Speaker 1: Dr. Radha Kishan Motkuri

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Google scholar:

https://scholar.google.com/citations?user=PACXq2QAAAAJ&hl=en&oi=ao

Dr. Radha Kishan Motkuri, a senior material scientist/ chemical engineer with the PNNL Energy and Environment Directorate. He serves as principal investigator (PI), Co-PI, and project manager in a diverse range of material chemistry and chemical security projects. He has over 20 years of experience in inorganic and material chemistry, emphasizing nanoporous materials such as zeolites, Metal-organic frameworks (MOFs), covalent organic frameworks, and mesoporous silica and hierarchical porous carbons(HPCs) for potential applications including sorption, separation, catalysis, detection, and sensing. Few examples including adsorption cooling/refrigeration, dehumidification, PFAS remediation (sensor-capture-destruction) CO2 capture, water cleaning, Xenon/Krypton separation, polar/non-polar solvents, etc., Recent success of his projects, including a series of cooling technology development projects and PNNL's **2017 R&D 100 Award**-winning thermal vapor-compression cooling technology. Dr. Motkuri has published more than **~95 peer-reviewed publications** (including **12** journal cover articles) with an **h-index of 27**. Also, Dr. Motkuri has **18 international patents,** while NINE of them are USA patents/applications. Dr. Motkuri organized or co-organized several sessions at American Chemical Society (ACS) meetings. He is an active reviewer for many ACS, Wiley, Springer, Elsevier journals and grants like DOE-BES, ARPA-e, ACS-PRF. Dr. Motkuri is an editorial board member for the prestigious inorganic and material journals: "**Inorganic Chemistry** (American Chemical Society)"; "**Inorganic Chimica Acta** (*Elsevier*)" and

"**Scientific Reports** (Nature Publishing Group)" and guest editor for "**Catalysis Today** "(*Elsevier*).

ABSTRACT

Engineering Nanoporous Materials for PFAS Adsorption, Sensing, and Remediation

Per- and polyfluoroalkyl substances (PFAS) are among the most abundant contaminant species that have become ubiquitous in the environment due to uncontrolled industrial and commercial use. Because of their low volatility, high water solubility, and extreme resistance to degradation have made their high concentrations in contaminated sites several orders of magnitude higher than the US EPA health advisory level (HAL) for drinking water. These compounds are linked to a variety of health risks, such as cancer, miscarriage, and liver damage. Contamination has been observed in water samples globally and often at concentrated levels that are several orders of magnitude higher than the US EPA health advisory level due to PFAS' low volatility, high water solubility, and extreme resistance to degradation. Rising global concerns about the public health effects of PFAS exposure motivate the development of strategies for reliable monitoring and effective removal. There is a growing need to reduce global concentrations of accumulated PFAS, especially in drinking water supplies. Traditional sensing techniques have shown inefficiencies such as long measurement times, are labor-intensive, carry high costs, and are limited to ex-situ analysis. We at Pacific Northwest National Laboratory (PNNL) have developed unique PFAS capture and sensing strategies based on improved capture probe technology with an affinity for fluorocarbons, including PFAS. For both sensing and removal, MOF-based capture probes allow for fine-tuning pore size and structure, along with the ability to molecularly tailor the overall framework to target specific PFAS compounds. This tailoring allows for high PFAS sensitivity, selectivity, and faster kinetics. Tunable capture probes with a range of detection sensitivities, embedded within a microfluidic platform design, have allowed us to achieve PFAS detection limits as low as 0.5 ng/L (compared to the U.S. Environmental Protection Agency HAL of 70 ng/L). This research established the molecular-level interactions at the origin of these unique adsorption properties by various experimental tools and molecular simulations.

Speaker 2: Amol D. Sonawane

Post-Doctoral Research Associate, Prof. Ghosh's Research Lab.,
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Biography: Amol received his M.Sc. (Organic Chemistry) degree in 2013 from H.P.T. Arts and R.Y.K. Science College, Nashik (Affiliated to Pune University, India). After master's degree he joined National Chemical Laboratory (NCL) Pune, Maharashtra as project assistant during the period 2013-2015. Further, in 2016 he joined Indian Institute of Science Education and Research (IISER-P) Pune as JRF fellow. He has completed his Ph.D. work in 'Cascade cyclization and photophysical properties of quinoline/ isoquinoline- based heteroacenes' under the supervision of Professor Mamoru Koketsu at Department of Chemistry and Biomolecular Science, Faculty of Engineering, Gifu University, Japan (Oct. 2016 to March 2020). From November 2020, he is working as post-doctoral research fellow with Professor Arun K. Ghosh at Purdue University, west Lafayette, Indiana, USA. His area of interest is synthetic organic chemistry, selenium chemistry and devlopement of new organic methodologies towards drug discovery. Currently, he is engaged in the research area of "design and synthesis of molecules for the treatment of COVID-19 and HIV/AIDS".

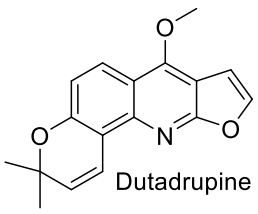
Abstract

Iron-Promoted Intramolecular Cascade Cyclization for the Synthesis of Selenophene-fused, Quinoline-based Heteroacenes

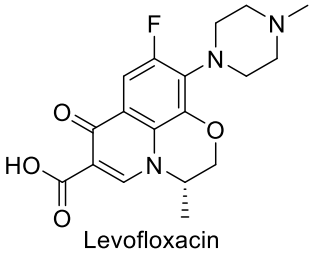
Amol D. Sonawane,[a] and Mamoru Koketsu [a*]

[a]*Department of Chemistry and Biomolecular Science, Faculty of Engineering, Gifu University, Gifu 501-1193 Japan.*

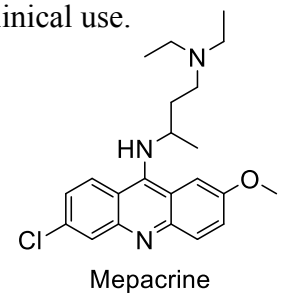
Quinoline nucleus occurs in several natural products (cinchona alkaloids), shows various biological activities such as antihistamine, anti-malerial, anti-bacterial. Some of the quinoline derivatives such as dutadrupine, mepacrine & levofloxacin are in clinical use.



Dutadrupine

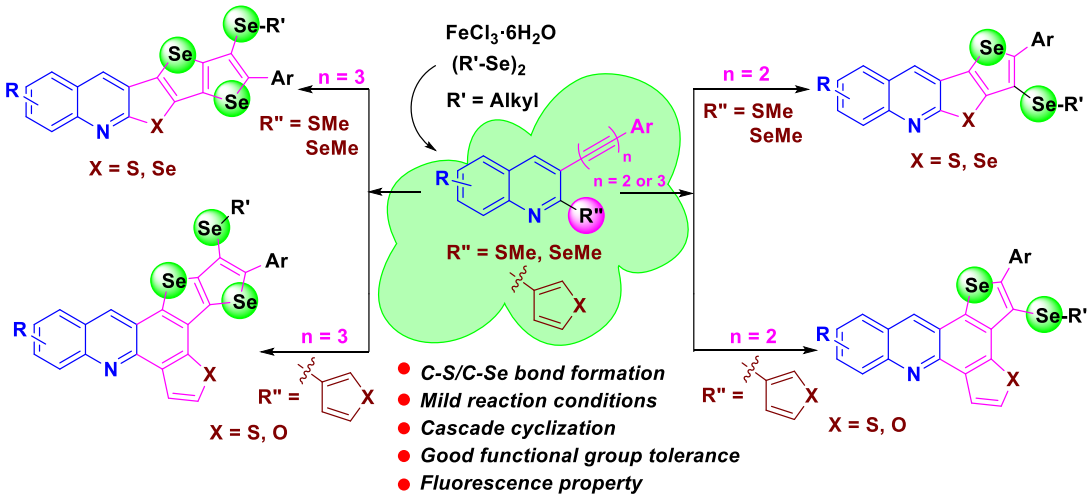


Levofloxacin



Mepacrine

Herein, we report the Fe(III)-promoted linear intramolecular cascade cyclization of 1,3-diyne and 1,3,5-triyne for the construction of selenophene-fused, quinoline-based heteroacene scaffolds. In one step 1,3-diyne and 1,3,5-triyne were cyclized *via* diversified internal nucleophiles by using diorganyl diselenides.



Speaker 3: Drasko Vidovic

Senior Lecturer, School of Chemistry, Monash University, Australia



Biography: Dr Vidovic has undertaken under-graduate studies (BSc) in Canada, before PhD studies in the USA and post-doctoral position in the UK. His first independent research group was established in Singapore before joining Monash as a Senior Lecturer in December 2017. Dr Vidovic is a trained inorganic chemist with the emphasis on green and sustainable catalysis. His main research interests lie in the development of various catalysts based on readily available and inexpensive elements such as aluminium. He became interested in the chemistry of fatty acids, in particular polyunsaturated analogues, when he established a collaborative project with a US based company (Retrotope) focusing on the use of fortified PUFAs as therapeutics for various neurodegenerative diseases.

Abstract

Site-selective deuteration of polyunsaturated fatty acids

Brief abstract: In recent years polyunsaturated fatty acids (PUFAs) that have been deuterated at the bis-allylic position(s) have shown tremendous promise in helping patients with various neurological diseases. However, the availability of these deuterated molecules has been limited to long and laborious total synthesis procedures that are prohibitively expensive. In this seminar, we reveal a one-step catalytic approach that performs, under exceptional kinetic control, site-selective H/D exchange using a wide range of naturally available PUFAs and the least expensive deuterium source (heavy water).

Speaker 4: Lim Seng Joe

Department of Food Sciences, Faculty of Science and Technology, Universiti Kebangsan Malaysia, 43600 UKM Bangi, Selangor, MALAYSIA

Innovation Centre for Confectionery Technology (MANIS), Faculty of Science and Technology, Universiti Kebangsan Malaysia, 43600 UKM Bangi, Selangor, MALAYSIA

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Biography: Seng Joe Lim currently works at the Department of Food Sciences, The National University of Malaysia. He is currently the Head of Innovation Centre for Confectionery Technology. Seng Joe does research in Functional Food Ingredients. Their current projects are 'Edible Bird Nest Hydrolysate', 'Seaweed Polysaccharides', and 'Tropical Fruits Vinegars'.

Abstract

Edible Bird's Nest: A novel Glycoprotein Source

Edible bird's nest (EBN) is the nest produced by swiftlets' saliva secreted from its salivary glands during mating season, to house their hatchlings. The EBNs are harvested after the young swiftlets mature and leave the nests. Interestingly, EBN is made up mainly of sialic acid-rich glycoproteins, making it one of the most expensive animal-based products in the world, which is worth up to USD 5,000 per kg. Glycoproteins are available in various sources, such as milk, eggs, and meat products. However, unlike EBN, the compositions of glycoproteins are usually very low in the other sources, making EBN a novel source of glycoprotein. Our work on EBN started nearly a decade ago, where our focus has been on EBN downstream research. To date, we have produced 3 patents derived from EBN and its products, all of which involved enzymatic technology to produce and recover high-value and bioactive EBN glycopeptides, glycans and sialic acid. These patents have attracted the interests from the EBN industry players, and thus living up to the true objective of downstream research.

Speaker 5: Mihaiela Stuparu

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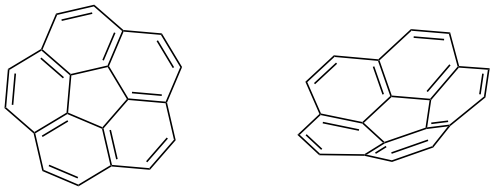


Biography: Mihaiela obtained her doctoral degree from ETH-Zürich. After a one-year postdoctoral stay with Prof. H. K. Hall Jr. at the University of Arizona, Mihaiela returned to Zürich and finished her habilitation work under the mentorship of Prof. J. S. Siegel at the University of Zürich. Since 2014, Mihaiela is a Nanyang Assistant Professor (NAP) at NTU Singapore. She is an Elected Council Member of Singapore National Institute of Chemistry (SNIC), member of the Women Chapter of SNIC, and Chair of the Singapore Chapter of the Royal Society of Chemistry (RSC).

Abstract

Mechanochemical Synthesis of Corannulene Derivatives

Corannulene ($C_{20}H_{10}$) is a polycyclic aromatic hydrocarbon that exhibits molecular curvature due to the arrangement of five six-membered rings around a central five-membered ring (Figure 1). It can, therefore, be considered as the cap region of fullerene C_{60}. This is the reason corannulene is sometime referred to as a 'buckybowl'. The nonplanarity of the structure endows corannulene (and C_{60}) with unique electronic properties that are not found in planar aromatic hydrocarbons such as anthracene and pyrene. In contrast to C_{60}, however, corannulene offers high solubility in common organic solvents and an avenue for multiple and well-defined substitutions on the aromatic nucleus. These two attributes are of high relevance to the synthetic and materials chemists as they allow for synthesis and unambiguous structural characterization of the synthesized materials. In this presentation, we will discuss our synthetic work



relating to mechanochemical synthesis of corannulene and its derivatives.

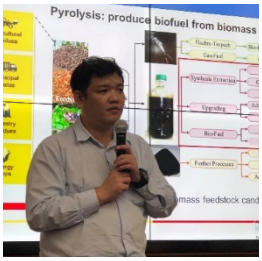
Figure 1. Chemical structure of corannulene.

Speaker 6: Chanatip Samart

Department of Chemistry, Faculty of Science and Technology, Thammasat University, Pathumtani 12120 Thailand

Thammasat University Research Unit in Bioenergy and Catalysis, Thammasat University, Pathumtani 12120 Thailand

E-mail: chanatip@tu.ac.th



Biography: Dr. Chanatip Samart is Assistant Professor in Department of Chemistry, Faculty of Science and Technology, Thammasat University (Thailand). His main research interests is conversion of biomass to chemical and fuel via chemical reaction using heterogeneous catalyst. Currently his research focuses on: Heterogeneous catalyst for biodiesel production from edible and non-edible oil, Chemical from biomass-based such as carbohydrate or xylose, Photovoltaic solar cells and Carbon nanosphere from biomass-based.

Abstract

Green carbon science through valorization biomass waste to energy storage application

Green carbon science proposed the high efficient carbon utilization and recycling for minimize CO_2 emission. Biomass and food waste were discarded in the environment and released the greenhouse gasses during degradation. The utilization of biomass and food waste via carbon recovery was an interesting solution approaching the green carbon science concept. Hydrothermal carbonization is a thermochemical conversion under water vapor for convert organic matter to carbonaceous material without any chemical used. The hydrothermal carbonization have been widely used for pretreatment the biomass or organic waste to enrich carbon contents. Hydrothermal carbonization of xylose (monomer of hemicellulose) and expired fresh milk were presented. The effects of porous formation and composite with metal on electrochemical performance were investigated. Sequential potassium hydroxide (KOH)-phosphoric acid (H_3PO_4) activation was applied to hydrothermal carbon from xylose solution to fabricate controllable porous structure. A uniform porous structure was formed without destruction of the spherical shape with large surface area up to 700 m^2g^{-1}. During activation, H_3PO_4 also reacted with the surface carbon to produce phosphoric acid sites. The excellence specific capacitance and energy density were obtained. The porous carbon was composite with Cu metal during hydrothermal carbonization. The presence of Cu (II)

ions had the Cu ions incorporated with the growth of carbon particles under the hydrothermal condition. Small Cu clusters were distributed along the carbon particles. The presence of Cu enhanced the specific capacitance up to 316.2 F g^{-1} which was higher than the biomass-based carbon electrodes. Hydrothermal carbonization was applied to food waste for sequestration of carbon to minimize the carbon emission. Expired milk was a promising material for the preparation of carbon electrodes for supercapacitors. Natural nitrogen-doped carbon from expired fresh milk was occurred which y the presence of phosphorous and nitrogen functional groups on the carbon surface played significant role to increase the specific capacitance. The specific capacitance of carbon from expired fresh milk was higher than that reported for carbon derived from other forms of organic waste. As our research work in hydrothermal carbonization of biomass waste was not only useful in the view of fabrication carbonaceous material in electrochemical supercapacitor but it also reduced biomass and food waste.

Speaker 7: Menaka Jha,

Institute of Nano Science and Technology (INST), Mohali, Punjab, India



Biography: Dr. Menaka Jha is working as Scientist-D at INST, Mohali, India. She has received her Ph.D. degree from IIT Delhi. Her research interests are based on nanostructured materials and their application to make electronic devices, Low temperature stabilization of boron based materials (b orane, boride and borates) and stabilization of higher oxidation states in binary and ternary metal oxides, Quantum dots based Colloidal nanostructures and their application in making flexible electronic devices, Production and storage of H_2 using nanostructured materials

Abstract

Extraction of nanostructured materials from waste natural products

In the past two decades, lot of efforts have been carried out to develop the synthetic strategies for nanostructured materials synthesis especially with well controlled size, shape, composition and spatial arrangement [1-3]. Also, our world is looking for the suitable techniques to treat waste materials especially domestic and industrial waste [4]. The major hurdle in the waste treatment is cost associated with it. So, in the present meeting, I would like to highlight our group work where we have utilized waste coir fibres for the synthesis of graphene oxide and its derivatives for energy related applications [5]. We have also designed the strategy to extract nanostructured materials from waste product using chemical route. The synthesis of nanostructured ternary metal oxide, metal, graphene, silica, sodium nitrate, and sodium carbonate derived from waste product will be discussed. Ternary metal oxide, Yttria stabilized zirconia (YSZ) nanostructures were synthesized at low temperature by using simple hydrothermal route from waste zircon mineral. The morphology changed has been observed by doping different mole percentage of yttria. The pure zirconia nanoparticles shows spherical shape morphology whereas pure yttria shows flake like structures. The morphology of YSZ nanoparticles in the form of rods and spindle like structures was observed after addition 3 to 8 mol % of yttria. Nanostructured metal,

silica, sodium nitrate, and sodium carbonate have also been extracted from waste using chemical techniques. These nanostructures shows very good photocatalytic and electro-catalytic behavior.

References

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Speaker 8: Dr. Ved Prakash Singh

Associate Professor, Department of Industrial Chemistry, School of Physical sciences, Mizoram University

E-mail: vpsingh@mzu.edu.in



Biography: Dr. Ved Prakash Singh has received his Ph.D from Banaras Hindu University, India and postdoctoral studies from Indian University, USA. His current focus is on drug discovery and is working as associate professor in Department of Industrial Chemistry, School of Physical Sciences, Mizoram University in India. He has published 26 papers in reputed journals, one chapter and one book. He qualified National Eligibility Test (NET) - CSIR. He is BHU-PG entrance all India rank holder in 2003. He also rank holder in 2003 in IIT-Roorkee PG-entrance. He is BHU-Combined Research Entrance Test (CRET) rank holder in entrance test in 2005. He received UGC fellowship from Banaras Hindu University, Varanasi, India. (2005-2008) and senior research fellowship from CSIR, New Delhi, India (2008-2010). He Selected in Chhattisgarh Public Service Commission in Higher education in 2012. He availed Raman fellowship Award to visit USA for one year from 2016-2017. He awarded best Oral presentation award in national Seminar on "conservation and sustainable use of Medicinal and Aromatic plants" in September 2018. Awarded Young Scientist Award in 12th Annual Convention of ABAP & International Conference on "Biodiversity, Environment and Human Health: Innovations and Emerging Trends"BEHIET-2018 in November 2018. He completed two projects funded from UGC and DBT. Now three projects are running funded from CSIR, DBT and ICMR.

Abstract

Drug design, synthesis and study of supramolecular self-assembly of pyridone and dihydropyridone

Synthesized and natural pyridones/pyridines derivatives exhibiting diverse biological activities. A series of dihydropyrimidine (DHPM) derivatives was synthesized, characterized,

and structural analysis is done through SCXRD & Hirshfeld surface analysis. Dihydropyridone is synthesized by the multicomponent condensation reactions (MCRs), followed by three different oxidation methods to synthesize pyridone. The 3-D self-assemblies of both the compounds were determined using the single-crystal X-ray diffraction method. Dihydropyridone products are found as a racemic mixture in synthesis and crystalized as co-crystal. Similar structural conformations are observed in both the compounds but stabilized with different non-covalent interactions. Hirshfeld surface analysis is done to analyze the various intermolecular interactions in both the structure. This study gives the clue of driving force in the self-assembly of molecules in crystal lattices. Further, compounds were docked with Survivin Protein and Kinesin Eg5 protein to analyze the binding affinity with targeted protein and *in vivo* was done to study anti-cancerous activity. Some of the analogues are showing better binding affinity and in *vitro* results revealed that some compounds might be promising anticancer drug candidates for treating different types of cancers, particularly for cancer **of the lung.**

Speaker 9: Albert Fahrenbach

Albert C. Fahrenbach Ph.D., School of Chemistry, University of New South Wales

Anzac Parade, Kensington NSW 2033, Australia

a.fahrenbach@unsw.edu.au



Biography: Albert received his PhD from Northwestern University in Organic Chemistry in 2013 under the mentorship of **Professor Sir Fraser Stoddart** investigating the molecular self-assembly and template-directed syntheses of artificial molecular switches and machines. Albert then moved to Boston to carry out research in origins-of-life chemistry as a postdoctoral scholar with **Professor Jack Szostak** at Harvard University and Massachusetts General Hospital. Thereafter, Albert spent about one and a half years at the Tokyo Institute of Technology with the Earth-Life Science Institute (ELSI) as an Associate Principal Investigator before moving to UNSW as a Lecturer in the School of Chemistry in 2018 where he currently resides.

Abstract

A Radiation-Driven Reaction Network that Generates RNA Precursors

Abiotic reaction networks on early Earth, that produced biologically important molecules like nucleic acids and peptides are hypothesised to have supported life's emergence. Experimental models for these reaction networks are currently undergoing rapid development. In this online seminar, a reaction network[1] that produces known synthetic precursors for ribonucleotides and amino acids will be discussed. This reaction network starts from a briny mixture containing dilute ammonium and phosphate salts in addition to HCN – the only source of carbon. This initial mixture is then made to evolve chemically by a combination of γ-radiolysis and dry-down. No well-timed addition of any other reagents is required. Model reaction networks of this sort can help us understand how important biomolecules like RNA and peptides may have arisen spontaneously, and serve as much needed platforms for better understanding the behavior of complex chemical systems.

[1] Yi, Tran, Ali, Yoda, Adam, Cleaves & Fahrenbach (2020), *Proc. Natl. Acad. Sci. USA* 117, 13267–13274.

Speaker 10: Dr. Ramesh Kataria

Assistant Professor, Department of Chemistry & Centre for Advanced Studies in Chemistry, Panjab University, Chandigarh, India,

E-mail: rkataria@pu.ac.in, katariapu@gmail.com,

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Biography: The research interest of Dr. Kataria is basically to develop the novel cost effective, sensitive, selective and easily available methods for the determination of metals at micro levels using various organic molecules, supramolecules, nanoparticles & Metal-Organic Frameworks (MOFs) as binding agents. As organic molecules, supramolecules, nanoparticles & Metal-Organic Frameworks are functional materials that have applications in water purification, gas absorber and dye degradation. MOFs are polymers formed by coordination between metal ions with polydentate organic linkers, producing extended three-dimensional structures with a porous network that can trap adsorbents. The extent and the availability of the porous network of the MOFs are responsible for their efficacy in devices or sensors. Hence, there is an unmet need to examine the MOF structure and sorption chemistry to complement the structural and morphological information on traditional characterization techniques like Single Crystal X-ray diffraction studies, SEM and TEM etc. I am also interested in reaction between organic compound with the metals and its bindings with new organic compound or existing agents at micro levels, its biological activity of bonded metals, extraction of metals and about concentrate on of constituent metals. Study the same complexes at macro level, elemental analysis, physico-chemical techniques; IR., NMR, UV-visible and thermal analysis.

Abstract

Functionalized gold nanoparticles as versatile sensing materials for heavy metal ions

Heavy metal contamination is becoming a crucial concern to human society due to its prolonged half-life, ability to accumulation to the human body, and non-biodegradability. Moreover, the majority of heavy metal ions are poisonous at low concentrations, and their continuous addition to the human environment through natural and manmade sources causes numerous hazardous health issues. For instance, mercury causes serious damage to human health such as brain

damage, kidney failure, Minamata disease, pink disease, and even death may occur. Excess of cadmium may cause metabolism disorder and renal dysfunctioning. A trace amount of lead can damage the immune and nervous systems, such as the brain and liver, copper is a biologically essential element but an excess concentration of copper may cause cancer and genetic disorders. The chromium oxyanions are highly soluble in water and can easily mobile in groundwater, it can increase the threat of DNA damage and hazard to human health due to their mutagenic and carcinogenic effect on most of the organisms. Hence, the development of reliable and inexpensive materials for the detection of heavy metal ions is a matter of great concern. To solve the above-cited problem, many chemical and optical-based methods have been established for the detection of toxic metals. Among the numerous reported methods, gold nanoparticles derived materials have fascinated great attention predominantly owe to biocompatibility, easiness in synthesis, and versatile tendency in surface functionalization that leads to considerable changes in their chemical/physical properties. The functionalization of gold nanoparticles has empowered speedy and simultaneous detection of metal ions with good accuracy with excellent sensitivity and selectivity. The sharp observation for heavy metal ions detection using AuNPs-functionalized materials can be explained based on inter-particle interactions (aggregation/anti-aggregation) and changes in surface modification.

Keywords: Functionalized gold nanoparticles, heavy metal, anti-aggregation, detection and aggregation

Speaker 11: Yun Yee Low, University of Malaya, Malaysia

Senior Lecturer, Department of Chemistry, Faculty of Science, University of Malaysia, Malaysia



Biography: Dr. Low had received his Ph.D. degree from University of Malaysia in 2012. Currently Dr. Low is working as Senior Lecturer at Department of Chemistry, Faculty of Science at University of Malaysia. His research interests are, Natural Products Chemistry (Natural Products, Alkaloids, Structure Elucidation) , Organic Chemical Synthesis (Biomimetic Partial Synthesis, Electro-organic Synthesis) and Characterization of Molecules (X-ray Crystallography).

Abstract:

Unusual encounters during the structure elucidation of two indole alkaloids (Mersiphylline A and Andransinine).

Structure elucidation of an unknown secondary metabolites involves utilizing wide variety of spectroscopic techniques (UV, IR, 1D and 2D NMR, MS, X-ray, CD, etc.). Chemical transformation will sometimes be carried out to assist in the structure elucidation process. An X-ray diffraction analysis will be the ultimate method in structure elucidation of an unknown compound, in the event if the compound forms suitable crystals. The structure elucidation of the pentacyclic alkaloids, mersiphyllines A and B (from *Kopsia singapurensis*) was assisted by the formation of an alkaloid-borane complex. This alkaloid-borane complex facilitates the determination of the relative configuration at the quaternary centre bearing an acid function. Andransinine, an indole alkaloid derivative obtained during isolation of alkaloids from *Alstonia angustiloba* and *Kopsia pauciflora*, was found to undergo spontaneous resolution when crystallized in ethyl acetate, forming racemic conglomerates. In other solvents (dichloromethane and methanol), andransinine formed a crystalline racemate.

Speaker 12: Ms. Rashim Bawa

University of Delhi, Delhi, India

Phone: +919953407567, E-mail: rashim.bawa@gmail.com



Biography: Ms. Rashim Bawa is pursuing Ph.D. from the Department of Chemistry, University of Delhi under the supervision of Dr. Rakesh Kumar. Her Ph.D. research work is based on design, synthesis and biological evaluation of Nitrogen containing heterocycles

Abstract

Isatin-Triazole Functionalized Rhodamine as a fluorimetric and a colorimetric sensor for Cu2+ and Fe3+ and Its Interaction Studies With Bovine Serum Albumin and Human Hemoglobin

A new isatin-triazole tethered rhodamine based fluorescent probe has been synthesised using click chemistry approach. The synthesized probe **R1** exhibits a selective binding towards Cu^{2+} and Fe^{3+} ions through turn-on fluorescence response. A significant color change from colorless to pink allows the naked eye identification of these metal ions. **R1** formed a 1:2 complex with Cu^{2+} and Fe^{3+} ions with a binding constant 8.0×10^{8} & 2.93×10^{7} M^{-2}, respectively. The binding mode is scrutinized through various spectroscopic techniques and further supported by theoretical calculations. The detection limit of **R1** for Cu^{2+} and Fe^{3+} ions could be determined as 12.2 nm and 0.33 μM, respectively. The probe was also applied in human primary glioblastoma brain cancinoma cells (UT-87) for monitoring of Cu^{2+} ions which further demonstrated its application in biological systems. Also, the bidning interactions between R1 and bovine serum albumin (BSA) or human hemoglobin (HHb) have been examined in aqueous solutions at pH=7.4 using various spectroscopic techniques, molecular docking and molecular dynamics simulation methods. Temperature-dependent fluorescence technique was found to be valuable in assessing the fluorescence quenching mechanism. All the values of the calculated parameters i.e. binding, fluorescence quenching and quenching rate constants suggested static quenching mechanism with moderate binding in both the systems. The thermodynamic parameters implied that the complex formation involves H-bonding and Van der Waals interactions between R1 and the proteins.