to find molecular membrane permeability, oral bioavailability, drug-likeness and drug score. In addition, DFT method was employed to calculate the PP structural geometries, molecular stability and electronics structures using online tool. Moreover, the docking method was used to determine voltage-dependent calcium channel blockers receptor-PP ligand interactions and molecular surface bonding were performed by online tool. The synthesized products were characterized by FT-IR, 1H NMR and 13C NMR spectral analysis. The synthesized analogs have also been evaluated for their bioassay against bacterial and fungal strains. SAR study relates features of PP structure to a property, effect and biological activity associated within moiety. In this summery, theoretical and experimental approaches brought together in order to synthesize target PP molecules with desired activity will serve as vital aid for future researchers working in the area of drug design.

Biography

Manojkumar K Rathod completed his MSc, MPhil in Bioinformatics; BSc, MSc in Chemistry and; PhD in Chemistry at Sardar Vallabhbhai National Institute of Technology, Surat, India. At present, he works as an Assistant Professor in Department of Chemistry at Marwadi University, Gujarat, India. He has two years of experience as an Assistant Professor and Head of Department of Chemistry at S S Agrawal College of Commerce & Management, Gujarat, India. He received scientific awards by RSC (2014) and BTISNET, DBT (2012). He has published four research paper and presented research article in nine national & international conference.

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Neha Manhas et al., Mod Chem Appl 2017, 5:3(Suppl)
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Full structural elucidation of quinazoline-Schiff bases using 2D-NMR studies

Neha Manhas, Parvesh Singh and **Neil A Koorbanally**
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Quinazoline nucleus is not only present in various therapeutic agents but also form an important structural component of natural products. The prazosin (anti-hypertensive), methaqualone (hypnotic), metolazone (diuretic), raltitrexed (anti-cancer) and (+)-febrifugine (anti-malarial) are few commonly used drugs that contains quinazoline ring as a core. Over the past few decades, the synthesis of quinazoline derivatives has attracted considerable attention of the synthetic chemists worldwide owing to its diverse medicinal activities including anticancer, anti-HIV, antibacterial, anti-inflammatory, anti-malarial, and anti-tubercular activities. The most established preparative methodologies for quinazoline synthesis involve its use. On the other hand, Schiff bases (>C=N), also known as imines or azomethines, are another widely explored intermediates in heterocyclic synthesis with various biological/medicinal applications such as anticancer, anti-tubercular and anti-inflammatory activities. Consequently, several research papers and review articles regarding the design and synthesis of new and promising quinazolines or Schiff bases or both as their hybrids have been documented in international peer-reviewed literature. In view of the above facts, we prepared a new series of quinazoline-tethered Schiff bases by condensation of 3-aminoquinazolinone with a variety of aldehydes. Predominantly, fluorinated Schiff bases were targeted owing to the property of fluorine atom to increase in metabolic stability and bioavailability of organic scaffolds. Additionally, the molecular hybrids of quinazoline with other pharmacophores such as quinolines, thiophene and indole were also prepared owing to their existence in biologically significant heterocycles and drug molecules.

The full structure elucidation of all synthesized compounds was subsequently performed using 2D NMR (HMBC, HSQC, COSY, and NOESY) techniques followed by the extensive analysis of the chemicals shifts and splitting patterns of all compounds. The 19F being NMR active splitted both the proton and carbon nuclei of the compounds, and played a significant role in characterization process.

Biography

Neha Manhas completed her Master's degree in Chemistry from Durban University of Technology (South Africa), and currently pursuing her Doctorate in the School of Chemistry and Physics at University of Kwazulu-Natal (UKZN), Durban, South Africa. Her PhD research focuses on "The synthesis, biological evaluation and molecular modeling of novel quinazoline based heterocycles". She has co-authored three research publications in the peer-reviewed journals.

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Hydrogen storage comparison of Cu-BTC and Fe-BTC

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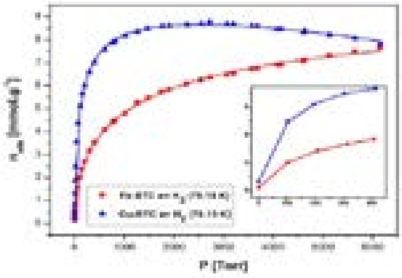
The search for materials with structural characteristics that allow for proper adsorption of either greenhouse gases (CO2, CH4) or energy carrier gases (H2) is nowadays one of the main research lines in the scientific community. This contribution reports a comparative study of the hydrogen storage in two metal organic frameworks (MOFs), Fe-BTC and Cu-BTC. Both materials were obtained by solvothermal technique and then characterized from XRD, FTIR, UV-vis, XPS, Mössbauer and magnetic measurements. A detailed analysis on the possible guest-host interactions for the hydrogen molecules in the porous framework of these materials is discussed. These frameworks present promising potential as storage materials due to large surface area (more than 10^3 m^2/g), accessible pore volume between 45 and 55% of the total volume and high chemical and thermal stability. Adsorption isotherms were recorded in order to determine the H2 maximum adsorption capacities (Qmax) and to evaluate the adsorption heats (Hads) by the isosteric method. Results yielded good Qmax values (150-200 cm^3/g) and intermediate Hads (7-9 kJ/mol), which make Fe-BTC and Cu-BTC promising candidates for H2 storage. With the obtained data, the nature of the adsorbate-adsorbent interactions is discussed.



Biography

Neil Torres Figueredo completed his Engineering in Nuclear and Energetic Technologies at Higher Institute of Technology and Applied Sciences in Havana, Cuba in July 2008 and his Master of Advance Technology at Research Center for Applied Science and Advanced Technology (CICATA-Legaria) of IPN, Mexico in December 2014. At present, he is a Researcher at Center of Applied Technology and Nuclear Development in Havana, Cuba and a PhD student at Research Center for Applied Science and Advanced Technology of IPN, Legaria Unit, Mexico. He has published two research articles and participated in about 10 international scientific meetings held in Cuba, Mexico, Brazil, Argentina and EEUU and has done research on the synthesis, characterization and evaluation of the porous materials promising for storage and gases capture.

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Parvesh Singh et al., Mod Chem Appl 2017, 5:3(Suppl)
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Synthesis and antioxidant activity of 2-mercaptothienopyrimidine-tethered-1,2,3-triazoles

Parvesh Singh and **Nagaraju Kerru**
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Thienopyrimidines are known to possess a wide-spectrum of medicinal activities including anti-TB, anti-cancer, anti-bacterial, anti-fungal, anti-oxidant, and anti-diabetic activities. Similarly 1, 2, 3-triazole nucleus has been exploited in the design of several medicinally and biologically active scaffolds including anti-oxidant compounds. Among different synthetic approaches being used in the drug discovery, molecular hybridization (MH) is gaining popularity owing to its ability to combine two or more bioactive scaffolds with different or novel mechanism of action. In view of the aforementioned significance of thienopyrimidine and 1,2,3-triazoline scaffolds, it was thought worthwhile to couple these two pharmacophores in a single molecular architecture to check the anti-oxidant effect of the resultant molecular hybrid. Accordingly, the desired molecular hybrids (5a-f and 6a-f) were prepared by copper catalyzed cycloaddition of alkynyl thienopyrimidine with various substituted aryl azides in the presence of CuSO4 and sodium ascorbate in THF/H2O (1:1). The synthesized compounds screened for their antioxidant activity using DPPH radical scavenging, NO and ABTS assays revealed several promising molecular conjugates with excellent antioxidant activity, even better than the standard drug (acarbose). The structure activity relationship studies further revealed the role of electron-donating (-CH3, Cl, I) groups in increasing the anti-oxidant activity of the compounds, whereas an opposite effect was observed for the electron-withdrawing substituents.

Biography

Parvesh Singh received his PhD degree in Organic Chemistry from the Guru Nanak Dev University, India. Currently, he is working as a Senior Lecturer of Organic Chemistry at University of KwaZulu Natal (South Africa). His research interests involve the synthesis, biological evaluation and molecular modeling of heterocyclic scaffolds. He is primarily using hetero Diels-Alder methodology to synthesize heterocyclic rings of different sizes. He has published 60 research articles in peer-reviewed journals of international repute including a book chapter and a book.

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Notes:

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Rima D Alharthy et al., Mod Chem Appl 2017, 5:3(Suppl)
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Synthesis of triazole-linked morpholine oligonucleotides via CuI catalysed cycloaddition

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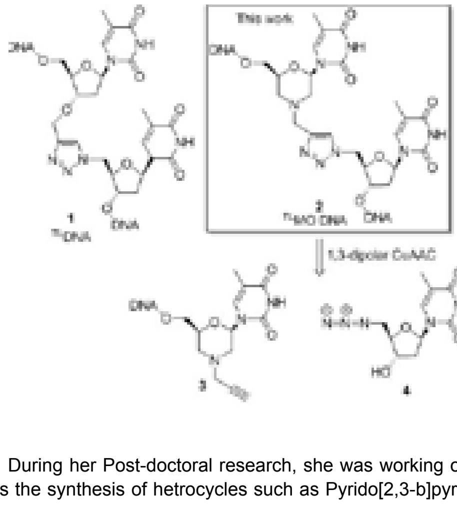
The Cu^{I} catalysed (3+2) azide–alkyne cycloaddition (CuAAC) has been used to construct modified inter nucleotide linkages, to prepare nucleic acid conjugates, and as a strand ligation tool. In particular, the artificial triazole-linked DNA ^{TL}DNA 1 retains good aqueous solubility, is stable towards enzymatic degradation, and can be read by polymerases. As part of our own research aimed at developing therapeutic nucleic acids, we decided to examine triazole-linked morpholino (^{TL}MO) hybrid structures 2 (Fig. 1) as they could combine the ease of synthesis of the ^{TL}DNAs 1 with the increased melting temperatures associated with morpholino drug candidates. Thus, triazole-linked morpholino (^{TL}MO) oligonucleic acids were synthesized using the CuAAC reaction. The ^{TL}MO hybrid 2 can be disconnected to reveal the azide 4 and the alkyne-substituted morpholine 3 as potential precursors for the proposed CuAAC reaction (Fig. 1). Synthesis strategy involved oxidative cleavage of ribose, reductive amination treatment with sodium cyanoborohydride/AcOH to build the propargylamine partner. The azido thymidine building block was accessed via a two-step sequence involving mesylate formation and displacement with sodium azide. Next, CuAAC was successfully applicable to obtain ^{TL}MO. A range of catalysts and solvents were initially screened, and it was quickly found that the use of copper(I) iodide in THF:tBuOH:H2O (3:2:1) with microwave heating (80°C) was optimal. Under these conditions, cycloaddition of the acetylene with the TBS-protected azide gave the ^{TL}MO dimer in good yield, and TBAF de-protection gave the desired alcohol in good yield. The modified DNA analogues were incorporated into 13-mer sequences via solid phase synthesis. UV melting experiments showed that the ^{TL}MO modification gives higher Tm values than the corresponding ^{TL}DNA modification. Thus, addition of the morpholine modification can regain half of the Tm lost by incorporating the triazole inter nucleotide linkage.



Biography

Rima D Alharthy is an Organic Synthetic Chemist. During her Post-doctoral research, she was working on the synthesis of attractive bioactive compounds and consequently evaluating their activity. This includes the synthesis of hetrocycles such as Pyrido[2,3-b]pyrazines, polyphenols, pyrazolo pyrimidine scaffolds and hybrid acridine-HSP90 ligand conjugates.

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Sanjeev Dhawan et al., Mod Chem Appl 2017, 5:3(Suppl)
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Synthesis of coumarin-tagged 1,3,4 oxadiazole conjugates

Sanjeev Dhawan, Srikanth Babu Jonnalagadda and **Parvesh Singh**
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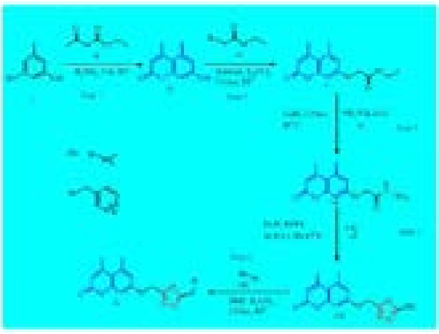
Coumarins are an important class of heterocyclic compounds with natural and synthetic origins. It has a unique benzo-α-pyrone which has demonstrated proliferative biological activity. Similarly, the 1,3,4-oxadiazole heterocycles exhibit remarkable pharmacological and biological properties, e.g., antibacterial, anti-viral, anti-cancer, anti-coagulation and anti-inflammatory activities. The 1,3,4-oxadiazole ring is highly lipophilic thus improving drug permeability across cell membranes, ensuring the drug reaches the biological target. Both classes of compounds form valuable leads in drug discovery i.e. coumarin fused 1,3,4-oxadiazole and their derivatives. Molecular hybridization techniques have been used in drug design and discovery. The method involves the combination of two or more bioactive pharmacophores to generate a single molecular scaffold with improved affinity and bioactivity, in comparison to the parent molecules. Accordingly, a series of novel 7-((5-mercapto-1,3,4-oxadiazol-2-yl)methoxy)-4,5-dimethyl-2H-chromen-2-one derivatives was synthesized. Using commercially available orcinol as the starting material, the key intermediate 7-((5-mercapto-1,3,4-oxadiazol-2-yl)methoxy)-4,5-dimethyl-2H-chromen-2-one was synthesized in four steps: condensation; esterification; hydrazidation and; cyclization; followed by alkylation and benzylation.



Biography

Sanjeev Dhawan is a PhD candidate at University of KwaZulu-Natal, School of Physics and Chemistry, Westville, Durban, South Africa. He was awarded the NRF-TWAS fellowship in 2016, to complete his PhD research in Medicinal Chemistry. He completed his B Pharmacy at Punjab Technical University, India. He completed his M Pharmacy in Medicinal Chemistry from Lovely Professional University, Punjab in 2013. He has worked as Research Associate in Jubilant Chemsys, Noida, India.

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Se-Jong Park et al., Mod Chem Appl 2017, 5:3(Suppl)
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Analysis of migrated 1-hexene and 1-octene from polyethylene food packaging into food simulants by HS-GC-MS

Se-Jong Park, So-Ra Park, Yu Mi Cho, Joung Boon Hwang, Jae-Chon Choi and **MeeKyung Kim**
Ministry of Food and Drug Safety, South Korea

Polyethylene (PE) is used in greater volume worldwide than any other plastic as food packaging. This might be due to PE is cheap, durable, flexible and easy to use. The polyethylene is manufactured by polymerizing ethylene with α-olefin monomers such as 1-butene, 1-hexene and 1-octene. Food contact materials may contain trace amounts of residual monomers during the formulation or manufacturing process. However, ethylene and 1-butene are very volatile and easily lost from processed PE polymer. 1-hexene and 1-octene could be migrated into the food when PE food packaging is used for cooking and storing. Therefore, it is necessary to determine migration levels of 1-hexene and 1-octene from food contact materials for food safety. The aim of this study was to determine 1-hexene and 1-octene from PE food contact materials by head space-gas chromatography-mass spectrometry (HS-GC-MS). Migration tests with three food simulants, deionized water, 4% acetic acid and 50% ethanol were examined at 70°C and 100°C for 30 min under the Korea regulation. Analysis of migration amounts of 1-hexene and 1-octene from samples was performed by HS-GC-MS (selected ion monitoring mode, HP-1 column). The method was validated by measuring the limit of detections (LODs), the limit of quantifications (LOQs), recovery, precision and uncertainty. Based on the optimized method, we monitored the migration of 1-hexene and 1-octene from PE food packaging materials such as food packaging films, wraps, bags and containers, All the samples were collected from manufactures and retailed stores. The result of this study can be used as valuable data for the safety control of the PE food contact materials in Korea.

Biography

Se-Jong Park is a Scientific Officer in Food Safety Evaluation department at Ministry of Food and Drug Safety (MFDS), South Korea. Her research focuses on food packaging safety. She has led projects involving development analytical methods, risk assessment and migration of hazardous substances from food packaging materials.

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Soon Kwan Jeong et al., Mod Chem Appl 2017, 5:3(Suppl)
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Amino-acids salt solutions for CO_2 capture from flue gases

Soon Kwan Jeong and **K T Park**
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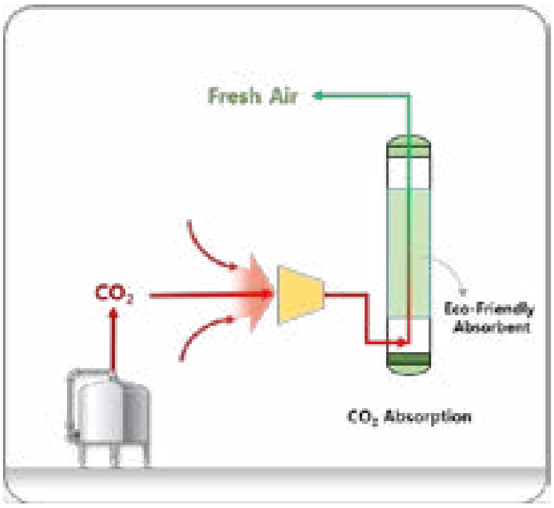
Anthropogenic carbon dioxide (CO_2) is a major greenhouse gas that acts as a blanket to absorb thermal radiation emitted by the earth's surface. Many studies have introduced new technologies for CO_2 capture; however, the quest for feasible capture technologies continues. Amino acid salt solutions have distinguished features such as fast reaction kinetics, high cyclic loading capacity, and good stability towards oxygen, low vapor pressure and biodegradable property. In this study, the CO_2 absorption capacity, absorption rate and heat of absorption of the aqueous potassium salts of amino acids were investigated using semi-batch absorption system, wetted wall column and a differential reaction calorimeter (DRC). The results were compared to amine solvents. The CO_2 loading capacity of amino-acids salts solutions showed higher than that of amine solutions. The CO_2 loading capacities were found to be 0.50 and 0.68 mol of CO_2/mol of solvent for aqueous MEA and potassium salt of L-alanine at 298 K, respectively. The heat of regeneration depends on the heat of absorption as well as sensible heat and latent heat. Therefore, the heat of absorption can be used as useful data for the continuous process. MEA and DEA showed 81.77 kJ/mol of CO_2 and 67.06 kJ/mol of CO_2, respectively. Among the amino-acids slats solutions, potassium salt of L-alanine showed the lowest heat of absorption of 53.26 kJ/mol CO_2. Amino-acids salts solutions had the higher CO_2 loading capacity and lower heat of absorption than those of MEA. Therefore, amino-acids salts solutions are deemed to be the potential CO_2 absorbent to replace the existing system.



Biography

Soon Kwan Jeong received BS degree in Chemical Engineering and PhD degree in Chemical Engineering both from Korea University, South Korea, in 1993 and 2000, respectively. From 1992 to 1994, he was a Researcher at Honkook Tire Co., Seoul. From 2005 to 2006, he was a Postdoctoral Fellow with Pratim Biswas at Washington University. He is currently a Principal Researcher at Korea Institute of Energy Research, South Korea. His research interests include “Biomimetics, material science and engineering for CO2 capture and conversion”.

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Susel Del Sol Fernandez et al., Mod Chem Appl 2017, 5:3(Suppl)
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Multifunctional nanoparticles composed of a mixed ferrite core and a mesoporous silica shell for RGD peptide to target alpha (v) beta (3) integrin in cancer therapy and diagnosis

Susel Del Sol Fernandez[1], **Herlys Viltres Cobas**[1], **Ricardo García Salcedo**[1], **Oscar F Odio Chacon**[2] and **Edilso Reguera Ruiz**[1]
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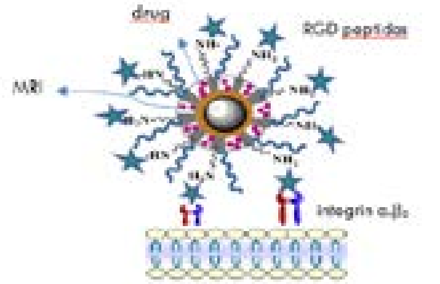
The integrin αvβ3 plays an important role in angiogenesis. It is expressed on tumoral endothelial cells as well as on some tumor cells. RGD peptides are well-known to bind preferentially to the αvβ3 integrin. In this context, targeting tumor cells or tumor vasculature by RGD-based strategies is a promising approach for delivering anticancer drugs or contrast agents for cancer therapy and diagnosis. A key challenge in developing theranostic nano platform is to achieve an optimal pharmacokinetic profile to allow sufficient targeting and to avoid rapid clearance by the reticuloendothelial system (RES). Recently, multifunctional nanostructured materials have been applied to multimodal imaging and simultaneous diagnosis and therapy. In this context, the integration of mesoporous silica with superparamagnetic monodisperse nanocrystals to form uniform core–shell composite particles has great potential for simultaneous bio imaging and drug delivery. In the present study, mixed ferrite ($MnFe_2O_4$) were coated with a mesoporous silica and polyethylene glycol (PEG), making them water soluble and function-extendable for future bio-conjugation with RGD peptide. $MnFe_2O_4$@$mSiO_2$-PEG particles were characterized by DRX, TEM, DLS and VMS. Results showed that a spherical, highly-ordered MnFe2O4 nanoparticles with a diameter of around 10 nm, and a narrow size distribution. Dynamic light scattering (DLS) analysis revealed that such $MnFe_2O_4$@$mSiO_2$-PEG has a hydrodynamic size of ˜20 nm in aqueous solution. The field dependent magnetism of at 300 K shows no hysteresis, demonstrating a superparamagnetic behavior, which is a desirable characteristic for T2 MR contrast agents. The integrated capability of the core–shell NPs to be used as MR and fluorescence imaging agents, along with their potential use as a drug delivery vehicle, make them a novel candidate for future cancer diagnosis and therapy.



Biography

Susel Del Sol Fernandez has expertise in the synthesis and characterization of nanomaterials and Medical Physics. She has completed her Master's degree at Center for Research in Applied Science and Advanced Technology (CICATA), Legaria Unit, National Polytechnic Institute, Mexico City, Mexico. Currently, she is a PhD student at CICATA, Legaria Unit. She worked on the synthesis and characterization of iron oxide nanoparticles (magnetite and mixed ferrites) for delivering anticancer drugs or contrast agents for cancer therapy and diagnosis.

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Elena A Vasileva et al., Mod Chem Appl 2017, 5:3(Suppl)
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Main products of echinochrome A oxidative degradation

Elena A Vasileva, **Natalia P Mishchenko** and **Sergey A Fedoreyev**
G.B. Elyakov Pacific Institute of Bioorganic Chemistry, Russia

In the last decade appeared a large number of publications on the therapeutic effectiveness of echinochrome A and drug preparations based on it, and that arouse the interest in the whole world to search and investigate biologically active quinonoid pigments of sea urchins. Therefore, the study of the chemical properties of echinochrome A, in particular the stability of its solutions, is an urgent task for modern pharmaceuticals. To investigate stability of echinochrome A in aqueous solutions, 200 mg of it was diluted 50-fold with distilled water saturated with atmospheric oxygen (pH 7.2), and was vigorously stirred at room temperature for 48 hours. Echinochrome A was removed from the reaction mixture by extraction with chloroform, its oxidation products were extracted with ethyl acetate and chromatographed on a Toyopearl HW-40 gel in a solvent system 20-50% EtOH containing 0.3% HCOOH. As a result, 7-ethyl-2,2,3,3,5,6,8-heptahydroxy-2,3-dihydro-1,4-naphthoquinone, 2-(carboxycarbonyl)-4-ethyl-3,5,6-trihydroxybenzoic acid, echinolactone A (7-ethyl-5,6-dihydroxy-2,3-dioxo-2,3-dihydrobenzofuran-4-carboxylic acid), 4-ethyl-3,5,6-trihydroxyphthalic acid and 4-ethyl-2-formyl-3,5,6-trihydroxybenzoic acid were isolated. The structures of compounds 2, 3, 5, 6 were established using high-resolution mass spectrometry (HR-ESI-MS) and NMR, and of compound 4–using X-ray crystallography.

Biography

Elena A Vasileva is a Junior Researcher in the Laboratory of Chemistry of Natural Quinonoid Compounds at G. B. Elyakov Pacific Institute of Bioorganic Chemistry, Vladivostok, Russia. She has an experience in identification, isolation and structure elucidation of natural quinonoid compounds from plants, their cell cultures and sea urchins.

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Mohamed O Amin et al., Mod Chem Appl 2017, 5:3(Suppl)
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Novel and versatile solid-state chemiluminescence sensor based on TiO2-Ru(bpy)32+ nanoparticles for pharmaceutical drugs detection

Mohamed O Amin, Entesar Al-Hetlani and **Metwally Madkour**
Kuwait University, Kuwait

This work describes a novel and versatile solid-state sensor for analytes detection using $Ru(bpy)_3^{2+}$-Ce(IV). Herein, we report the synthesis, characterisation, optimisation and application of a new type of hybrid nanoparticles (NPs). Mesoporous TiO_2-$Ru(bpy)_3^{2+}$ NPs were prepared using a modified sol-gel method by incorporating $Ru(bpy)_3^{2+}$ into the initial reaction mixture at various concentrations. The resultant bright orange precipitate was characterised via: TEM, N_2 sorpometry, ICP-OES, Raman and UV-Vis spectroscopy techniques. The concentration of $Ru(bpy)_3^{2+}$ complex in the NPs was quantified and its chemiluminescence (CL) response was compared to the same concentration in the liquid phase using oxalate as model analyte. The results showed that this type of hybrid material exhibited higher CL signal compared to the liquid phase due to enlarged surface area of the hybrid NPs (~149.6 m^2/g). The amount of TiO_2-$Ru(bpy)_3^{2+}$. NPs and the effect of the oxidant flow rate were also investigated to optimize the CL signal. The optimized system was further used to detect oxalate and two pharmaceutical drugs; imipramine and promazine. The linearity of both drugs was in the range of 1-100 pM with limits of detection (LoD) of 0.1 and 0.5 pM, respectively. This approach is considered simple, low cost, facile and can be applied to a wide range of analytes.

Biography

Mohamed O Amin completed his Graduation at Kuwait University and currently pursuing MSc in Medicinal Chemistry.

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Global Chemistry 2017

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Identifying, developing, and moving sustainable communities through application of bioenergy

Abdeen Mustafa Omer
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In the present communication, an attempt had also been made to present an overview of present and future use of biomass as an industrial feedstock for production of fuels, chemicals and other materials. We may conclude from the review paper that biomass technology must be encouraged, promoted, invested, implemented, and demonstrated, not only in urban areas but also in remote rural areas. This article discusses a comprehensive review of energy sources, environment and sustainable development. This includes all the renewable energy technologies, energy efficiency systems, energy conservation scenarios, energy savings and other mitigation measures necessary to reduce climate change.

The study was a step towards achieving this goal. The adoption of green or sustainable approaches to the way in which society is run is seen as an important strategy in finding a solution to the energy problem. The key factors to reducing and controlling CO2, which is the major contributor to global warming, are the use of alternative approaches to energy generation and the exploration of how these alternatives are used today and may be used in the future as green energy sources. Even with modest assumptions about the availability of land, comprehensive fuel-wood farming programmes offer significant energy, economic and environmental benefits. These benefits would be dispersed in rural areas where they are greatly needed and can serve as linkages for further rural economic development. The nations as a whole would benefit from savings in foreign exchange, improved energy security, and socio-economic improvements. With a nine-fold increase in forest – plantation cover, the nation's resource base would be greatly improved.

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DOI: 10.4172/2329-6798-C1-006

Effect of cimetidine on the pharmacokinetics of paracetamol in human subjects

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Statement of the Problem: the recognition of a drug interaction is usually the result of either enhanced or diminished therapeutic effect. This may be from the concomitant administration of another agent, an alteration in physiology or from the effect of diseases.Purpose of the study is to study the effect of *Cimetidine* on the pharmacokinetics of *paracetamol* in human subjects..

Methodology & Theoretical Orientation: The study was divided into two phases. The non-invasive method of estimating drug levels in plasma was used.

Findings: The results of this study have shown that *cimetidine* affected the pharmacokinetics of *paracetamol* in delayed treatments than in concurrent treatment.

Conclusion & Significance: *Cimetidine* has affected the pharmacokinetics of *Paracetamol* which was obvious when it was administered an hour before Paracetamol tablets.The rationale of single dose study here is to observe the profile of the interaction without any disturbance by the multiple regimen. Recommendations are made to administer cimetidine and paracetamol concurrently.

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A novel continuous flow route for the synthesis of phase pure brushite calcium phosphate nanoparticles

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Dicalcium phosphate dehydrate: CaHPO4.2H2O (brushite) nanoparticles (~ 35 nm) were rapidly synthesised using a rapid novel two pump continuous plastic flow synthesis (CPFS) at room temperature (22 °C) in 3 minutes residence time at the conditions of pH 5.5 from aqueous solution of calcium nitrate tetrahydrate and diammonium hydrogen phosphate. The product was collected as a phase pure material with Ca:P molar ratio of 0.8 , without the need for an ageing step. Highly crystalline brushite nanoparticles exhibiting spherical chain like morphology were observed, which had high surface area of 160 m2 g-1. These brushite nanoparticles were also transformed to monetite and calcium pyrophosphates by additional steps such as heat treatments. The final product was physically characterized by using different techniques such as transmission electron microscopy (TEM), BET surface area analysis, X-ray diffraction analysis (XRD), and FTIR spectroscopy. In addition, X-ray photoelectron spectroscopy (XPS) was also used to analyze the chemical structure. The employed system shows promise for the rapid production of high surface area, smaller nanoparticles for use in bone regeneration strategies.

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Influence of biochar on Chinese cabbage (Brassica rapa L.) and wheat (Triticum aestivum L.) seeds germination with Cd(II) in water

Baowei Zhao, Hurynovich Volha and Xiaohong Tang
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The biochars were derived from Gossypium *barbadense* straw, Z. mays straw and pig manure through pyrolysis at temperatures 300˚C and 500˚C under limited oxygen condition. The influences of the biochars on seed germination and early seedling growth of Chinese cabbage (*Brassica rapa L.*) and wheat (*Triticum aestivum L.*) in the aqueous solutions containing Cd(II) were evaluated under laboratory conditions. The research comprised 4 amount rates (0, 0.5%, 1% and 2%/glass) of 6 types of biochars. Cd(II) was added as chloride salt in solution in concentration 10 mg/L. The results of sowing seeds showed that addition of biochar changed such characteristics as pH, electroconductivity (EC), availability of ammonium and Cd(II). It was determined that germination and root length had been decreased with higher amount of biochar, at the same time lower amount showed increase. A large amount of biochar (2%/glass) had negative effect on the root length of *Brassica rapa L.* and *Triticum aestivum L.* while fewer biochar (0.5 g/glass) indicated a better result, increased or no effect. The percentage of germination did not show regularity. Pearson's correlation coefficient showed association between pH and Chinese cabbage germination and root length had weak positive relationship ($0.2 < r > 0.29$), between EC and Cd(II) and root length and germination of both seeds had strong positive relationship ($0.40 < r > 0.69$), another all had no or had negligible relationship ($0 < r > 1.9$).

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Carbon dot - Unique reinforcing filler for polymer with special reference to physico-mechanical properties

Dinesh Kumar Kotnees, P R Sreenath, Seema Singh, M S Satyanarayana and **Prolay Das**
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This work reports the reinforcing efficiency of carbon dots (CDs) in carboxylated acrylonitrile butadiene (XNBR) latex at very low concentration. Amine and carboxyl functionalized CDs have been synthesized from citric acid and glycine. The CDs are covalently conjugated to XNBR latex using 1-(3-dimethylaminopropyl)-3-ethylcarbodiimide hydrochloride (EDC.HCl) and N-hydroxysuccinimide (NHS) as coupling agents. The covalent conjugation of CDs with XNBR latex has been confirmed by Fourier transform infrared spectroscopy (FTIR), dynamic light scattering (DLS) and X-ray photoelectron spectroscopy (XPS). The optical properties of CDs and XNBR-CDs conjugate have been characterized by ultraviolet (UV) - visible, fluorescence spectroscopy, time-resolved fluorescence spectrophotometer and haze meter. The tensile stress-strain properties of XNBR latex dramatically increases by the addition of CDs to XNBR latex. The maximum tensile stress of 2 phr of CDs loaded XNBR latex is nearly 215 % higher than the maximum tensile stress of neat XNBR latex. There is a concomitant decrease in the tan δ peak height and increase in the tan δ peak temperature of XNBR latex with the incorporation of CDs to XNBR latex. In addition, the storage modulus (G') value of sample containing 2 phr of CDs is 161 % higher than the storage modulus value (G') of neat XNBR latex. The onset of degradation temperature (Ti) value of sample containing 4 phr of CDs is 40 C higher than the Ti value of neat XNBR latex. On the other hand, the maximum degradation temperature (Tmax) of XNBR latex containing 1 phr of CDs is 11 C higher than the Tmax value of neat XNBR latex. Morphology of pristine CDs and XNBR-CDs conjugate has been analyzed using transmission electron microscopy (TEM). To the best of our knowledge, this is the first report which analyzes the effect of CDs on the physico-mechanical properties of elastomer contrary to the other novel fillers of carbon family.

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Development of green method for the defluoridation of groundwater

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Engineering of chitosan by praseodymium has been investigated to improve the adsorption properties as well as physical Characteristics of chitosan. Modification of chitosan changes the original properties of chitosan so that it can be more suitable for adsorption of fluoride ions. In this study, chitosan-lanthenoids (Chi- La,Pr,Nd,Ce,Dy, Al, Ba,) was synthesized by impregnation method. The Chi complex was characterized by scanning electron microscopic-energy dispersive X-ray spectroscopy (SEM-EDX), Fourier transform infrared (FTIR) and employed as an adsorbent for removal of fluorides ions from water in the batch system. The variables such as contact time, concentration of Pr, adsorbent dose, initial concentration of fluoride ions, and competitor anions were studied. Preparation low cost green deflourinating technique like preparation soil pot, Tea Bag, Brick use as removal flourine in drinking Water by used of Chitosan complex.

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Nano-$TiCl_2$/cellulose as an eco-friendly and bio-based catalyst for one-pot synthesis of ethyl-2-amino-4-aryl-4H-chromene-3-carboxylate derivatives

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Recently heterogeneous catalysts have attracted paramount importance in many aspects including chemical and energy industries. It is noteworthy to mention that these catalysts are valuable due to their simple handling and storage, easy separation and regenerability. Among these heterogeneous catalysts, polysaccharides especially cellulose has been widely studied as it is the most abundant natural carbon-based biopolymers in the world. It has different fascinating properties including mechanical robustness, biodegradability, hydrophilicity and biocompatibility. Therefore, cellulose has found a wide application in a variety of areas such as pharmacy, agriculture, medical science, industries and so many other related branches.3-5 Also, cellulose susceptible to bond with Lewis acids because of its free OH groups. Hence, with important properties of cellulose in hand and some appealing features of nano-scale materials, chemists can approach to their goal. In recent years, we have been trying to conduct synthetic methodologies under environmentally friendly conditions. In this regard, we have reported convenient procedutres using various efficient nano catalysts.6-8 Based on these achievements and in continuation of our previous experiences, we would like to report nano-TiCl4/cellulose as a bio-based and eco-friendly Lewis acid catalyst for synthesis of ethyl-2-amino-4-aryl-4H-chromene-3-carboxylate derivatives. The catalyst was prepared via reaction of nano-cellulose and TiCl4 in dichloromethane as solvent under room temperature conditions. This catalyst has been characterized by fourier transform infrared spectroscopy, field emission scanning electron microscopy, powder X-ray diffraction, energy dispersive X-ray spectroscopy, X-ray fluorescence techniques, and transmission electron microscopy. Nano-TiCl2/cellulose has been shown to effectively promote multi-component synthesis of ethyl-2-amino-4-aryl-4H-chromene-3-carboxylate derivatives by reaction of aldehydes, resorsinol, and ethylcyanoacetate under ethanol reflux. All prepared compounds were characterized with melting points, 1H NMR and 13C NMR. Simple methodology, an eco-friendly catalyst, a clean procedure, easy work-up, and excellent yields are some of the important advantages of this protocol.

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DBU/H_2O as an efficient, eco-friendly and inexpensive catalyst for trans-esterification and trans-acylation reactions

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Transesterification or alcoholysis reaction in the production of alkyl esters or biodiesel is the process of exchanging alkoxy moiety between two carboxyl groups which is often superior to direct synthesis of esters from carboxylic acids and alcohols. This method especially can applicable for labile and difficult to separate carboxylic acids, polymerization of lactones, the preparation of oils and fats, the curing of alkyd resins in the paint industry, and the preparation of polyesters [1, 2]. There are several available procedures in the literature as catalysts for this reaction [3,4]. However, many of the present methods have drawbacks and disadvantages such as long reaction times, harsh reaction conditions, toxicity and difficulty in product isolation. We recently reported the use of mild Lewis acid for efficient room-temperature transesterification and transacylation reactions [5]. Also, we introduced aqueous organocatalysts for dihydrothiopyran-4-one system conducting parallel competitive MBH and diastereoselective aldol reactions [6]. Based on these achievements and in continuation of our previous experiences, we would like to report here a simple and convenient transesterification and transacylation procedure conducted at room-temperature under DBU/H2O catalysis. These reactions proceed at room temperature in suspension of an ester and alcohol through catalytic quantities of DBU. Completion of the reaction followed by TLC or GC experiments and the structure of the products assigned based on their spectroscopic data.

In summary, we have demonstrated that a very stable and mild reagent which can undergoes rapid reaction under mild and eco-friendly conditions with high yields. The products are directly obtained from the reaction mixtures by evaporation of the volatile portion.

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Chemical constituents from the rhizomes of Curcuma zedoaria and assessment of their biological activities The influence of preparation methods on halloysite nanotubes supported Ni catalysts for hydrogenation of benzene

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Phytochemical investigation of C. zedoaria resulted in the isolation of 21 compounds. Isolated compounds includes eighteen sesquiterpenes and three labdane diterpenes. Various chromatographic techniques were used for the detection and isolation of the compounds. Extensive spectroscopic methods including NMR, IR, UV, GC-MS, LC-MS were used for the identification of the isolated compounds. Isolated compounds were subjected to cytotoxicity, anti-oxidant and neuroprotective assays. Curcumenol and dehydrocurdione showed the highest protection (100%) against hydrogen peroxide induced oxidative stress in NG108-15 cells at the concentrations of 4 and 8 μM, respectively. In the oxygen radical antioxidant capacity assay, zerumbone epoxide showed the highest antioxidant activity with a Trolox equivalent (TE) of 35.41 μM per 100 μg of sample. In the MTT based cytotoxicity assay against four cancer cell lines (Ca 41 Ski, MCF-7, PC-3 and HT-29), curcumenone and curcumenol displayed strong antiproliferative activity (IC50 8.3 and 9.3μg/ml, respectively). A quantum chemical study was performed to investigate their relationship with cytotoxic activity and revealed that the dipole moment (μ), molecular volume (V), molecular area (A), polarizability (α) and hydrophobicity (log P) are the most important descriptors that influence the cytotoxic activity of the compounds under investigation. The two most active compounds; curcumenol and curcumenone were investigated for their binding to human serum albumin (HSA). The spectroflurometric analysis, in conjunction with molecular docking study suggested that both curcumenol and curcumenone could bind to binding sites I and II of HSA with intermediate affinity while site I was the preferred binding site for both molecules.

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Selective hydroformylation of alkyl acrylates using [2,2′-bis(dipyrrolylphosphinooxy)-1,1′-(±)-binaphthyl]/Rh catalyst: reversal of regioselectivity

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Hydroformylation of alkyl acrylate could provide 1,3- and 1,4-bifunctional carbonyl compounds, which could transform to malonic acids, 1,4-dicarboxylic acid, lactones, 2-methyl-1,3-propanediol and 1,4-butanediol. Nevertheless, acrylate was regarded as a kind of less reactive substrate compared with general olefins, and the problem might lies in the formation of thermodynamically stable five- or six-membered rings through the coordination of carbonyl group to the Rh center [1], hence high temperature or high pressure was required. And the hydroformylation generally gave the branched aldehyde as the major product [2]. Hence, it is highly desirable to seek an accessible ligand/Rh system that affords linear aldehyde as the major product with high efficiency due to the wide application of 1,4-bifunctional compounds. Herein, a series of P-N ligands (Fig. 1) were synthesized and applied to Rh-catalyzed hydroformylation of alkyl acrylate. Intriguingly, highly selective hydroformylation of alkyl acrylate could be realized by an accessible ligand 2,2'-bis(dipyrrolylphosphinooxy)-1,1'-(±)-binaphthyl (ligand L1) with the presence of Rh(acac)(CO)2, that is, elevating the temperature to 90 oC, this Rh system could preferentially afford the linear aldehyde with 96.1% regioselectivity, and the TOF could reach up to 9000 h-1. More importantly, the regioselectivity could be readily controlled just through altering the temperature or the pressure, for instance, a high selectivity (> 99%) to branched aldehyde was obtained under 20oC and 2 MPa. In addition, L1/Rh system had benign substrate compatibility. These results enable the L1/Rh system to be a potential candidate for selective hydroformylation of functionalized olefin. Deuterioformylation was conducted to explore the mechanism of regioselectivity reversal, and the results established that the reversible rhodium hydride addition to form the Rh-alkyl species might play a vital role on this reversal. The β-hydride elimination of branched Rh-alkyl species was comparatively stronger than that of linear one under increased temperature, probably because that L1 could cause comparatively larger steric repulsion in branched Rh-alkyl species under high temperature, due to its bulky and rigid binaphthyl backbone characteristics. In turn, the linear Rh-alkyl species progress to linear aldehyde was facilitated.

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Determination of heavy metal (PB) content in mineral water produced in Iran by flameless atomic absorption spectroscopy

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There are some limitations about quantity of heavy metals in food and drugs specially in mineral water. High concentrations of heavy metals in food, drugs and mineral water can cause peripheral neuropathy ,decrease in learning ability and memory ,nephritis, anemia and growth deficiency during a long time. So everybody who drinks mineral water with lead content more than maximum contaminant level is high risk of lead cumulation and chronic toxicity by it. As there is not process control during mineral water production, we decided to assay lead quantity in products of 14 mineral water companies of Iran, by atomic absorption spectroscopy. The maximum average of lead content (0.0935±0.0018 ppm) was found in crystal mineral water and the minimum average of lead content(0.0222±0.00099 ppm) in Sepidan mineral water. Results showed that the mean lead content, in 14 types of mineral water were higher than approvable concentrations(0.0015 ppm) so none of these samples have a satisfactory lead concentration.

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Synthesis, structural characterization and DFT studies of coordination polymers with nitrogen based ligands

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Coordination polymer or Metal-Organic Frameworks (CP/MOFs), which are generally obtained by (self)-assembling of oligonuclear metal clusters (the so-called Secondary Building Units or SBUs), are the subjects of an increasing number of studies due to their interesting properties and promising applications in numerous important fields, such as gas storage, molecular recognition and catalysis.[1] An interesting class of polynucleatingappropriate ligands able to drive the self-assembly of MOFsis represented by N-donor units containing two moieties interconnected by various spacers. Such ligand can afford different lengths, present linear or non-linear geometries and exhibit conformationally rigid or flexible molecular skeletons withan infinite one-(1D), two-(2D) or three-(3D) dimensional framework or periodic nets.[2] Yaghiet al. have successfully developed porous materials (such as metal carboxylate) with controllable shape and size of the cavities.[3] Some of these metal carboxylates appeared to have unusual magnetic properties [4a] while others exhibited high efficiency for gas absorption such as dihydrogen and dinitrogen.

In this context, we have designed, synthesized and characterized new CP/MOFs by treatment ofthe trinuclear core$[Cu_3(\mu\text{-}C_3H_3N_2)3(\mu_3\text{-}OH)(H_3CCOO)_2(C_3H_4N_2)]$ (A) [4b] with different either rigid or flexibleN-donor containing ligands.One of the targeted species, the supramolecule$[Cu_3(4,4'\text{-bipy})(HCOO)(HO)(\mu\text{-}4,4'\text{-bipy})_2(\mu_3\text{-}OH)\ (\mu\text{-pz})3]\infty.nH_2O$ (C), obtained by reaction of SBU with 4,4'-bipyridine (B), consists of a 3D supramolecular material, in which themonomeric unitsare connected bynon-covalent bonds such as π-π stacking intermolecular interactions and/or C-H…π and C-H…O weak contacts.

In this contribution, we will present the fascinating waved channel structural architecture exhibited by these compounds, which are CP/MOFs or supramolecular self-assembly.The aptitude of the dinitrogen ligandtake-upof theseMetal-Organic-Frameworks will be discussed

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Selective TNT fluorescent sensor from benzimidazole-isoquinolinone derivatives

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Three new pyrene-substituted benzimidazole-isoquinolinones which are different in the positions and numbers of the pyrene groups are designed and synthesized via imidation-condensation reaction and Suzuki coupling. The compounds are fully characterized by spectroscopic and spectrometric techniques. Interestingly, these compounds exhibit Aggregation-Induced Emission Enhancement (AIEE) in highly aqueous THF media and selective fluorescent quenching towards trinitrotoluene (TNT). The compound with two pyrene units has the best selectivity towards TNT and has a quenching efficiencies (Ksv) of 60,000 M-1, which leads to the estimation of the detection limit of 0.25 ppm TNT. The sensing mechanism involves the - interaction between the pyrene moieties and electron-poor TNT. In addition, the solid-state sensors are prepared by pipetting a solution of this sensor into 1-cm circular fluid reservoirs patterned by wax-printing technique on a piece of filter paper. The easy-to-use sensor can readily detect TNT in aqueous media by naked-eye observation at the concentration as low as 50 μM. It can also detect TNT vapor in closed chamber within 5 minutes of exposure at room temperature.

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Single particle spectroscopic studies on two-photon photoluminescence of plasmon coupled gold nano triangle dimers

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Surface plasmon resonance (SPR) coupling between adjacent metal nanoparticles in aggregated nanoclusters results in significant enhancements in many optical responses, such as fluorescence, surface enhanced Raman scattering (SERS) and two-photon photoluminescence (2PPL). Here, 2PPL properties of gold nanotriangle (Au NT) dimers with different spatial arrangements have been investigated on single particle level to understand their different plasmon coupling effects on 2PPL enhancement mechanism and explore the limit of maximum achievable enhancement factor.

Compared to NT monomer, scattering spectra of both side-by-side and tip-to-tip coupled NT dimers are red-shifted by 101 nm and 175 nm respectively with strong polarization dependence along their assembly axis, which can be understood in terms of plasmon hybridization theory. A close resemblance between scattering spectra and 2PPL spectra indicated SPR is the origin of observed 2PPL signal. 2PPL intensities of side-by-side and tip-to-tip dimers are enhanced by 1.0×10^3 fold and 2.6×10^4 fold respectively, compared to the NT monomer. Such a huge enhancement in tip-to-tip dimer is a combined effect of plasmon-coupling-induced red-shifted SPR band which has better overlap with the excitation wavelength and giant local electric field amplification due to the presence of sharp tips in interparticle gap. The influence of sharp tips has been further demonstrated by comparing Au NT monomer and dimers with Au nanosphere (NS) monomer and dimer of similar dimensions. The 2PPL intensity of Au NT monomer is 20 times stronger compared to Au NS monomer, where as that of Au NT tip-to-tip dimer is 93.5 times stronger compared to Au NS dimer. All our experimental results show excellent agreement with numerically calculated integrated $|E/E0|4$ results. These findings offer a deeper insight in fundamental understanding of plasmon coupling enhanced 2PPL properties and provide a platform for various sensing and imaging applications.

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The influence of preparation methods on halloysite nanotubes supported Ni catalysts for hydrogenation of benzene

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A series of halloysite nanotubes supported nickel catalysts (Ni-HNT) were prepared using classical (C) and non-classical (NC) methods via impregnation technique. The Ni content was varied between 2-14 wt %. Catalysts were characterized via Atomic Absorption Spectroscopy (AAS). The catalysts prepared via NC methods contained a lower amount of Ni species. Furthermore, electron microscopy images showed that although the Ni species were scattered with some agglomeration in both the C and NC catalysts, the Ni species were more aggregated in the NC catalysts. These occurrences are attributed to the preparation method employed and is related to the mobility of the Ni species during preparation of the catalysts. The surfaces of the catalysts were characterized using Hydrogen Temperature-Programmed Desorption (H_2-TPD), Hydrogen Temperature-Programmed Reduction (H_2-TPR) and H_2 Chemisorption techniques. The H_2-TPR analysis demonstrated the availability of bulk NiO species in the C catalysts while surface oxides were available in the NC catalysts. H_2-chemisorption studies indicated that the total surface area of the Ni active phase in the C catalysts were larger than the NC catalysts. Even so, the H_2-TPD analyses reveal that different active sites were available in the C and NC catalysts. These different active sites influenced the catalytic reactivity of the catalysts. The catalysts prepared using the NC method showed high amounts of H_2 spillover. In addition, the 7.7 wt% Ni-HNT/NC catalysts exhibited additional active sites and the largest amount of desorbed H_2. This resulted in the better catalytic reactivity for the hydrogenation of benzene to cyclohexane when compared to the C catalysts.

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Kinetics and mechanism of Pt(II)-sulfur adduct formation with bio-relevant molecules *in vitro* aqueous medium: Their anticancer activity, DNA binding, drug reservoir property and a theoretical approach

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Synthesis and cytotoxic property of Pt(II)-sulfur adducts are significant in biological aspect. In order to investigate their relevance, two Pt(II) model complexes were considered for detailed study. *In-vitro* kinetics and their mechanism, drug reservoir property of the complexes [Pt(ambim)(H2O)2]X2 1A, [Pt(MAMP)(H2O)2]X2 2A (where, AMBIM= 2-aminomethylbenzimidazole, MAMP = 2-[(N-methylamino)methyl]pyridine and X= NO3- or ClO4-) with sulfur containing bio-molecules DL-methionine (DL-meth), DL-penicillamine (DL-pen) and Glutathione (GSH) were studied to explore the 'drug reservoir' mechanism. The complexes [Pt(ambim)(DL-pen)] 1B, [Pt(ambim)(GSH)] 1C, [Pt(MAMP)(DL-meth)] 2B and [Pt(MAMP)(DL-pen)] 2C were synthesized from complexes 1A and 2A, which was obtained from the hydrolysis of complexes [Pt(ambim)Cl2] and [Pt(MAMP)Cl2] and characterized by spectroscopic methods. Interaction mechanism between the diaqua complexes with S-containing ligands have been established by kinetic study. Two step consecutive reaction rate constants (k1 and k2) and corresponding activation parameters (ΔH and ΔS) for both the steps were calculated and an associative mechanism was proposed. Theoretical investigations like structural optimization, HOMO-LUMO energy calculations, NBO analysis were performed to get an insight into their electronic structure. The coordination mode of the biomolecules via (S, O) were established by spectroscopic methods and confirmed by NBO analysis. DNA binding property of the complexes 2-4 were investigated by UV-Vis spectra, competitive binding experiment, gel electrophoresis and their corresponding binding constants (kb and ksv) were calculated. The computational molecular docking study was carried out for the complexes with B-DNA to confirm their DNA binding mode. Cytotoxic property of the proposed complexes were investigated on HeLa, HepG2 and A549 cell lines. Their corresponding IC50 values were calculated and compared with the well known anticancer drug cisplatin.

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NIR-emitting quinone-fused coumarin dyes: aqueous mediated, catalyst free synthesis and their optical properties

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Water mediated organic synthesis is a fascinating approach in chemistry. We have attempted catalyst free synthesis of thermally stable near infra-red (NIR) emitting quinone fused coumarins with a benzothiazole/benzimidazole acceptor in aqueous medium. The synthesis was attempted using naturally occurring 2-hydroxy-1, 4-naphthoquinone (Lawsone). It is an efficient and environmentally friendly approach for the diversity oriented synthesis of 5, 6-quinone fused 2-pyrone containing compounds. It is a highly productive one pot synthetic method at room temperature that avails commercially accessible materials. In addition, this method has a very short reaction time and milder reaction conditions with an easy separation process. The composition of catalyst free and room temperature condition ensure a green approach towards the excellent practice of the synthetic method. These reactions offer functional NIR emitting fused coumarin compounds extended emission to 810 nm. Structural, spectroscopic and morphological characterization of the material confirms the purity, integrity and future potential materials for high technological applications. Eventually this method gives structurally interesting compounds having optical and pharmacological significance.

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Cross-linked polyacrylamide film as gel polymer electrolyte for rechargeable hybrid aqueous batteries

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Nowadays, rechargeable aqueous lithium-ion batteries (RALB) are attracting an increasing interest. Main challenges faced in conventional Li-ion batteries research are related to safety concerns associated with usage of organic electrolytes, high productions costs as well as overall need for enhancement of physical and electrochemical properties. Replacing of flammable, toxic and expensive organic electrolytes by aqueous has several advantages in ecological and economical point of view. Earlier the system of lithium iron phosphate (LFP) and Zn metal which has promising results have reported [1]. But after numerous cycles on surface of Zn metal occurs dendrites and water loses from system negatively effects on cyclability and capacity of RALB. Therefore, it is interesting to use stable polyacrylamide gel (PAAG) instead of widely used AGM separator. Composite gel polymer electrolytes PAAG for RALB (RALBs) have been prepared by simple ionic polymerization and cross-linking methods and absorbing an aqueous electrolyte solution. Several compositions with different cross-linking degree were investigated. The batteries were assembled from a cathode containing LiFePO4 – a lithium intercalation compound, a zinc metal foil anode and a electrolyte containing Zn2+ and Li+ ions. Stability and morphology of the membranes and an electrolyte uptake and retention properties were tested. The RALBs assembled from gel polymer electrolyte provided high specific discharge capacity, up to 140 mAh (g LiFePO4) at 0.5 C, and the cyclability of such systems was significantly enhanced compared to the RALBs assembled with AGM and liquid electrolytes.

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