27th ISCB International Conference (ISCB-2022)

Research and Innovation in Chemical, Pharmaceutical and Biological Sciences

ABSTRACT BOOK

Date: 16 - 19 November, 2022

Venue: Birla Institute of Technology,
Mesra, Ranchi, India

Jointly Organized by:

Indian Society of Chemists & Biologists (ISCB)
Department of Chemistry, Birla Institute of Technology,
Mesra, Ranchi

Website: www.iscbindia.com, www.iscbconference.com

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Ex-Vice Chancellor,
Gujarat Vidyapeeth, Ahemdabad
President, ISCB

Dr. P.M.S. Chauhan
Ex. Chief Scientist and Professor,
CDRI, Lucknow
General Secretary, ISCB

Message

We are very happy to inform you that the Indian Society of Chemists and Biologists, Lucknow and Department of Chemistry, Birla Institute of Technology, Mesra, Ranchi, India is jointly organising **27th ISCB International Conference (ISCBC-2022)** at Birla Institute of Technology, Mesra, Ranchi, India from 16th – 19th November, 2022.

It is a matter of great pleasure that the focal theme of the 27th International Conference of ISCB on "**Research and Innovation in Chemical, Pharmaceutical and Biological Sciences**". During above conference researcher are going to discuss self-reliance, sustainability & affordability of pharmaceutical substances by improving process chemistry through innovation so that India can be more competitive and self-reliant on Pharma products, drug intermediates & finished formulations. Scientists across the globe, especially from USA, Greece, UK, France, Poland, Slovenia, Belgium, Sweden, Italy and many other countries will participate as keynote/invited speakers to address above mentioned issues. The entire conference will be addressed by more than 80 senior scientists & professors as key-note/invited speaker while it will attract more than 500 young researchers & post-doctoral researchers from entire country who will take part as oral/poster presentations.

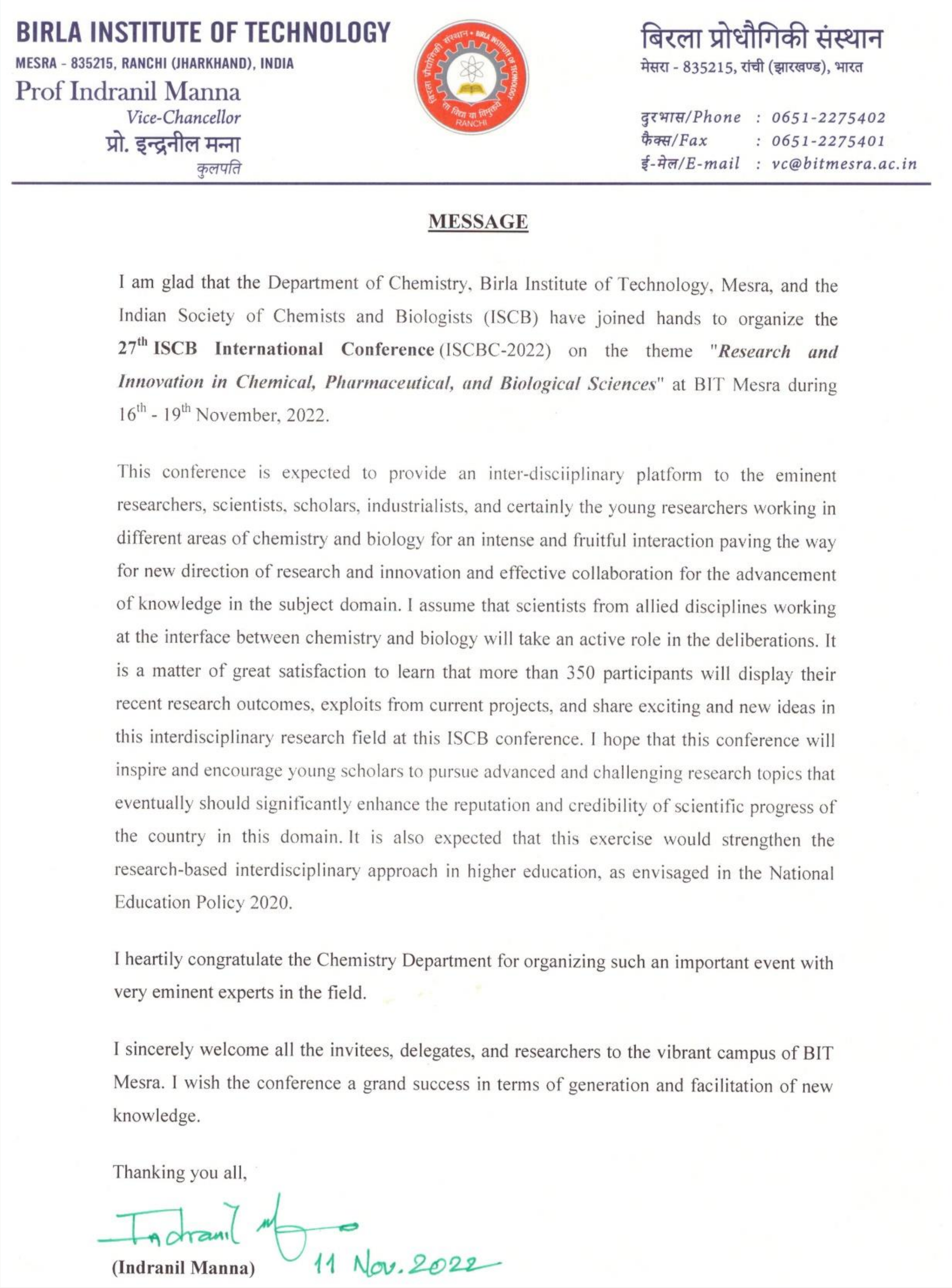
We are glad that the scientific committee is bringing out an abstracts book covering the presentations to be made during ISCBC-2022. Our sincere thanks are due to the members of organizing committee. During this conference a number of eminent scientists and technologists of the country and overseas will be discussing the trends, prospects and future directions of research. We look forward to fruitful deliberations in extremely interesting areas of scientific research. We are happy that an extensive and comprehensive scientific program is arranged. The scientific program beside inaugural function includes 14 plenary lectures, 65 invited lectures and 12 short gun lectures by the eminent scientists from India and abroad. 67 Oral presentations by the young researchers are scheduled. The most heartening feature of the conference is that it is being participated with a number of young scientists and Ph. D. students and presentations are schedules in three poster sessions. On behalf of ISCB we are looking for the galaxy of speakers and young participants who made this conference a memorable event. We extend our warm welcome to all National and International delegates from pharmaceutical companies, research organization, universities and academic institutes wish them very happy stay at Jaipur. Now Finally I take this opportunity to express my sincere thanks and gratitude to members and office bearers of organizing committee of 27th ISCB International Conference (ISCBC-2022).

Anamik Shah

PMSchauhan

(Prof. Anamik Shah)
President, ISCB

(Dr. P.M.S. Chauhan)
General Secretary, ISCB



BIRLA INSTITUTE OF TECHNOLOGY
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Prof Indranil Manna
Vice-Chancellor
प्रो. इन्द्रनील मन्ना
कुलपति

बिरला प्रोधौगिकी संस्थान
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MESSAGE

I am glad that the Department of Chemistry, Birla Institute of Technology, Mesra, and the Indian Society of Chemists and Biologists (ISCB) have joined hands to organize the **27th ISCB International Conference** (ISCBC-2022) on the theme "***Research and Innovation in Chemical, Pharmaceutical, and Biological Sciences***" at BIT Mesra during 16th - 19th November, 2022.

This conference is expected to provide an inter-disciiplinary platform to the eminent researchers, scientists, scholars, industrialists, and certainly the young researchers working in different areas of chemistry and biology for an intense and fruitful interaction paving the way for new direction of research and innovation and effective collaboration for the advancement of knowledge in the subject domain. I assume that scientists from allied disciplines working at the interface between chemistry and biology will take an active role in the deliberations. It is a matter of great satisfaction to learn that more than 350 participants will display their recent research outcomes, exploits from current projects, and share exciting and new ideas in this interdisciplinary research field at this ISCB conference. I hope that this conference will inspire and encourage young scholars to pursue advanced and challenging research topics that eventually should significantly enhance the reputation and credibility of scientific progress of the country in this domain. It is also expected that this exercise would strengthen the research-based interdisciplinary approach in higher education, as envisaged in the National Education Policy 2020.

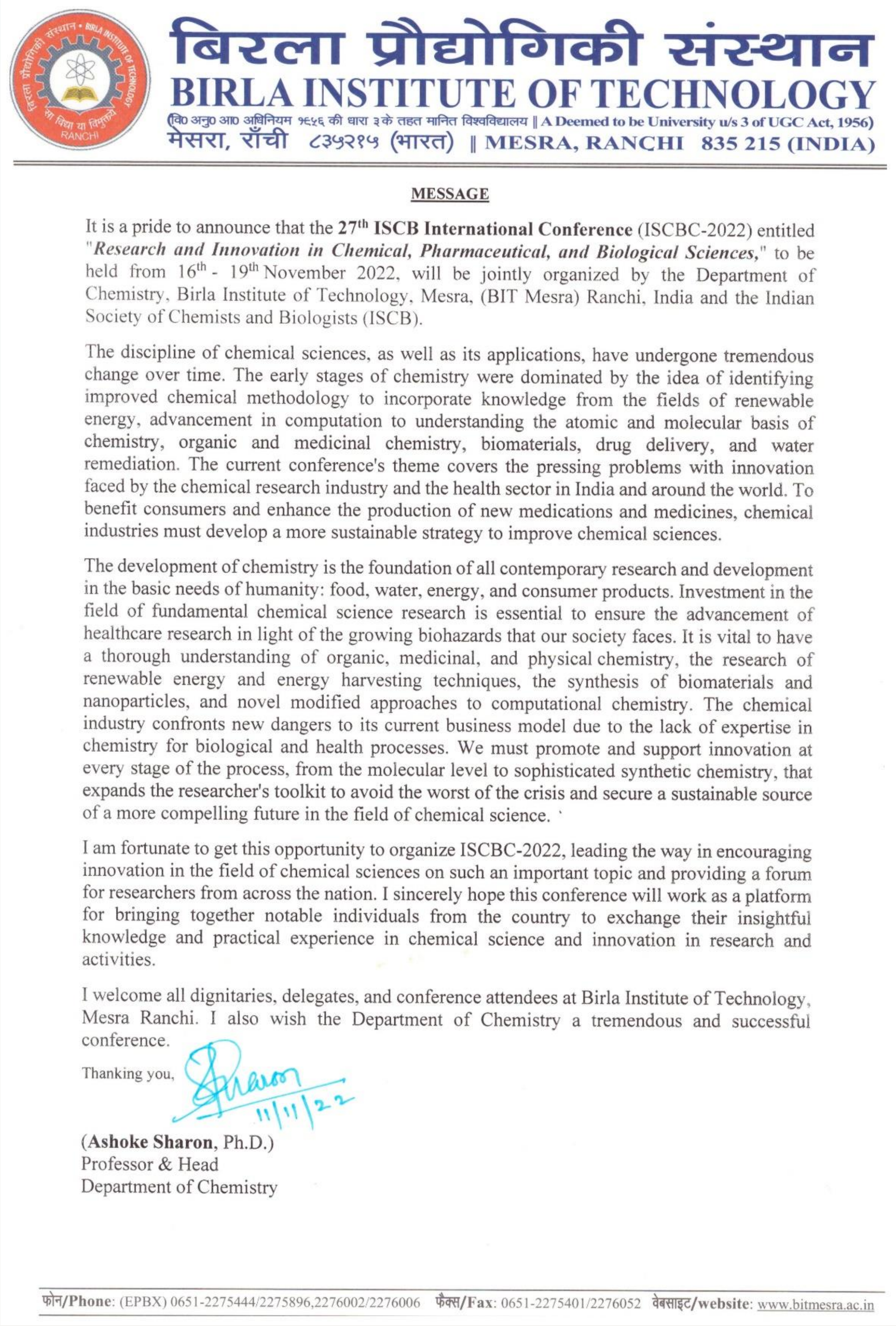
I heartily congratulate the Chemistry Department for organizing such an important event with very eminent experts in the field.

I sincerely welcome all the invitees, delegates, and researchers to the vibrant campus of BIT Mesra. I wish the conference a grand success in terms of generation and facilitation of new knowledge.

Thanking you all,

Indranil

(Indranil Manna) 11 Nov. 2022



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MESSAGE

It is a pride to announce that the 27th **ISCB International Conference** (ISCBC-2022) entitled "***Research and Innovation in Chemical, Pharmaceutical, and Biological Sciences,***" to be held from 16th - 19th November 2022, will be jointly organized by the Department of Chemistry, Birla Institute of Technology, Mesra, (BIT Mesra) Ranchi, India and the Indian Society of Chemists and Biologists (ISCB).

The discipline of chemical sciences, as well as its applications, have undergone tremendous change over time. The early stages of chemistry were dominated by the idea of identifying improved chemical methodology to incorporate knowledge from the fields of renewable energy, advancement in computation to understanding the atomic and molecular basis of chemistry, organic and medicinal chemistry, biomaterials, drug delivery, and water remediation. The current conference's theme covers the pressing problems with innovation faced by the chemical research industry and the health sector in India and around the world. To benefit consumers and enhance the production of new medications and medicines, chemical industries must develop a more sustainable strategy to improve chemical sciences.

The development of chemistry is the foundation of all contemporary research and development in the basic needs of humanity: food, water, energy, and consumer products. Investment in the field of fundamental chemical science research is essential to ensure the advancement of healthcare research in light of the growing biohazards that our society faces. It is vital to have a thorough understanding of organic, medicinal, and physical chemistry, the research of renewable energy and energy harvesting techniques, the synthesis of biomaterials and nanoparticles, and novel modified approaches to computational chemistry. The chemical industry confronts new dangers to its current business model due to the lack of expertise in chemistry for biological and health processes. We must promote and support innovation at every stage of the process, from the molecular level to sophisticated synthetic chemistry, that expands the researcher's toolkit to avoid the worst of the crisis and secure a sustainable source of a more compelling future in the field of chemical science.

I am fortunate to get this opportunity to organize ISCBC-2022, leading the way in encouraging innovation in the field of chemical sciences on such an important topic and providing a forum for researchers from across the nation. I sincerely hope this conference will work as a platform for bringing together notable individuals from the country to exchange their insightful knowledge and practical experience in chemical science and innovation in research and activities.

I welcome all dignitaries, delegates, and conference attendees at Birla Institute of Technology, Mesra Ranchi. I also wish the Department of Chemistry a tremendous and successful conference.

Thanking you,

Sharon
11/11/22

(**Ashoke Sharon**, Ph.D.)
Professor & Head
Department of Chemistry

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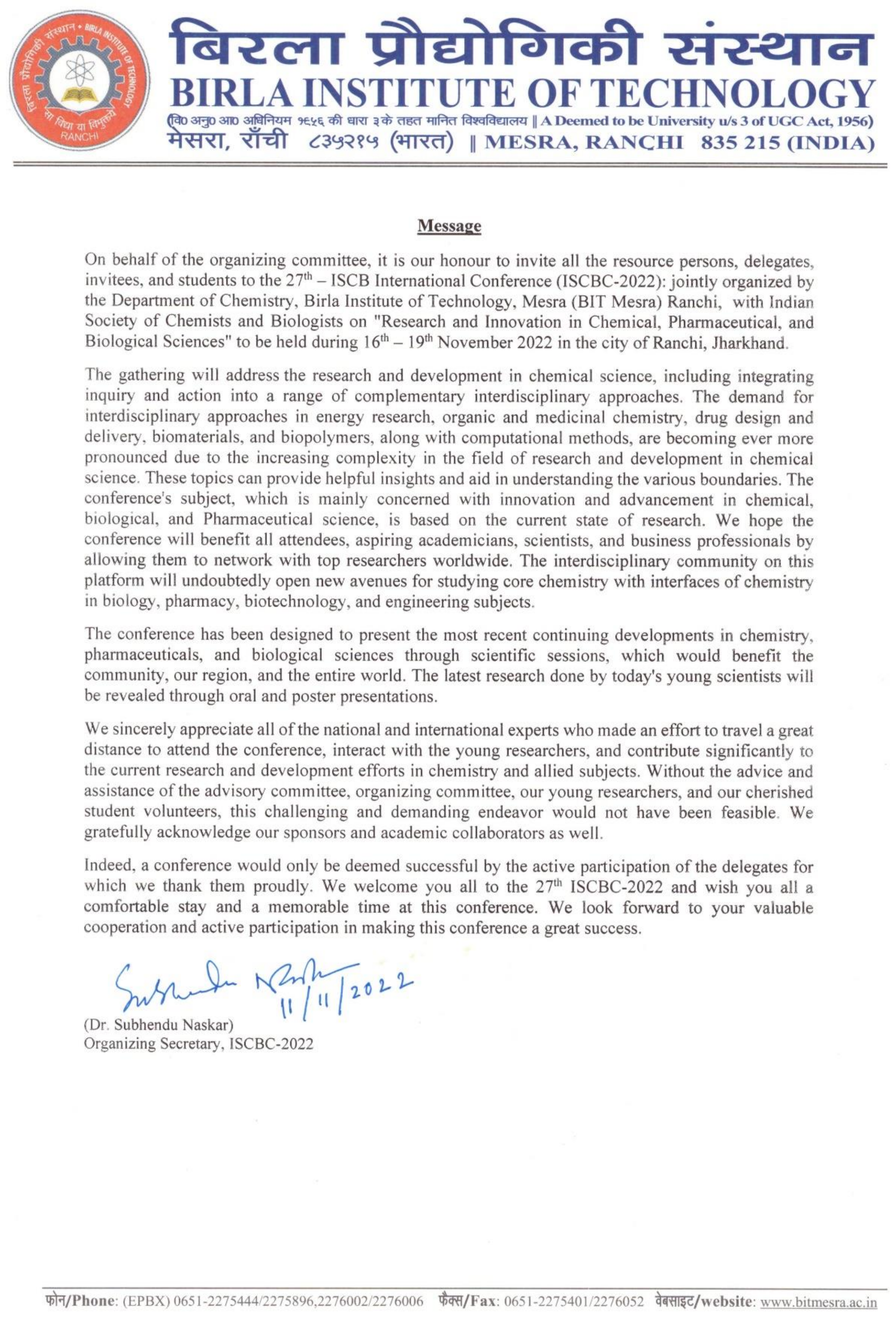

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मेसरा, राँची ८३५२१५ (भारत) || MESRA, RANCHI 835 215 (INDIA)

Message

On behalf of the organizing committee, it is our honour to invite all the resource persons, delegates, invitees, and students to the 27th – ISCB International Conference (ISCBC-2022): jointly organized by the Department of Chemistry, Birla Institute of Technology, Mesra (BIT Mesra) Ranchi, with Indian Society of Chemists and Biologists on "Research and Innovation in Chemical, Pharmaceutical, and Biological Sciences" to be held during 16th – 19th November 2022 in the city of Ranchi, Jharkhand.

The gathering will address the research and development in chemical science, including integrating inquiry and action into a range of complementary interdisciplinary approaches. The demand for interdisciplinary approaches in energy research, organic and medicinal chemistry, drug design and delivery, biomaterials, and biopolymers, along with computational methods, are becoming ever more pronounced due to the increasing complexity in the field of research and development in chemical science. These topics can provide helpful insights and aid in understanding the various boundaries. The conference's subject, which is mainly concerned with innovation and advancement in chemical, biological, and Pharmaceutical science, is based on the current state of research. We hope the conference will benefit all attendees, aspiring academicians, scientists, and business professionals by allowing them to network with top researchers worldwide. The interdisciplinary community on this platform will undoubtedly open new avenues for studying core chemistry with interfaces of chemistry in biology, pharmacy, biotechnology, and engineering subjects.

The conference has been designed to present the most recent continuing developments in chemistry, pharmaceuticals, and biological sciences through scientific sessions, which would benefit the community, our region, and the entire world. The latest research done by today's young scientists will be revealed through oral and poster presentations.

We sincerely appreciate all of the national and international experts who made an effort to travel a great distance to attend the conference, interact with the young researchers, and contribute significantly to the current research and development efforts in chemistry and allied subjects. Without the advice and assistance of the advisory committee, organizing committee, our young researchers, and our cherished student volunteers, this challenging and demanding endeavor would not have been feasible. We gratefully acknowledge our sponsors and academic collaborators as well.

Indeed, a conference would only be deemed successful by the active participation of the delegates for which we thank them proudly. We welcome you all to the 27th ISCBC-2022 and wish you all a comfortable stay and a memorable time at this conference. We look forward to your valuable cooperation and active participation in making this conference a great success.

Subhendu Naskar 11/11/2022

(Dr. Subhendu Naskar)
Organizing Secretary, ISCBC-2022

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SCIENTIFIC PROGRAMME

Wednesday, November 16, 2022	
9.00 AM - 10.00 AM	**Registration**
10.00 AM - 10.30 AM	**Tea Break**
10.30 AM - 12.30 PM	**Inaugural Session with Plenary Talk by Chief Guest**

1.00 PM - 2.15 PM	**Lunch**

Parallel Session – IA (Chairpersons: Prof. Anamik Shah and Dr. P. M. S. Chauhan) Wednesday, Nov 16, 2022	
PL-1 2.20 PM - 2.50 PM	**Keshav Deo** Executive Director, Almelo Private Limited, Hyderabad, India **LifeViroTreat: An innovation for life**
IL-1 2.50 PM - 3.10 PM	**Bimlesh Lochab** Professor, Shiv Nadar University, India **Smartly Designed Materials for Biological Applications**
IL-2 3.10 PM - 3.30 PM	**RameshBabu Boga** BogaR Laboratories LLC, PO Box 1554, Suwanee, GA 30024, USA **Challenges of Antimicrobial Resistance (AMR) and Biofilm control**
IL-3 3.30 PM –3.50 PM	**Abu Salim Mustafa** Department of Microbiology, College of Medicine, Kuwait University, Kuwait **Chemical and Biological characterization of *M. tuberculosis*-specific ESAT6-like proteins and their potentials in prevention of tuberculosis and asthma**
IL-4 3.50 PM – 4.10 PM	**Monika Dwivedi** Department of Pharm. Sci and Technology, BIT Mesra, Ranchi **Stimuli responsive microbubbles for programmed delivery of nanocarriers: Redirecting diagnostic modality for drug delivery**

Parallel Session – IB (Chairpersons: Prof. Mahesh Sharma) Wednesday, Nov 16, 2022	
PL-2 2.30 PM - 3.00 PM	**Shyamal Kumar Chattopadhyay** Professor (HAG), Department of Chemistry, Chairman, SPGC, IIEST, Shibpur, India **Biomimetic catalysis using copper and vanadium complexes**
IL-5 3.00 PM - 3.20 PM	**Indresh Kumar** Associate Professor, Department of Chemistry, BITS Pilani, India **Direct Synthesis of β-(C3)-Functionalized Pyrrole**
IL-6 3.20 PM –3.40 PM	**Hemant Joshi** Department of Chemistry, Birla Institute of Technology and Science, Pilani, Rajasthan, India **Molecular Rotors for Site-selective Organic Transformations**
IL-7 3.40 PM - 4.00 PM	**Devesh M. Sawant** Asst. Professor, Department of Pharmacy, School of Chemical Sciences and Pharmacy, Central University of Rajasthan, Ajmer, India **Pd-Catalyzed Azide-Isocyanide Cross Coupling Reaction: Applications in Medicinal Chemistry and Bioimaging**

Parallel Session – IC (Chairpersons: Prof. Asha Jain) Wednesday, November 16, 2022	
PL-3 2.30 PM - 3.00 PM	**Debashish Haldar** Professor, Chemical Sciences, IISER Kolkata, India **Innovative Materials to Mimic Biology's Adaptive Properties**
IL-8 3.00 PM - 3.20 PM	**Ravindra V. Singh** Director and Head- India R&D, Technology and Innovation, Sigma-Aldrich Chemicals Pvt. Ltd (Merck KGaA, Darmstadt, Germany), India **Artificial Intelligence (AI) powered technologies and innovations in chemistry, transforming every walk of chemist's life**
IL-9 3.20 PM –3.40 PM	**Divya Vohora** Professor, Department of Pharmacology, School of Pharmaceutical Education and Research (SPER), Jamia Hamdard, New Delhi, India **Abstract Awaited**

IL-10 3.40 PM - 4.00 PM	**Satpal Singh Badsara** Assistant Professor, Department of Chemistry University of Rajasthan, Jaipur, Rajasthan, India **Electroorganic Synthesis of Thioethers, Selenoethers and Bis(Indolyl)methanes**
OL-1 4.00 PM - 4.10 PM	**Arpita Roy** Department of Chemistry and Chemical Biology, Indian Institute of Technology (ISM) Dhanbad, India **An Ultra-highly Stretchable, Adhesive Transparent, Flexible, Pressure and Electro sensitive Hydrogel for Motion Sensing**

Poster Session (Chairpersons: Dr. Jaybir Singh and Dr. Animesh Ghosh) Wednesday, Nov 16, 2022	
4.10 PM – 6.00 PM	**Poster Session With High Tea**

6.30 PM – 8.00 PM	**Cultural Programme**
8.00 PM	**Dinner**

Thursday, November 17, 2022

Parallel Session – IIA (Chairpersons: Dr. Manas Ghorai) Thursday, Nov 17, 2022	
IL-11 9.00AM - 9.20 AM	**Amit Kumar** Department of Chemistry, Indian Institute of Technology Patna, Bihar, India **Decoding the Chemistry of Primary Amide/Imidates for Functionalization Reactions**
IL-12 9.20AM - 9.40AM	**Ajay K. Sah** Department of Chemistry, Birla Institute of Technology and Science, Pilani, Pilani Campus, Rajasthan, India **Mo(VI) complexes of N-glycoconjugates and their catalytic application in selective oxidations of organic sulfides**
PL-4 9.40 AM - 10.10 AM	**Amit Basak** INSA Senior Scientist IISER Kolkata, Former Professor, Department of Chemistry, School of Bioscience, IIT Kharagpur, India **Cycloaromatization Reactions: A Perfect Platform for Exploring Design-Synthesis-Reactivity Cascade**
OL-2 10.10AM - 10.20AM	**Gaurav Sheth** Department of Chemistry, Faculty of Science, The M.S. University of Baroda, Vadodara, India **Development of potent and selective Malic enzyme 3 inhibitors for the treatment of pancreatic cancer**
OL-3 10.20 AM–10.30 AM	**Komal M. Vyas** Department of Chemistry, Sardar Patel University, Vallabh Vidyanagar, India ***In Vitro* Evaluation of Cytotoxicity and Anti-Metastatic Properties of Novel Arene Ruthenium(II)-Tetrazolato Compounds on Human Cancer Cell Lines**
OL-4 10.30 AM –10.40AM	**Priya Kumari** Department of Chemistry, Dayalbagh Educational Institute, Dayalbagh, Agra, India **An Insight into Binding of Chrysophanol and Aloe-emodin to G-Quadruplex DNAs (HTel-22 and wHTel-26) using Spectroscopic and Molecular Docking Techniques**
OL-5 10.40AM –10.50AM	**Rafika Yasmin** Department of Molecular Biology and Biotechnology, Tezpur University, Tezpur, Assam, India **Antiplatelet Activity Of An Anticoagulant Pla$_2$ From *Daboia Russelii* Venom**
OL-6 10.50AM –11.00AM	**Asmita Mondal** Department of Chemistry, Durgapur Government College, J. N. Avenue, Durgapur, Paschim Bardhaman, West Bengal, India **Unveiling the synthesis of isoxazolidines from intramolecular [3+2] nitrone cycloadditions in terms of molecular electron density theory**
11.00 AM - 11.10 AM	**Tea-Break**

Parallel Session – IIB (Chairpersons: Dr. Ram Sagar Misra) Thursday, Nov 17, 2022	
IL-13 9.00AM - 9.20 AM	**Dalip Kumar** Department of Chemistry, Birla Institute of Technology and Science, Pilani, India **Efficient syntheses of porphyrin-based photosensitizers for near infrared photodynamic cancer therapy**
IL-14 9.20AM - 9.40AM	**Mukesh Nandave** Associate Professor, Department of Pharmacology, Delhi Pharmaceutical Sciences and Research University (DPSRU), New Delhi, India **Abstract Awaited**
PL-5 9.40 AM - 10.10 AM	**Amalendu Chandra** Dean of Faculty Affairs,Professor of Chemistry, IIT Kanpur, India **Nonlinear vibrational spectroscopy of aqueous surfaces using a combination of classical and quantum methods**
OL-7 10.10AM - 10.20AM	**Ruchita V. Patel** Department of Chemistry, Hemchandracharya North Gujarat University, Patan, India **Synthesis, Characterization and Application of Graphene/Zr Composite Supported on Activated Carbon for Efficient Removal of Fluoride from Drinking Water**
OL-8 10.20 AM–10.30 AM	**Anuvasita Parikh** Department of Chemistry, Birla Institute of Technology and Science, Pilani; Pilani Campus, Rajasthan, India **Hetero-coordination assisted self-assembly of Mo(VI)-glycoconjugate complex into polymeric single-crystal and its catalytic application: a combined experimental and computational studies**

OL-9 10.30 AM –10.40AM	**Amit Shard** Assistant Professor, Department of Medicinal Chemistry, National Institute of Pharmaceutical Education and Research (NIPER), Ahmedabad, India **Development of Imidazopyrimidine-based compounds towards tumor pyruvate kinase-M2 modulation**
OL-10 10.40AM –10.50AM	**Kesur R. Ram** Department of Chemistry, Sardar Patel University, Vallabh Vidyanagar, Gujarat, India **Ultrasound-promoted and [BMIM]BF_4assisted green synthesis of functionalized pyrazolo quinoline core via one-pot multicomponent reaction, DFT study and pharmacological evaluation**
OL-11 10.50AM –11.00AM	**Dheeraj Pandey** Department of Medicinal Chemistry, NIPER-Raebareli, Transit Campus Lucknow, Uttar Pradesh, India **Quinoline based fluorescent chemosensor for selective detection of hydrazine and diethyl cyanophosphonate in aqueous medium**
11.00 AM - 11.10 AM	**Tea-Break**

Parallel Session – IIC (Chairpersons: Dr. Debashish Haldar) Thursday, Nov 17, 2022	
IL-15 9.00AM - 9.20 AM	**Deepak Kumar** School of Pharmaceutical Sciences, Shoolini University, India **Design and synthesis of natural product and heterocyclic compounds for its biological activity**
IL-16 9.20AM - 9.40AM	**Prasanta Ghosh** Dept. of Chemistry, R. K. M. Residential College, Narendrapur, Kolkata, India **Redox Active Fragments and Redox Cascades**
PL-6 9.40 AM - 10.10 AM	**Partha Sarathi Mukherjee** Professor, Inorganic and Physical Chemistry Department,Indian Institute of Science, Bangalore, India **Chemistry in Self-Assemble Molecular Vessels**
OL-12 10.10AM - 10.20AM	**Sreelatha Thonthula** Advanced Research, L'Oréal Research and Innovation India, Bangalore, India **A natural antioxidant for the skin: *Salvianolic acid B enriched Red Sage extract***
OL-13 10.20 AM–10.30 AM	**Subrata Munan** Molecular Sensors and Therapeutics (MST) Research Laboratory, Department of Chemistry, School of Natural Sciences, Shiv Nadar Institution of Eminence deemed to be University, Delhi NCR, India **A unique Ratiometric Fluorescent Probe for Mitochondrial pH Mapping during Mitophagy**
OL-14 10.30 AM –10.40AM	**Sarita Maurya** University of Allahabad, Prayagraj, UP, India **Destabilization of *Staphylococcus aureus* biofilm by DNase/or Tween-80 adsorbed antibiotics loaded solid lipid nanoparticles**
OL-15 10.40AM –10.50AM	**Snehasish Debnath** CSIR-CSMCRI, G. B. Marg, Bhavnagar, India **Towards the Development of a Point-of-Care Diagnostic Kit for Hyperhomocysteinemia: Clinical Validation of Cardiac Patients' Samples**
OL-16 10.50AM –11.00AM	**Dhananjay S. Nipate** Department of Chemistry, Birla Institute of Technology & Science, Pilani, India **Rh(III)-Catalyzed Dehydrogenative Annulation of 2-Arylquinoxalines with Allyl Alcohols: Synthesis of Benzo[*a*]phenazine-6-carboxylic Acids**
11.00 AM - 11.10 AM	**Tea-Break**

Parallel Session – IIIA (Chairpersons: Dr. Keshav Deo) Thursday, Nov 17, 2022	
IL-17 11.10 AM –11.30AM	**Rafique Ul Islam** Professor, Department of Chemistry, School of Physical Sciences, Mahatma Gandhi Central University, India **Metal-nanocomposites: Synthesis and its application in Catalysis**
IL-18 11.30AM - 11.50 AM	**Rajeev Sakhuja** Department of Chemistry, Birla Institute of Technology and Science, Pilani, Rajasthan, India **Metal-Catalyzed Strategies for Fostering Fused Diazaheterocycles as Promising Pharmacophores**

OL-17 11.50AM–12.00	**Taur Prakash Pandurang** Department of Chemistry, Birla Institute of Technology and Science, Pilani, India **Synthesis of Visible Light Triggered Pheophorbide-a Tryptamine Conjugate Photosensitizer for Photodynamic Therapy**
OL-18 12.00PM–12.10PM	**Ankita Tripathi** Department of Chemistry, School of Natural Sciences, Shiv Nadar University, Gautam Buddha Nagar, Uttar Pradesh, India **Deciphering a dissociative path to phosphoryl transfer mechanism catalysed by promiscuous Homoserine Kinase**
OL-19 12.10PM -12.20PM	**Brinda Goda Lakshmi Didugu** Department of Biotechnology, GITAM School of Science, GITAM (Deemed to be University), Visakhapatnam, Andhra Pradesh, India **Posterior silk glands of *Bombyx mori* show decreased levels of polyamines during degradation**
OL-20 12.20PM –12.30PM	**Prashant N. Bavachikar** Biotechnology Laboratory, Andhra Pradesh State Sericulture Research and Development Institute, Kirikera, Hindupur, Andhra Pradesh, India **Impact of heat stress on the development of embryo and its effect on the commercial traits of silkworm *Bombyx mori* L**
OL-21 12.30PM –12.40PM	**Hetal Jebaliya** Department of Chemistry, Marwadi University, Rajkot, India **UPLC is an effective tool for simultaneous analysis of Anxiolytic drugs**
OL-22 12.40 PM 12.50 PM	**Ashok Kumar Acharya** Department of Chemistry, Dr. Shyama Prasad Mukherjee University, Ranchi **Synthesis and characterization of Rare earth Doped Potassium Sodium Niobate for electronic application**
OL-23 12.50 PM - 1.00 PM	**Juhi Rais** Department of Nuclear Medicine, SGPGI, Lucknow **Natural substance as a Tyrosine Kinase Inhibitor (TKI) and its efficacy in Thyroid Cancer**
1.00 PM – 2.15 PM	**Lunch Break**

Parallel Session – IIIB (Chairpersons: Dr. Ashok K Jha) Thursday, Nov 17, 2022	
IL-19 11.10 AM –11.30AM	**Sandeep Chaudhary** Department of Medicinal Chemistry, NIPER, Raebareli **Oxidant-Promoted, Palladium-catalyzed, Regioselective Synthesis of Bioactive Heterocycles via C–H Bond Activation: Chemistry on 1-Aryl-1*H*-indazoles and 2-Aryl-2*H*-indazoles**
IL-20 11.30AM - 11.50 AM	**Sartaj Tabassum** Department of Chemistry Aligarh Muslim University, Aligarh, India **Progress in Metallic Chemotherapeutic Agents, Structural Elucidation, In vivo and In vitro Investigations**
OL-24 11.50AM–12.00	**Amit K. Yadav** Nano-Bio Laboratory, Special Centre for Nanoscience, Jawaharlal Nehru University, New Delhi, India **Fabrication of disposable and sensitive electrochemical biosensor based on (3-Aminopropyl)trimethoxysilane for new cancer biomarkerdetection, sperm protein 17**
OL-25 12.00PM–12.10PM	**Arnab Mukherjee** Nanomaterials Research Lab, Department of Chemistry, Sidho-Kanho-Birsha University, Purulia, India **Wastewater treatment (photodegradation/fluoride removal) via 3D rod-like Fe-Al bimetallic metal-organic-framework prepared through solvothermal route**
OL-26 12.10PM -12.20PM	**Anurup Mukhopadhyay** School of Medical Science and Technology, Indian Institute of Technology Kharagpur, Kharagpur, West Bengal, India **Sticky Hydrophobic Surface Patterning in Synergy with Biochemical Cue Augment Mesenchymal Stem Cells Proliferation, Differentiation, Epithelial Transition, and Curb Senescence**
OL-27 12.20PM –12.30PM	**Umesh Kumar** Catalysis and Bioinorganic Research lab, Department of Chemistry, Deshbandhu College, University of Delhi, New Delhi, India **A novel Ni(II)-thiocyanate complex with functionalized carbon nanotube as efficient catalytic activator for oxygen evolution reaction**

OL-28 12.30PM –12.40PM	**Ayan Gope** Advanced Technology Development Center, Indian Institute of Technology Kharagpur, Kharagpur, West Bengal, India **Honey ghee incorporated double stabilized alginate hydrogel to accomplish regenerative repair of full-thickness cutaneous wounds**
OL-29 12.40 PM- 12.50 PM	**Baban Dey** Department of Chemistry, BIT Mesra, Ranchi, Jharkhand, India **Flexible and freestanding Co (II) based metal-organic framework/ carbon nanofiber hybrid mat for uric acid sensing**
OL-30 12.50 PM- 1.00 PM	**Nilmadhab Roy** Department of Chemistry, Vellore Institute of Technology Tamilnadu, Vellore, India **A Glimpse on Effective Synthetic Strategy for Developing a Variety of Mitochondria Specific Ru(II)/Ir(III)/Re(I)-based Mixed Metallic Luminescent Complexes as Highly Efficient Cancer Therapeutic Agents**
1.00 PM – 2.15 PM	**Lunch Break**

Parallel Session – IIIC (Chairpersons: Dr. Diwan S Rawat) Thursday, Nov 17, 2022	
IL-21 11.10 AM –11.30AM	**Raj Kumar** Department of Pharmaceutical Sciences and Natural products, Central University of Punjab **Design and Synthesis of Quinoline-based Dual Inhibitors of Topoisomerase and Histone Deacetylases as Anticancer Agents**
IL-22 11.30AM - 11.50 AM	**Fateh Veer Singh** Assistant Professor, Chemistry, VIT Chennai, India **Hypervalent Iodine Reagents as key Replacements of Transition Metals in Organic Synthesis**
OL-31 11.50AM–12.00 PM	**Pinky Gupta** Department of Biotechnology, Kalinga University, Raipur, Chhattisgarh, India **A CLINICAL STUDY OF BACTERIAL PATHOGENS FROM HOSPITAL ACQUIRED INFECTIONS IN ANM MEDICAL COLLEGE AND HOSPITAL, GAYA**
OL-32 12.00PM–12.10PM	**Kumari Chandrika** Department of Life Sciences, Central University of Jharkhand, Ranchi, India **SCREENING AND PARTIAL PURIFICATION OF CRUDE BACTERIOCINS**
OL-33 12.10PM -12.20PM	**Sasmita Sabat** Department of Biotechnology, PES University, 100 Feet Ring Road, Banashankari III Stage, Bangalore, India **Influence of Gut Microbiome on Parkinson’s Disease due to the intake of Pesticides using Quorum Sensing Pathway**
OL-34 12.20PM –12.30PM	**Vicky Jain** Department of Chemistry, Marwadi University, Rajkot, India **Development of 1,2-bis(hydroxymethyl)benzo[g]pyrrolo[2,1-a] phthalazine hybrids as potent anticancer agents to small cell lung cancer**
OL-35 12.30PM –12.40PM	**John J. Georrge** Associate Professor & Head, Dept. of Bioinformatics, University of North Bengal, Darjeeling, WB, India **Designing of a novel Curcumin Analog to inhibit MAPK 1 and MAPK 3: A Cheminformatics Approach**
OL-36 12.40 PM - 12.50 PM	**Kiranmayi Patnala** Department of Biotechnology, GITAM School of Science, Visakhapatnam, AP, India **Exploring the role of endophytic fungi in remediating industrially polluted soils using *Catharanthus roseus***
OL-37 12.50 PM – 1.00 PM	**Smita Singh** Department of Chemistry, Birla Institute of Technology, Mesra, Ranchi, Jharkhand, India **Synthesis, Characterization and Environmental applications of a graft copolymer of Guar gum**
1.00 PM – 2.15 PM	**Lunch Break**

Parallel Session – IVA (Chairpersons: Dr. Partha Sarathi Mukherjee) Thursday, Nov 17, 2022	
PL-7 2.20 PM - 2.50 PM	**Abhisek Dey** Professor, School of Chemical Sciences, Indian Association for the Cultivation of Science, Kolkata, India **Bio-inspired Chemistry on Electrodes: Methods to Functional Modelling**
PL-8 2.50 PM - 3.30 PM	**Vinit Kunte** Sr. Customer Support Specialist – ACSI India Pvt. Ltd. **Big data searching using CAS SciFinder Discovery Platform**

IL-23 3.30 PM – 3.50 PM	**Indra Bahadur** Professor in Physical Chemistry, Faculty of Natural and Agricultural Sciences, North-West University, South Africa **Ionic Liquids and Deep Eutectic Solvents as Green Solvent for Separation of Close Boiling Point Mixtures**
OL-38 3.50 PM – 4.00 PM	**Lalji H. Baldaniya** Department of Pharmaceutics, Anand Pharmacy College, Anand, Gujarat, India **EXPLORATION OF FOAM GRANULATION TECHNIQUE FOR PRODUCING FAST DISINTEGRATING TABLETS CONTAINING FLUPIRTINE MALEATE**
OL-39 4.00 PM – 4.10 PM	**Anindita Mukherjee** Department of Chemistry, Birla Institute of Technology Mesra, Ranchi 835215, India. Synthesis and characterization of APTES modified ZnO loaded PVDF composites for energy storage application
4.10 PM - 4.20 PM	**Tea-Break**

Parallel Session – IVB (Chairpersons: Dr. Bimlesh Lochab) Thursday, Nov 17, 2022	
PL-9 2.30 PM - 3.00 PM	**Rakeshwar Bandichhor** Vice President, Dr. Reddy's Laboratories, Hyderabad, India **Process Chemistry Innovation**
IL-24 3.00 PM - 3.20 PM	**Devdutt Chaturvedi** Department of Chemistry, School of Physical Sciences, Mahatma Gandhi Central University, Motihari (East Champaran), Bihar, India **Versatility of hetero-allenes: An easy access for the syntheses of biologically potent scaffolds.**
IL-25 3.20 PM - 3.40 PM	**Debasish Mandal** School of Chemistry and Biochemistry, Thapar Institute of Engineering and Technology, Patiala, Punjab, India **The Role of primary and secondary sphere ligands on the C-H activation reactivity, quantum mechanical tunneling of Fe(IV)O complexes**
OL-40 3.40 PM - 3.50 PM	**Pallavi Singh** Department of Biotechnology, Graphic Era, Dehradun, Uttarakhand, India **Repurposing of Anti Cancerous Drugs against Alzheimers disease for Targeting Tyrosine Kinase receptors**
OL-41 3.50 PM- 4.00 PM	**Prachi Thakur** Department of Chemistry, Birla Institute of Technology, Mesra, Ranchi, India **Modeling studies of Hsp90 inhibitors with subtype selectivity**
OL-42 4.00 PM – 4.10 PM	**Chandana Chintu** Department of Biotechnology, GITAM School of Science, Visakhapatnam, AP, India **Potential of marine fungi to biodegrade oil spillages in the most commonly contaminated sites of Visakhapatnam Port**
4.10 PM - 4.20 PM	**Tea-Break**

Parallel Session – IVC (Chairpersons: Prof. Amit Basak) Thursday, Nov 17, 2022	
PL-10 2.30 PM - 3.00 PM	**Manas K Ghorai** Professor, Department of Chemistry Indian Institute of Technology Kanpur, India **Abstract Awaited**
IL-26 3.00 PM - 3.20 PM	**Diwan S Rawat** Department of Chemistry, Dean Examinations, University of Delhi, Delhi, India **Discovery of Nurr1 agonist and development clinical candidate for the treatment of Parkinson disease**
OL-43 3.20 PM - 3.30 PM	**Shobhana Sharan** Chemistry Department, Ranchi Women's College, Circular Road, Ranchi, Jharkhand **Use of Tropical Peptides for Cosmetic Medicine**
OL-44 3.30 PM - 3.40 PM	**Sunil Pani** KIIT School of Biotechnology, Kalinga Institute of Industrial Technology, Patia, Bhubaneswar-751024 **Does perinatal development of locomotory muscles differ from postural muscles? Implication towards metabolic diseases and muscle defects**
OL-45 3.40 PM - 3.50 PM	**Noopur Pandey** Department of Pharmaceutical Sciences and Technology, Birla Institute of Technology, Mesra, Ranchi, Jharkhand, India. **Tailoring Permeability of Acetazolamide Through Cocrystallization**

OL-46 3.50 PM- 4.00 PM	**Punyadhara Pani** KIIT School of Biotechnology, Kalinga Institute of Industrial Technology, Patia, Bhubaneswar-751024 **Using free-ranging birds as model organism towards identification of targets in the skeletal muscle for countering metabolic diseases**
OL-47 4.00 PM – 4.10 PM	**Vikash Kumar Sonu** Department of Chemistry, Lalit Narayan Mithila University, Darbhanga, Bihar **Interaction of Sulfadiazine with Bioconjugates**
4.10 PM - 4.20 PM	**Tea-Break**

Session – V (Chairpersons: Prof. Venkatesan J.) Thursday, Nov 17, 2022	
IL-27 4.30 PM – 4.40 PM	**Anurag Tiwari** Chemistry Of Heterocyclic Compounds & their Biological Importance **Thermo Fisher Scientific India Pvt. Ltd., Kolkata.**
IL-28 4.40 PM – 4.50 PM	**Mandar Bodas** Solution Consultants, Research Solutions-Life Sciences, Elsevier. **Expediting Research with Accuracy and Confidence**
IL-29 **4.50 PM – 5.00 PM**	**LC-MS in Advance Purification, Separation and Characterization.** Thermo Fisher Scientific India Pvt. Ltd., Kolkata**.**
IL-30 **5.00 PM – 5.10 PM**	**Sandip Jagtap** Labindia Analytical Instruments Pvt. Ltd., Kolkata **Bench Top Non-Cryo NMR in Research**
PL-11 **5.15 PM – 6.00 PM**	**Prof. Samir Kr. Barahmachari** Founder Director, CSIR-IGIB & Former Director General, CSIR **Disruptive Innovation in Healthcare Technologies for India to Pole Vault with Soft Landing: Can BIT Play its Role?**

8.00 PM	**Dinner**

Friday, November 18, 2022

Parallel Session – VIA (Chairpersons: Parthasarathi Das) Friday, Nov 18, 2022	
IL-31 9.00AM - 9.20 AM	**Hardik G. Bhatt** Associate Professor & Head, Dept. of Pharmaceutical Chemistry, Institute of Pharmacy, NIRMA University, Ahmedabad, India **Exploration of THQ Derivatives as Potent mTOR Inhibitors for Lung Cancer**
IL-32 9.20AM - 9.40AM	**Ramendra Pratap Singh** Department of Chemistry, University of Delhi, New Delhi, India **Synthesis of various functionalized carbocycles and heterocycles from cyanomethylarenes**
PL-12 9.40 AM - 10.10 AM	**Tarun Kanti Panda** Professor, Department of Chemistry, IIT Hyderabad, India **Metal and Non-Metal Catalyzed Activation of Organic Nitriles**
OL-48 10.10 AM - 10.20 AM	**Vivek Panwar** Department of Pharmaceutical Sciences, Shoolini University, Solan (HP), India **Overexpressed Kinases (EGFR) as Therapeutic Tool in Targeting Oncogenesis**
OL-49 10.20 AM – 10.30 AM	**Suchanda Dey** Centre for Biotechnology, School of Pharmaceutical Sciences, SOA University), Bhubaneswar, Odisha, India. **Pangenome analysis of ST147 Klebsiella pneumoniae reveals its genome evolution and functional diversity**
OL-50 10.30 AM – 10.40 AM	**Pratigyan Dash** Institute of Life Sciences, DBT-ILS, Bhubaneswar, Odisha, India **Bisphosphonates beyond Osteoporosis: Emergence as an anti-cancer agent and future potential upon nanoencapsulation**
OL-51 10.40 AM – 10.50 AM	**Kumari Neetu Singh** Department of Chemistry, Ranchi Women's college, Ranchi **Polymerization Kinetics and Swelling-Contraction of Acrylate based Hydrogels**
OL-52 10.50 AM – 11.00 AM	**Suman Kumar** Department of Chemistry, Central University of South Bihar, Gaya, Bihar-823001 **Near-IR Plasmonic and Anisotropic Silver Nanocrystals: Zero rpm Synthesis and the Effect of Sequence of Reagent Addition**
11.00 AM - 11.10 AM	**Tea-Break**

Parallel Session – VIB (Chairpersons: Dr. Poulami Roy) Friday, Nov 18, 2022	
IL-33 9.00 AM - 09.30 AM	**Vani Barahmachari** Former Professor, ACBR, Delhi University **Peptide signatures for Cellular function of Proteins.**
IL-34 9.30AM - 9.50 AM	**Lokman H. Choudhury** Professor & Head, Chemistry, IIT Patna, India **Diversity Oriented Synthesis by Multicomponent Cyclization Reactions**
PL-13 9.50 AM - 10.20 AM	**Pradyut Ghosh** Professor, Department of Inorganic Chemistry, IACS, Kolkata **Abstract Awaited**
OL-53 10.20 AM - 10.30 AM	**Reena Bhadani** Department of Chemistry, Ranchi Women's College, Ranchi, Jharkhand, India **Functional 3-D Smart Materials: Properties, absorption investigation, and usage**
OL-54 10.30 AM – 10.40 AM	**Sruthi Swaminathan** Department of Chemistry, Birla Institute of Technology, Mesra, Ranchi, Jharkhand, India **Synthesis and Study of a Novel Graft Copolymer With Mosaic Grafting And Assessment Of Its Suitability Towards Sugarcane Juice Clarification**
OL-55 10.40 AM – 10.50 AM	**Arya C G** Department of Chemistry, NIT Calicut, Kerala **Solvent Effects on Regioselectivity: Sodium Fluoride Catalysed Synthesis of Mono- and Di-Substituted Benzimidazoles**
OL-56 10.50 AM – 11.00 AM	**Siddharth Goswami** Department of Biotechnology, Graphic Era Deemed to be University, Dehradun, Uttarakhand **Design and Development of effective drugs against Histone deacetylases in Alzheimer's disease using Computational Biology tools**
11.00 AM - 11.10 AM	**Tea-Break**

Parallel Session – VIC (Chairpersons: Dr. Raj Kumar) Friday, Nov 18, 2022

IL-35 9.00AM - 9.20 AM	**Dina Nath Singh** Associate Professor, Department of Chemistry, K.S.Saket PG College, Dr. RML Avadh University, Ayodhya, India **Integrated Approach toward the Discovery of Drugs from Medicinal Plants**
IL-36 9.20AM - 9.40AM	**Pankaj Kumar Koli** Assistant Professor, Department of Chemistry, IISER Tirupati, India **Why Intermolecular Nitric Oxide (NO) Transfer? Exploring the Factors and Mechanistic Aspects of NO Transfer Reaction**
IL-37 9.40AM - 10.00AM	**Brajendra K. Singh** Associate Professor, Department of Chemistry, University of Delhi, Delhi 110007, India **Palladium Catalysed Regioselective Monohalogenation of 1-methyl-3-phenylquinoxalin-2(1*H*)-ones via C-H activation under microwave radiations**
OL-57 10.00 AM - 10.10 AM	**Debatrayee Dasgupta** Department of Chemistry, The Maharaja Sayajirao University of Baroda, Vadodara, India **Designing of nano drug delivery system based on polyoxometalates and MCM-48 for poorly soluble drug, Glipizide**
OL-58 10.10 AM – 10.20 AM	**Md. Adnan Khan** Department of Chemistry, Birla Institute of Technology, Mesra, Ranchi, Jharkhand, India **Poly pyridyl based Cobalt complexes as electrocatalysts for water oxidation**
OL-59 10.20 AM – 10.30 AM	**Sahanwaj Khan** Department of Chemistry, Birla Institute of Technology, Mesra, Ranchi, Jharkhand, India **Monomeric RuII complexes with anionic ligand: Electrocatalysts for water splitting reaction**
OL-60 10.30 AM – 10.40 AM	**Madhuram Ayush** Department of Chemistry, Shri Venkateshwara University, Gajraula, Amroha **Green Synthesis, Antimicrobial Activity and Corrosion Inhibition of Divalent Transition Metal Complexes of A Bidentate Amide Ligand**
OL-61 10.40 AM – 10.50 AM	**Shalinee** Department of Chemistry, Faculty of Science, Jai Prakash University, Chapra, Bihar, INDIA **Eco-Friendly Synthesis and Antimicrobial Activity of A Schiff Base Ligand & it's Divalent Transition Metal Complexes**
OL-62 10.50 AM – 11.00 AM	**Archana P K** Department of Chemistry, National Institute of Technology, Calicut **Synthesis, Characterization, Cytotoxicity, and In Vitro Antibacterial Activity of Novel N'(di-2-pyridylmethylene) morpholine-4-thiocarbohydrazide Complex of Manganese**
11.00 AM - 11.10 AM	**Tea-Break**

Parallel Session – VIIA (Chairpersons: Prof. Rafique Ul Islam) Friday, Nov 18, 2022	
IL-38 11.10 AM – 11.30 AM	**Priyankar Paira** Sr. Assistant Professor, Vellore Institute of Technology, Department of Chemistry, School of Advanced Science, Vellore, Tamilnadu, India **Development of Novel Synthetic Approaches for Establishing a variety of Luminescent mono metallic and bimetallic Complexes as Cancer Theranostics**
IL-39 11.30 AM - 11.50 AM	**R. Nagarajaprakash** Centre for Research, Dhanalakshmi Srinivasan University, Samayapuram, Tiruchirapalli, India **Abstract Awaited**
IL-40 11.50 AM – 12.10 PM	**Rakesh Kumar Parashar** Bio-Organic Lab, Department of Chemistry, University of Delhi, New Delhi, India **Synthesis of Isatin and 1,4-Dihydropyridne Scaffolds as Anti-Breast Cancer Agents and Their Applications as Chemosensors**
IL-41 12.10 PM – 12.30 PM	**Poulami Roy** Senior Scientist; CSIR-CMERI, Durgapur, India **Extracting Green Hydrogen as Clean Fuel from Seawater by Electrocatalytic Water Splitting**
OL-63 12.30PM –12.40PM	**Pranati Gupta** Department of Chemistry, Central University of South Bihar, Gaya, India **Zero-rpm synthesis of Hollow Silver Nanocubes with high monodispersity and Near-IR Plasmon Tunability**
OL-64 12.40PM –12.50PM	**Dr. Tasneem Parvin** Department of chemistry, NIT-Patna; **One-pot synthesis of pyrazole fused polyclic heterocycles**

OL-65 12.50PM –1.00PM	**Madhavi Kasa** Bivoltine Silkworm Breeding Laboratory, Andhra Pradesh State Sericulture Research and Development Institute, Kirikera-515 211, Hindupur, AP, India **Spermidine supplementation helps performance of sex-limited breeds of *Bombyx mori* (Lepidoptera: Bombycidae)**
1.00 PM – 2.00 PM	**Lunch Break**

Parallel Session – VIIB (Chairpersons: Dr. Prasoon Kumar Gupta) Friday, Nov 18, 2022	
IL-42 11.10 AM – 11.30 AM	**Arun K Sinha** Pro Vice-Chancellor, Kolhan University, Chaibasa, Jharkhand, India **“Green” and Click-Chemistry Approaches: Opportunity for Simplification and Innovation Towards Step-Economical Synthesis of Natural Polyphenols & Thiophenols-Based Small Molecules of Biological and Commercial Importance**
IL-43 11.30 AM - 11.50 AM	**Ratnesh Das** Professor of Chemistry, Dr. Harisingh Gour University, Sagar (M.P.), India **Nanomaterial a Versatile Innovation as a Electrochemical sensor, Catalyst & Electrode material**
IL-44 11.50 AM – 12.10 PM	**Ravindra Kumar** Senior Scientist, Medicinal and Process Chemistry Division, CSIR-CDRI, Lucknow, India **1,3-Site-Selective Functionalization of Phenols to Multi-functional Arenes via Oxidation-NGP Strategy**
IL-45 12.10 PM – 12.30 PM	**Saranjit Singh** Ex-Professor & Head, Department of Pharmaceutical Analysis, NIPER, Mohali, India **PHARMACEUTICALS IN THE ENVIRONMENT: A problematic requiring attention of chemists, biologists, and pharmaceutical scientists**
IL-46 12.30 PM – 12.50 PM	**Manish Dixit** Sanjay Gandhi Post Graduate Institute of Medical Sciences, Lucknow (SGPGIMS), India **The Role of Radiometal Isotopes: Concept For Theragnostic Radiopharmaceuticals**
IL-47 12.50 PM – 1.00 PM	**Dr. Sumita Hazra** Department of Chemistry, St. Xavier's College, Ranchi, Jharkhand **Ru(II) complexes of anthracene linked pyrazolyl pyridine and benzimidazolyl pyridine: Absorption and Emission spectroscopy**
1.00 PM – 2.00 PM	**Lunch Break**

Parallel Session – VIIC (Chairpersons: Dr. Devdutt Chaturvedi) Friday, November 18, 2022	
IL-48 11.10 AM – 11.30 AM	**Parthasarathi Das** Department of Chemistry and Chemical Biology, Indian Institute of Technology (ISM) Dhanbad, India **Expanding the Medicinal Chemistry Toolbox: From Method Development to Delivery of Drug Like Molecules**
IL-49 11.30 AM - 11.50 AM	**Hitendra M. Patel** Professor, Department of Chemistry, Sardar Patel University, Gujarat, India **one-pot reactions for 2-pyridone and pyrano[2,3-c]pyrazole scaffolds enabling *In-vitro* anti-glioma activity**
IL-50 11.50 AM – 12.10 PM	**Shovan Mondal** Assistant Professor, Department of Chemistry, Syamsundar College, Bardhaman, India **Synthesis of five- and six-membered heterocycles and their bioactivities**
IL-51 12.10 PM – 12.30 PM	**Anand S. Aswar** Department of Chemistry, Sant Gadge Baba Amravati University, Amravati, India **Abstract Awaited**
IL-52 12.30 PM – 12.50 PM	**Amit Rajput** Department of Chemistry, J. C. Bose University of Science & Technology, YMCA, Faridabad **Electronic Structure and Electron Transfer in Transition Metal Complexes with Non-innocent (Redox-active) Ligands**
1.00 PM – 2.00 PM	**Lunch Break**

Short Gun Session – VIII (Chairpersons: Dr. Manas Ghorai and Dr. Ashoke Sharon), Friday, Nov 18, 2022	
SG-1 2.30 PM –2.40 PM	**Dr. Anirban Pradhan** Department of Chemistry, Birla Institute of Technology (BIT) Mesra, Ranchi **Activated porous carbon materials /graphene /nanoribbons synthesis for energy production and storage applications**

SG-2 2.40 PM - 2.50 PM	**Dr. Manas Kumar Panda** Jadavpur University, Kolkata-700032 **Photo-mechanical molecular crystals: a future machinery tool**
SG-3 2.50 PM - 3.00 PM	**Dr. Bishnu P. Biswal** School of Chemical Sciences, NISER, Bhubaneswar, India **Storage and stabilization of biomacromolecules in a nanotubular ionic covalent organic framework**
SG-4 3.00 PM - 3.10 PM	**Dr. Alok Jain** Department of Bioengineering and Biotechnology, BIT Mesra, Ranchi, India **A riveting combination of various computational approaches to design, optimize and predict the bioactivity of highly selective and potent PKM2 modulators**
SG-5. 3.10 PM - 3.20 PM	**Dr. Binitendra Naath Mongal** School of Engineering and Sciences, GD Goenka University, Gurugram **Cobalt bis(terpyridine) complex as an efficient photosensitiser for photocatalytic hydrogen evolution**
SG-6. 3.20 PM - 3.30 PM	**Dr. Animesh Ghosh** Department of Pharmaceutical Science and Technology, BIT Mesra **Exploring The Application of Pirfenidone-Fumaric acid Cocrystal in Developing a Sustained Release Formulation by Comparative Bioavailability Study: From Bench-side to Bedside**
SG-7. 3.30 PM - 3.40 PM	**Dr. Madhulika Gupta** IIT (ISM) Dhanbad **Understanding Biomolecular Recognition in Human Interleukin for Therapeutic Intervention**
SG-8. 3.40 PM -3.50 PM	**Sanjay Swain** Central Instrument Facility, BIT Mesra, Ranchi. **Simplified & Affordable Arsenic Filter (SAAF): A solution to prevent arsenic poison**
SG-9. 3.50 PM **-4.00** PM	**Dr. Venkataraman Ganesh** Department of Chemistry, Indian Institute of Technology Kharagpur **Copper-Catalyzed hydroboration of 1,3-Diynes as a Platform for Iterative Functionalization**
SG-10. **4.00** PM **-4.10** PM	**Dr. Tamas Kumar Panda** Vellore Institute of Technology, Vellore **Mechanochemistry: An Opportunity to do Engineering in Metal Organic Frameworks (MOFs)**
SG-11. **4.10** PM **-4.20** PM	**Dr. Naga Rajiv Lakkaniga** Department of Chemistry and Chemical Biology, IIT-ISM, Dhanbad, India 826004 **Discovery of a potent first-in-class inhibitor of Aurora B Kinase for triple negative breast cancer**
SG-12. **4.20** PM **-4.30** PM	**Dr. Anupam Roy** Department of Chemical Engineering, BIT Mesra **Fortification in India: Current trend and future prospect**
4.30 PM -4.40 PM	**Tea-Break**

Parallel Session – IXA (Chairpersons: Dr. Naresh Chandra Bal) Friday, November 18, 2022	
IL-53 **4.40**PM -5.**00**PM	**S. Venkata Mohan** CSIR-Indian Institute of Chemical Technology Hyderabad, India **Abstract Awaited**
IL-54 5.**00**PM -5.**20**PM	**Hitesh D. Patel** Department of Chemistry, Gujarat University, Ahmedabad, India **Pre-Clinical Phase : DSST – In-silico Designing, Synthesis, Screening and Toxicity for NCE**
IL-55 5.**20** PM -5.**40**PM	**Amiya Priyam** Associate Professor, Chemistry, Central University of South Bihar, Gaya, India **Tunable Plasmonic and Luminescent Nanocrystals : Soft Chemical Synthesis and Theranostic and Photocatalytic Applications**
OL-66 **5.40 PM-5.50 PM**	**Sudha Kumari** P. G. Department of Chemistry, V. K. S. University, Ara, Bihar, India **Chalcone Complexes as Anticancer Agents**
OL-67 **5.50 PM-6.00 PM**	**Prerna Srivastava** BIT Mesra, Ranchi **Expression Profile of Differentially Expressed Genes associated with Oral Submucous Fibrosis.**

Parallel Session – IXB (Chairpersons: Dr. R. Bandichhor) Friday, Nov 18, 2022	
IL-56 **4.40**PM -5.**00** PM	**Ashok Kumar Jha** Sai Life Sciences Ltd, Hyderabad **Carbocyclic nucleosides: Search for novel synthetic methodologies**
IL-57 5.00 PM -5.20 PM	**Naresh Chandra Bal** Associate Professor, KIIT School of Biotechnology, Kalinga Institute of Industrial Technology (KIIT), Bhubaneswar, India **Targeting skeletal muscle based NST towards countering metabolic diseases: Identifying mechanisms and molecules**
IL-58 5.**20** PM -5.**40**PM	**Dibyendu Das** Chemistry Sciences, IISER Kolkata, India **Substrate-induced catalyst formation under non-equilibrium conditions**
IL-59 **5.40 PM -6.00PM**	**Pabitra Baran Chatterjee** Central Salt & Marine Chemicals Research Institute, Bhavnagar, Gujarat, India **Abstract Awaited**

Parallel Session – IXC (Chairpersons: Dr. Sandeep Chaudhary) Friday, Nov 18, 2022	
IL-60 **4.40**PM -5.**00** PM	**Sagar Pal** Professor, Department of Chemistry and Chemical Biology Indian Institute of Technology (ISM) Dhanbad **Abstract Awaited**
IL-61 5.**00**PM -5.**20**PM	**Ram Sagar Misra** Professor, School of Physical Sciences, Jawaharlal Nehru University (JNU), New Delhi, India **Stereoselective Synthesis of Natural Product Inspired Glycohydrids as Anticancer Agents**
IL-62 5.**20**PM -5.**40**PM	**Prasoon Kumar Gupta** Principal Scientist, Natural Products & Medicinal Chemistry Division, CSIR – Indian Institute of Integrative Medicine, Canal Road, Jammu, India **High-throughput Identification of Novel Anticancer Molecules from *Roscoea purpurea***
IL-63 **5.40 PM -6.00 PM**	**Brajesh Kumar** HOD Chemistry, Department of Chemistry, TATA College, Chaibasa Jharkhand, India **Catalysis, Sensing and Phytofabrication of metallic nanoparticles: From Green Synthesis to Environmental Remediation**

7.00 PM	**Award Session & Gala Dinner**

Saturday, November 19, 2020

Chairpersons:	**(Chairpersons: Prof. Anamik Shah) Saturday, Nov 19, 2022**
PL-14 9.00 AM – 9.30 AM	**Pratim Kumar Chattaraj** Professor, Department of Chemistry, Indian Institute of Technology, Kharagpur, India **All-metal Aromaticity and Hydrogen Storage**
IL-64 9.30 AM – 9.50 AM	**R. K. Singh** Ex. Vice Chancellor, Sardar Bhagwan Singh University, Balawala Dehradun (Uttarakhand), India **Safety Evaluations of Herbal Preparations in Experimental Animals**
IL-65 9.50 AM – 10.10 AM	**Nivedita Jena** COO, DBT-ILS Bioincubator, Institute of Life Sciences Nalco Square, Bhubaneswar, Odisha **Bioentrepreneurship - Platform beyond business!**
10.15 AM - 11.00 AM	**Valedictory Session and ISCB Scientific Committee Meeting**
11.00 – 11.15 AM	**Tea-Time**
11.15 AM	**Visit and Learn Trip: SPECIAL LAB SESSION** Reaxy by Elsevier (HANDS-ON) NMR Facility (Structure Solution and Analysis) Separation Science Lab High-Performance Chromatography including Flash) Protein Simulation Demonstration (High-Performance Cluster Computing) Computer-Aided Drug Design on Schrodinger
1.30 pm - 2.30 pm	**Lunch**

…………………………………..End of Program…………………………………………..

PLENARY

PL-1

LifeViroTreat: An innovation for life

Dr. Keshav Deo

Executive Director, Almelo Private Limited, Hyderabad, India
Cell: +91 8888657999
E-mail: kdeo35@yahoo.com

Abstract:

The last three pandemic year has seen a major transformation in the area of Anti-viral innovation in pharmaceutical industry worldwide. COVID-19 pandemic is a public health emergency that is causing a stressful and a difficult time for everyone.

Coronavirus Cases: **61.5 Cr**
Deaths: **65.4 L**

What is at stake for India: Today, in India alone, over 4.46 Cr people are COVID-19 infected and over 5.29 lakh people are dead. THEREFORE, TIME IS OF ESSENCE and every day lost is a day resulting in hundreds of thousands being Covid-19 infected, tens of thousands dead due to COVID-19 and consequent huge negative impact on National Economy and job losses.

LiveViroTreat, an inovative medicine to cure viral infection in respiratory system. Kill all strain's of corona virus. An aerosol based medicine, invented in India, is brilliant solution that can bring hope in millions of people worldwide.

PL-2

Biomimetic catalysis using copper and vanadium complexes

Shyamal Kumar Chattopadhyay

Department of Chemistry, Indian Institute of Engineering Science and Technology, Shibpur
Howrah, West Bengal, India-711103

Metallo-enzymes carry out diverse kind of reactions in biology, one of them being catalytic oxidation of substrates. These reactions are carried out under ambient conditions, with high degree of selectivity and specificity. Synthetic chemists very often try to mimic the biological chemistry to produce environmentally benign catalysts of industrial importance. In this lecture we shall discuss few examples of biomimetic oxidation catalysis by copper and vanadium complexes. Vanadium dependent haloperoxidases, like bromoperoxidase, catalyse oxidative bromination of organic compounds using bromide and hydrogen peroxide. Several organobromo compounds are known to possess antimicrobial and medicinal properties making them attractive candidates for pharmaceutical applications. We shall discuss few model complexes of vanadium, showing bromoperoxidase activity, in this lecture. We shall also discuss some model complexes of Cu(II) which show catalytic oxidation of ascorbate acid and catechol oxidase activities.

PL-3

Innovative Materials to Mimic Biology's Adaptive Properties

Debasish Haldar*

Department of Chemical Sciences, Indian Institute of Science Education and Research Kolkata
Mohanpur-741246, West Bengal, India
E-mail: deba_h76@iiserkol.ac.in; deba_h76@yahoo.com

The fabrication of peptide based molecular architectures and nanoarchitectures in high precession, environment friendly and low cost synthesis has drawn significant importance because of their irresistible applications in biology, chemistry, medicine and material sciences.[1] These new methods for the fabrication of sustainable advance functional materials from assembly of molecular building blocks, has appeared as the next generation approach beyond nanotechnology. Generally two distinct schools of thoughts, the “top-down” approach and the “bottom–up” approach have been employed to fabricate molecular architectonics and nanoarchitectonics. The non-covalent interactions such as hydrogen bonding, π-stacking, hydrophobic and van der Waals interactions play very important role to achieve the production of the nanoarchitectures from the recognition and organization of molecular building blocks. In addition, the self-immobilization based on self-assembly and array formation of building blocks results in soft architectures with advance functions.[2] Among all building blocks, amino acids, peptides and peptide mimetics are highly promising owing to their wide structural diversity, self-assembly propensities, biocompatibility and biodegradability. The layer-by-layer assemblies, Langmuir–Blodgett films, nano porous materials, soft rods, nano tubes are some of the best architectures for controllable functions. Moreover, the balance between these non-covalent interactions can tune the shape, size and morphology of the sustainable nanoarchitectures. Artificial enzymes and enzymemimicks are briefly analyzed as examples of biology’s adaptive properties and applications. This presentation mainly focuses on the role of amino acids or small peptides as building blocks to develop sustainable materials (Figure 1).[3] Emphasis will be given on both advantages and limitations. The recent advances and future scope in this area will be discussed briefly.

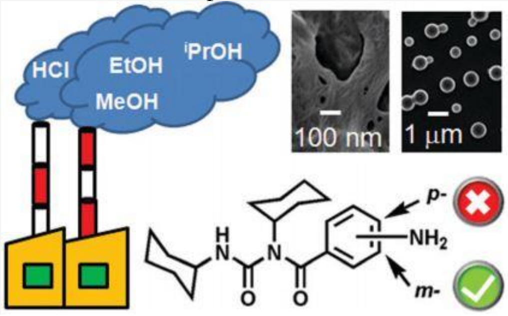

Figure 1. Impact of the isomerism of peptide mimetics on the assembly and properties: quick and onsite gas phase detection of acid and alcohols.

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PL-4

Cycloaromatization Reactions: A Perfect Platform for Exploring Design-Synthesis-Reactivity Cascade

Amit Basak*

Department of Chemical Science, Indian Institute of Science Education and Research, Kolkata
(E-mail: absk@iiserkol.ac.in)

Abstract:

Nature’s molecular engineering expertise continue to inspire chemists involved in research with various molecular architectures. With every passing day, new molecules are isolated from natural sources with diverse structures and reactivity profile which in turn pose new challenges and also at the same time, providing us the way to solve many unresolved burning problems. One such example is the discovery of the enediyne class natural products in the late 1980s showing extraordinary potency against various types of tumours via a diradical based cycloaromatization reaction. Over the last three decades, spectacular advances have been made in the area of synthetic, mechanistic and theoretical chemistry, biology, materials science and finally drug discovery. Currently, two semisynthetic enediyne based antitumour drugs are in the market. This lecture will take a tour on the diverse chemistry of cycloaromatization reactions, especially the enediynes and related systems along with our own efforts in this area.

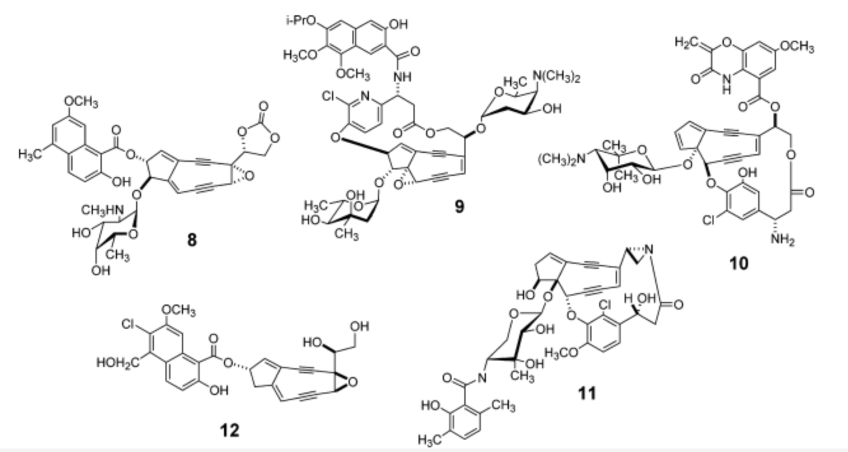

Figure 1: Few examples of Naturally occurring enediynes

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PL-5

Nonlinear vibrational spectroscopy of aqueous surfaces using a combination of classical and quantum methods

Amalendu Chandra

Department of Chemistry
Indian Institute of Technology Kanpur, Uttar Pradesh India 208016

We will discuss our recent studies of nonlinear vibrational spectroscopy of aqueous surfaces using a combination of classical molecular dynamics, ab initio quantum calculations and spectral mapping methods. Specifically, we will present a brief overview of our calculations of one- and two-dimensional surface specific vibrational sum frequency generation spectroscopy of stretch modes of water in the mid-IR region and how our theoretical results compare with available experiments in the literature.

PL-6

Chemistry in Self-Assemble Molecular Vessels

Partha Sarathi Mukherjee*

Inorganic and Physical Chemistry Department, Indian Institute of Science
(Email: psm@iisc.ac.in)

Abstract:

Physical and chemical properties of chemical entities in confined nanospace are expected to be different from their usual bulk properties due to restricted rotational and translational motions. This restricted degree of freedom along with other non-covalent interaction/s may allow to stabilize unusual conformations of compounds in confined nanospace of molecular cavity. Unusual properties of photochromic spiropyrans in water soluble molecular barrels and stabilization of transient merocyanines in such molecular barrels will be discussed.[1-4] Our recent efforts on designing chiral molecular flasks including their chiral recognition will be discussed in my lecture. A recently developed strategy on constructing enantiopure cage (Figure 1) without using chiral donor/acceptor will be highlighted in the lecture.[5-7]

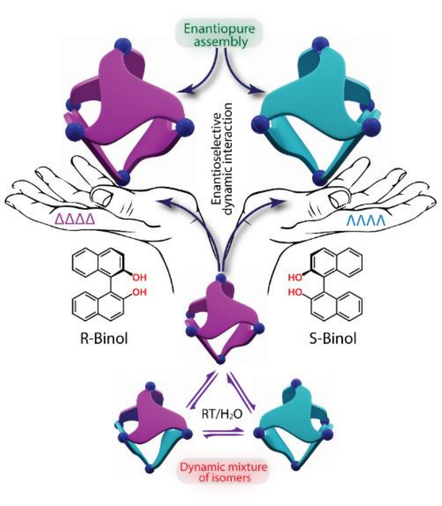

Figure 1 Guest induced enantiopure cage formation.

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PL-7

Bio-inspired Chemistry on Electrodes: Methods to Functional Modelling

Abhishek Dey

School of Chemical Science, Indian Association for the Cultivation of Science, Kolkata, WB, India, 700032
E-mail: abbeyde@gmail.com

One of the major goals of bio-inspired chemistry has been to mimic the function of elegant metallo-enzymes. Such functional modelling has been difficult to attain in solution for reactions that require multiple protons and multiple electrons (nH^+/ne^-). Using a combination of heterogeneous electrochemistry, electrode and molecule design one may control both electron transfer (ET) and proton transfer (PT) of these nH^+/ne^- reactions. In this perspective, the work of this group in creating functional models of hydrogenases ($H^+ + e^-$ à ½ H_2), cytochrome c oxidase ($O_2 + 4e^- + 4H^+$ à $2H_2O$), monooxygenases ($RCH_2 + O_2 + 2e^- + 2H^+$ à $R\text{-}CHOH + H_2O$) and dioxygenases ($S + O_2$ à SO_2; S = organic substrate), which work in aqueous medium and room temperatures, are discussed. In addition, these constructs allow probing unnatural reactions by these constructs and estimation of inner and outer-sphere reorganization energy.

PL-8

Big data searching using CAS SciFinder Discovery Platform

Vinit Kunte

Sr. Customer Support Specialist
ACSI India Pvt. Ltd.

Abstract:

SciFinder-n helps researchers locate latest discoveries and competitive intelligence, empowers them to locatemost relevant, actionable literature advance their research ideas forward. A global network of expert scientist'scurate and aggregate the world's scientific patent and journal content daily and make it fully discoverable throughthe advanced technology contained in SciFinder-n. This ensures researchers have the most current and accurateinformation available quickly supporting their critical research activities. SciFinder-n has access to workflow toolsdesigned to support multiple scientific research functions and requirements. This includes many exciting newfeatures like Biosequence Search, Chemscape Analysis, MethodsNow synthesis etc.

About Presenter:

Vinit is working with American Chemical Society International India Pvt. Ltd. – Representing CAS as a Sr. Customer success specialist, and he is looking after customized trainings of CAS's products training, demos and support. Vinit has completed his M.Sc. Organic chemistry from Mumbai university and PG diploma in Patent Law from NALSAR, Hyderabad. Vinit has total 4 years of industrial experience working in Indian as well as MNC's in Research and development department prior to joining ACS.

PL-9

Process Chemistry Innovation

Rakeshwar Bandichhor

IPDO, Dr. Reddy's Laboratories Limited
Email: rakeshwarb@drreddys.com

Abstract: Chemistry plays key role by being at the epicentre of Pharamecutical Industry. Most of the challenges eventually boil down to chemistry understanding and solution to the problems lies in process chemistry and engineering at scale. Process chemistry innovation provides levers to access IP, lower PMI and lower cost. Needless to mention that manufacturing medicines typically generates a large amount of waste to make unit quantity of API. Minimizing the amount of waste reduces not only disposal costs but also results in more cost-effective production. At a time when resources are becoming sparser and more expensive and the disposal of waste has become more energy demanding, the pharmaceutical industry has started to prioritize more sustainable development of manufacturing processes. This presentation will feature multifactorial strategies to design synthetic route enabling manufacturing process of medicines amenable to scale up.

Keywords: API, Process Chemistry, PMI.

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PL-10

Manas K Ghorai

Professor, Department of Chemistry Indian Institute of Technology Kanpur, India

Abstract Awaited

PL-11

Disruptive Innovation in Healthcare Technologies for India to Pole Vault with Soft Landing: Can BIT Play its Role?

Prof. Samir Kr. Barahmachari

Founder Director, CSIR-IGIB & Former Director General, CSIR

Abstract Awaited

PL-12

Metal and Non-Metal Catalyzed Activation of Organic Nitriles

Suman Das,[a] Jyotirmoy Maity[b] and Tarun K. Panda*[a]

[a]*Department of Chemistry, Indian Institute of Technology Hyderabad, Kandi, Sangareddy 502285. (tpanda@chy.iith.ac.in)*
[b]*Department of Chemistry, St. Stephen's College, University of Delhi, Delhi – 110 007, India.*

Abstract: Nitrile activation is a prominent topic in recent developments in chemistry, especially in organic, inorganic, biological chemistry, as well as in the natural synthesis of products and in the pharmaceutical industry. The activation of nitriles using both metal and non-metal precursors has attracted several researchers, who are exploring newer ways to synthesize novel compounds. Nitrile activation can be achieved by combining various catalytic double hydroelementation reactions, such as hydrosilylation, hydroboration, and hydrogenation of organonitriles using silanes, pinacolborane, and other sources of hydrogen. These methodologies have garnered considerable attention since they are effective in the reduction of organonitriles, whose end products are extensively applied in synthetic organic chemistry. In this presentation, the development of selective hydroborylation, hydrosilylation, dihydroborysilylation, and hydrogenation of organonitriles, as well as their reaction mechanisms and the role of metal complexes in the catalytic cycles will be discussed. Various synthetic methodologies applied toward the reduction of organonitriles into corresponding amines will also be covered.

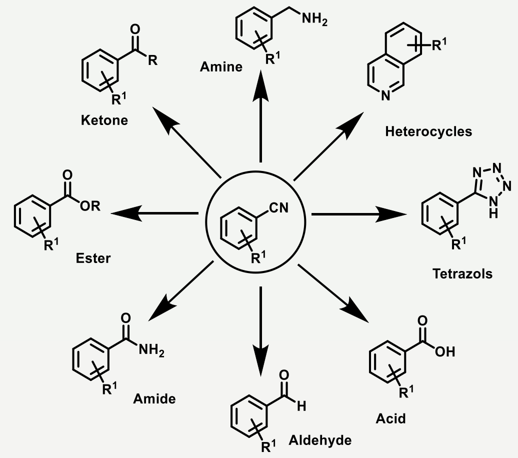

Figure 1: Synthetic application of organic nitriles to various functional groups and structural moieties.

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PL-13

Pradyut Ghosh

Professor, Department of Inorganic Chemistry, IACS, Kolkata

Abstract Awaited

PL-14

All-metal Aromaticity and Hydrogen Storage

Pratim Kumar Chattaraj

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E-mail: pkc@chem.iitkgp.ac.in

Abstract

Several metal clusters exhibit aromatic behaviour. Conceptual density functional theory has been found to be useful in analyzing the behaviour of all- metal aromatic compounds like Al_4^{2-} and all-metal antiaromatic compounds like Al_4^{4-} and their complexes in terms of different global and local reactivity descriptors as well as the nucleus independent chemical shift. Aromaticity and antiaromaticity in cyclic alkali clusters like Na_6 and K_6, polyacene analogues of inorganic ring compounds, multivalent superatoms, trigonal cyclic π- bonded dianions like Be_3^{2-} and Mg_3^{2-} as well as their different sandwich and multi- decker complexes are analyzed in terms of those reactivity descriptors and the associated electronic structure principles. A connection between aromaticity and fluxionality has been explored. Hydrogen has been considered to be an efficient fuel for combating two important problems of the modern age, viz., energy and environment. Storage of hydrogen in a reversible fashion has caused serious impediments. The hydrogen storage ability of these clusters has been explored.

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INVITED

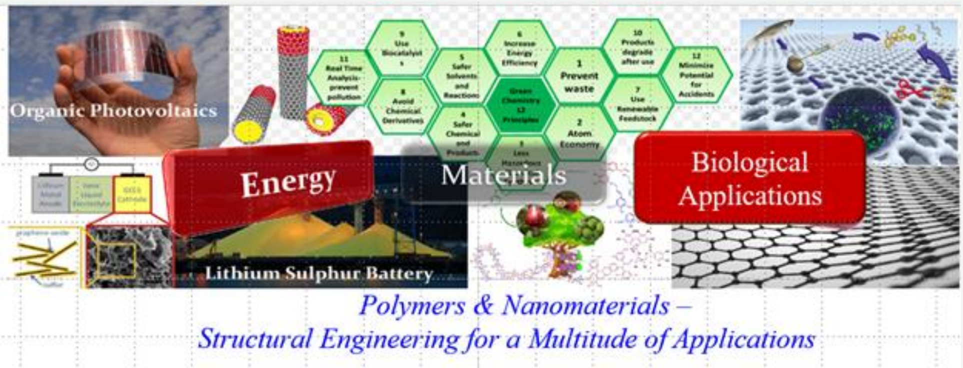
IL-1

Smartly Designed Materials for Biological Applications

Bimlesh Lochab

Materials Chemistry Laboratory, Department of Chemistry, Shiv Nadar Institution of Eminence, Uttar Pradesh
bimlesh.lochab@snu.edu.in

Drug delivery to antibacterial coatings, usage of materials holds great relevance. In particular, nanotherapeutics is most appealing and viable approach to enhance the potential of existing drugs, thereby minimizing the efforts required in designing and synthesizing new drug molecules to counter diseases. Simultaneously, benign approaches to modify and utilize naturally abundant polymer materials gaining advantages in several biological applications. Our lab is extensively working in Materials Chemistry. In this talk, I will discuss our research work in exploration of smartly designed nanoparticles, and few other approaches, synthesized via relatively safer, easier, less-energy intensive protocols and their advancement in biomedical applications.



IL-2

Challenges of Antimicrobial Resistance (AMR) and Biofilm control

RameshBabu Boga, Ph.D.,

BogaR Laboratories LLC, Suwanee, GA 30024, USA;
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Antimicrobial resistance (AMR) is commonly recognized as a global healthcare challenge and estimated to kill ten million people annually by 2050. Apart from mortality, economic hardship is another major concern for AMR and related drug resistance forcing 24 million people into extreme poverty by the year 2030. Therefore, AMR is becoming an alarming threat worldwide in every year and the developed drug resistant super-bugs have no treatment to most with the existing drugs. Several strains of methicillin-resistant *Staphylococcus aureus* (MRSA), multi-drug resistant *Acinetobacter baumannii*, and *tuberculosis* (MDR-TB or XDR-TB), and others have emerged as riskier and already untreatable with available drugs, and new approaches are highly necessitated to discover powerful and smarter drugs.

Developing such AMR and drug resistance has several explanations, and it is time for us to question ourselves that why the AMR is happening at first place, and whether it is caused by human-made or evolutionary development and all together or something else of unknown. Most of the drug-resistant diseases and AMR are due to unnecessary and widespread overuse of antibiotics/drugs, pollution, and other life-style changes by humans including even the cigarette smoke exposure develops significant resistance to the drugs for *S. Aureus.* It is better to recognize such patterns now than the later and the ramifications are severe in the future that either ignored or missed to treat such AMR or drug-resistant diseases. On the other hand, evolutionary development of drug resistance is still murky and there are no clear evidences as such to claim in confidence. However, systematic understanding of epigenetics and evolutionary process could find the clues to selected population where such prevalence of drug resistance and identifies the selection over genotype versus phenotype. Majority of the explanations on AMR are associated with human-made and that could trigger faster pace to influence the evolutionary process.

In order to overcome such AMR and biofilm formation, new approaches of developing antibiotics are essential and robust antibacterial pipeline are necessary with new class of molecules. Further to that promotion of good medical guidelines and avoid excess usage of antibiotics are required to overcome AMR along with stringent regulatory on quality of the marketed drugs. In the presentation, new development of antibacterial(s) that are smarter than the bacteria and minimize the resistance by designing with hybrid functions of drug candidates and recent research efforts overcoming efflux of the drug and other biofilm controlling agents will be discussed.

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IL-3

Chemical and Biological characterization of *M. tuberculosis*-specific ESAT6-like proteins and their potentials in prevention of tuberculosis and asthma

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ESAT6 (6 KDa early secretory antigenic target) is a protein secreted by the bacteria causing tuberculosis, i.e. *Mycobacterium tuberculosis*. It was first detected in the culture filtrates of in vitro grown *M. tuberculosis*. ESAT6 (ESXA) was found to be highly immunogenic in various animal species. Experiments in humans showed that ESXA was recognized by immune cells of tuberculosis patients as well. Furthermore, it was found specific for *M. tuberculosis* and absent in other bacteria, including various mycobacterial species. The gene for ESAT6 contains 288 base pair DNA, which encodes the protein containing 98 amino acids. Another highly immunogenic culture filtrate protein whose gene is linked to ESAT6 is known as CFP10 (ESXB). Because of their high immunogenicity and specificity to *M. tuberculosis*, they been proposed as a vaccine to prevent tuberculosis and diagnosing the disease. However, the same proteins cannot be used for both prevention and diagnosis because the immunized but healthy people will show a positive response and will be falsely reported as diseased. Therefore, the search was made to identify if other ESAT6-like proteins existed in *M. tuberculosis* genome. The search identified 21 additional ESAT-like proteins, i.e. ESXC to ESXW. All of them are low molecular weight proteins containing 90 to 125 amino acids in their sequence, and they are organized in a similar fashion in *M. tuberculosis* genome as ESXA and ESXB. Homology searches did not identify significant sequence identity between ESXA, ESXB and other ESAT-6 like proteins, suggesting that these proteins were similar in organization but different in function. However, immunological characterizations have shown that some of them (especially ESXV) were able to induce strong immune responses in vitro with peripheral white blood cells obtained from tuberculosis patients. Further work with 25-mer overlapping synthetic peptides (synthesized by using Fmoc solid-phase peptide synthesis) showed that multiple epitopes of ESXV were recognized by the immune cells and the immunogenic epitopes were present throughout the sequence of the protein. When the protein ESXV was tested in different recombinant forms (expressed in *Escherichia coli*, *Mycobacterium smegmatis* and DNA plasmids) and injected in mice, the immune responses were induced to multiple epitopes of the protein. Furthermore, immunization of mice with ESXV protected them from infection with *M. tuberculosis*. The same protein was also able to protect mice against the induction of asthma. These results suggest that ESXV has potentials to protect against two major diseases of the world, i.e. tuberculosis and asthma, and hence may be used as a common vaccine.

The study was supported by grants from the College of Graduate Studies and the Research Sector, Kuwait University.

IL-4

Stimuli responsive microbubbles for programmed delivery of nanocarriers: Redirecting diagnostic modality for drug delivery

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Abstract Awaited

IL-5

Direct Synthesis of β-(C3)-Functionalized Pyrrole

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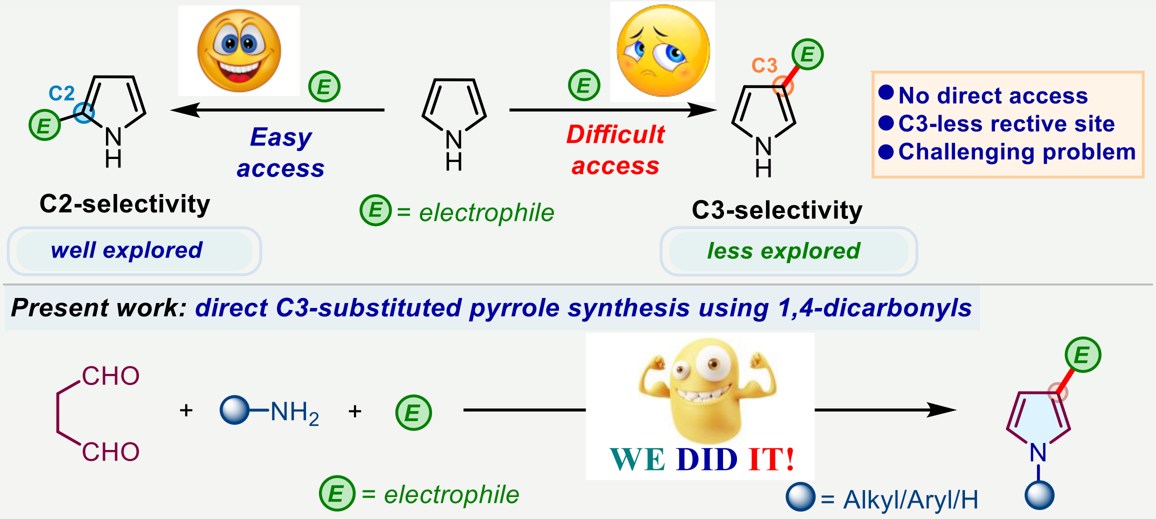
Due to mitigated nucleophilicity, the C3-position of pyrrole is usually considered a non-reactive site in conventional chemistry, thus the majority of S_EAr/Friedel-Craft reactions occur at the C2-(α)-position of pyrrole. Therefore, achieving functionalization at the β-(C3)-position of pyrrole is a challenging task in synthetic chemistry and requires multistep/indirect strategies.[1] These methods can be strictly distributed in two ways: (i) directed functionalization using bulky or electron-withdrawing on pyrrole, and (ii) C3-functionalization-aromatization of *N*-substituted pyrrolidine. We have been exploring the chemistry of 1,4-dicarbonyls as donor-acceptor (D-A) precursors for synthesizing five-membered *N*-heterocycles in asymmetric and non-asymmetric fashion using amine-catalyzed annulation reactions.[2] Recently, we have developed a stimulating and straightforward method to access β-(C3)-functionalized pyrrole using mild Lewis acid and catalyst-free conditions.[3] Details of the concept, design and synthetic strategy for accessing C3-substituted pyrrole in a non-asymmetric/symmetric fashion will be presented here.



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IL-6

Molecular Rotors for Site-selective Organic Transformations

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A new class of molecular rotors, having palladium dichloride rotor unit attached to air-stable bulky organoselenium stator ligands was designed. The new ligands and complexes are well characterized using various spectroscopic techniques. The structure of molecular rotors and bonding of ligands with palladium dichloride was authenticated using single crystal X-ray diffraction technique. The variable temperature NMR studies of molecular rotors show selenium inversion in the molecules with a barrier of~15.5 Kcal mol^{-1}.[1] The potential energy surface (PES) calculations were used to examine chlorine rotation in the molecular rotors. The barrier for chlorine rotation was found to be in the range of ~12.00-24.00 Kcal mol^{-1}.[2] The variation in the rotational barrier was attributed to the bulkiness of organoselenium ligands and the clearance available for the rotation. The molecular rotors were used as catalysts for site-selective organic transformations. Since palladium dichloride is available in sterically confined space and incoming reactants need to approach the metal through specific directions, it was envisioned that the molecular rotors could be used as a site-selective catalyst for the reactions where selectivity of product is an issue. The reaction of 2-arylimidazo[1,2-*a*]pyridines with diphenylacetylene derivatives resulted in an annulated product with reverse regioselectivity. Further, the efficiency of the molecular rotor catalyst was also tested for the decarboxylative Heck-coupling of coumarin with styrene derivatives under mild reaction conditions. Overall, these molecular rotors showed a promising outlook for use in catalysis to enable unique selectivity paradigms.

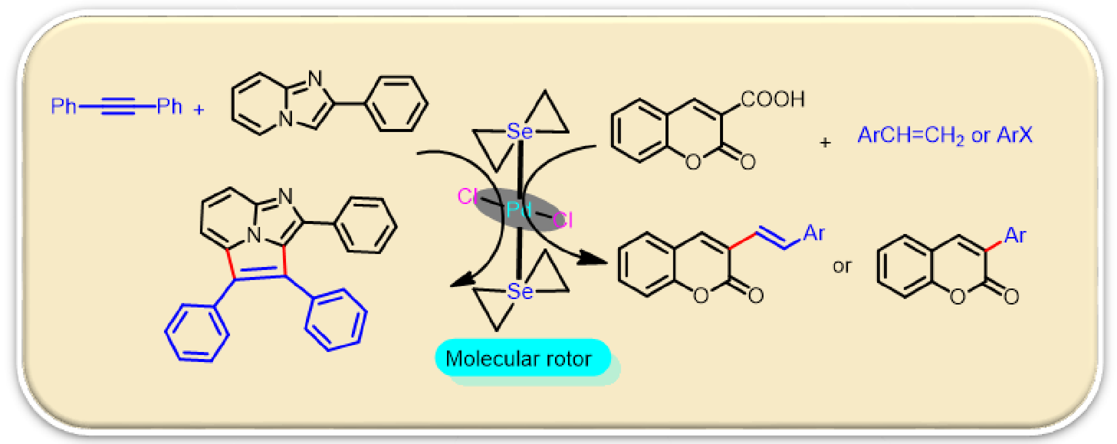

Figure 1. Molecular rotor catalyzed organic transformations.

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IL-7

Pd-Catalyzed Azide-Isocyanide Cross Coupling Reaction: Applications in Medicinal Chemistry and Bioimaging

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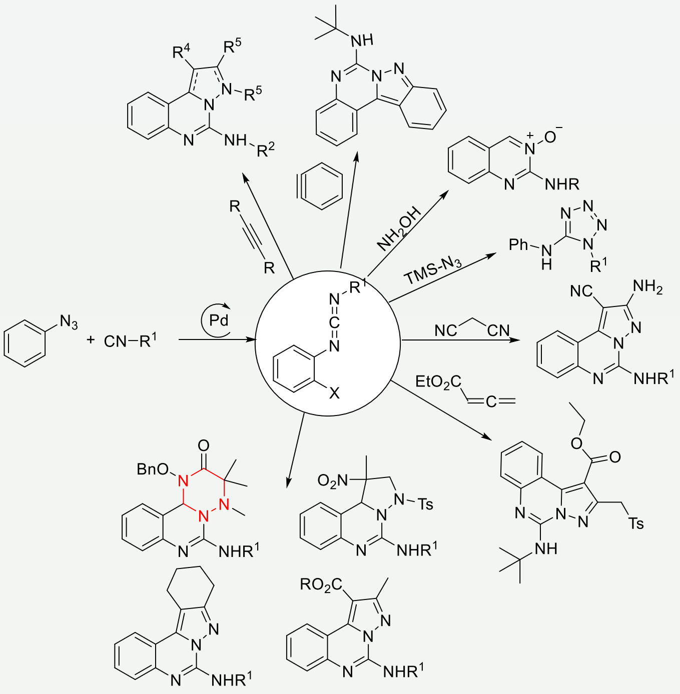
Abstract:



We recently studied transition metal-catalyzed azide-isocyanide cross-coupling reaction in detail.[1] The study revealed that the transfer of nitrene, generated in situ from azide, on isocyanide is a concerted process rather than a two-step process involving a metallaaziridine intermediate as proposed in the literature. The study helped us to fine-tune an elegant method for the synthesis of carbodiimide, a versatile intermediate, in quantitative yield. Encouraged by the result, we devised a four-component reaction promoted by bimetallic relay catalysis for the synthesis of pyrazolo[1,5-*c*]quinozolines.[2] The tricyclic relay cascade involves the formation of five new chemical bonds and concatenation of six discrete chemical steps. Interestingly, pyrazolo[1,5-*c*]quinozolines selectively inhibit EGFR, exhibit apoptosis through the ROS-induced mitochondrial-mediated pathway, and arrest the cell cycle at the G1 phase. The relay catalysis based on nitrene-transfer on isocyanide also provided rapid access to a variety of heterocycles that have application in medicinal chemistry and live-cell imaging.[3]

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IL-8

Artificial Intelligence (AI) powered technologies and innovations in chemistry, transforming every walk of chemist's life

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Abstract: Technological advancements, automation and digital transformation has now become a central topic of discussion for many industries, businesses, and subjects all around the globe, and chemistry is no exception. Artificial intelligence (AI) and its application to chemistry has grown enormously in last few years, helping students, researchers, professors, and scientists working in chemical research domain, industry, or academia.[1,2] In 2019, WIPO reported that Artificial Intelligence was the most prolific emerging technology in terms of number of patent applications and granted patents. Since its emergence in the 1950s, ~340 thousands AI-related patent applications were filed by innovators, in ~20 different application fields, interestingly, ~12 % patents were field in the life and medical sciences, including chemistry. COVID-19 pandemic has shown that it is possible for chemical industry to become innovative, agile and resilient through tech-enabled business models keeping data at the center. Furthermore, researchers and organizations working in chemistry domain are fast realizing the fact that whether this services or solution, or products, no matter how technically strong they are, won't serve the purpose in the future. Artificial Intelligence can feasibly be applied to various tasks in many areas of chemistry, like AI-driven ROS (Route of Synthesis) design for complex target molecules using retrosynthesis tools, prediction of the solubility of a new compound either through equations based on empirical data or by using theoretical calculations. The use of AI for tasks, such as property prediction have proliferated in recent years due to explosive growth in computing power, open-source machine-learning frameworks, and increasing data literacy among chemists. AI implementations have proven to dramatically reduce design and experimental effort by enabling laboratory automation, predicting bioactivities of new drugs, optimizing reaction conditions.[3] Application and advantage of Artificial Intelligence (AI) powered technologies and innovations in chemistry, and the future perspective of AI in chemistry will be discussed in this presentation.

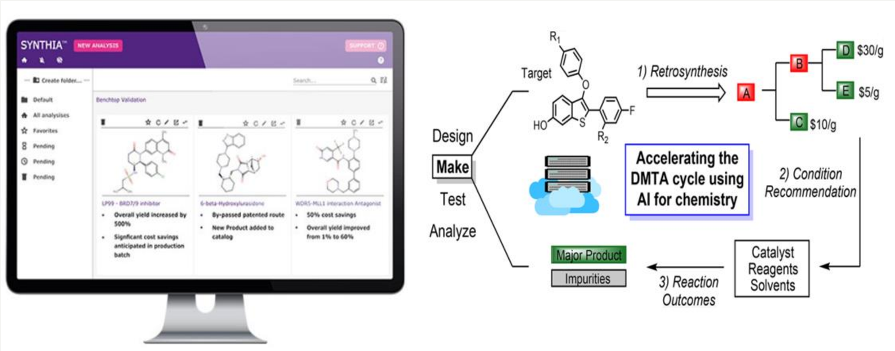

Figure 1: Artificial Intelligence (AI) enabled advanced chemical synthesis

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IL-9

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Abstract Awaited

IL-10

"Electroorganic Synthesis of Thioethers, Selenoethers and Bis(Indolyl)methanes"

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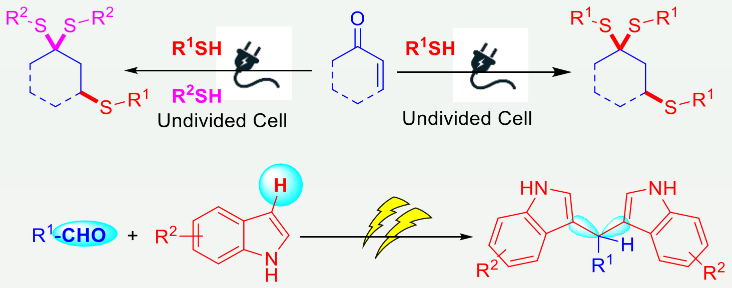
Abstract: Electro-organic synthesis has emerged as an environmentally benign technique for the development of novel organic methods due to its benefits such as high atom economy, mild synthetic route, avoiding redox reagents, ligands or catalyst- free synthetic procedures over traditional reagents-based methodologies.[1] This talk will cover the recent findings of electrcity promoted synthesis of thioethers, selenoethers and bis(indolyl)methanes from our laboratory.[2]



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IL-11

Decoding the Chemistry of Primary Amide/Imidates for Functionalization Reactions

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Abstract:

Functionalized organic molecules are an important class of compounds that are ubiquitously present as a key structural motif in natural products, and biologically active compounds. The introduction of the required functional motif into the desired system with satisfying the parameters of sustainable chemistry such as cost and atom economy is high in demand. Therefore, the direct functionalization of robust and unreactive C-H (sp^2/sp^3) bonds provides an alternate, effective, and desirable tool to organic chemists to convert them into valuable chemical commodities.[1] However, major challenges lies with these methods regio- and chemo-selective functionalization of C-H bonds. To overcome these issues, the concept of directing group was introduced, which offers chemoselective transformations.

Hence, in the past decade, a variety of DGs have been introduced for regioselective C-H transformation. In general, these strategies required the preinstallation of directing groups followed by their uninstallation, which demands two extra steps, resulting in the eventual reduction in the atom and step economy of the complete transformation. Despite the ubiquitous presence of primary amide/imidates functionality, has been rarely utilized as a DGs owing to its least reactive nature and makes an unattractive and challenging synthon. Considering the high abundance and challenges, we became interested in exploring the chemistry of primary amide/Imidates as optimal directing groups for the synthesis of high value-added derivatives of organic compounds.[2] The scope and limitations of such chemistry will be discussed using selected examples.

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IL-12

Mo(VI) complexes of N-glycoconjugates and their catalytic application in selective oxidations of organic sulfides

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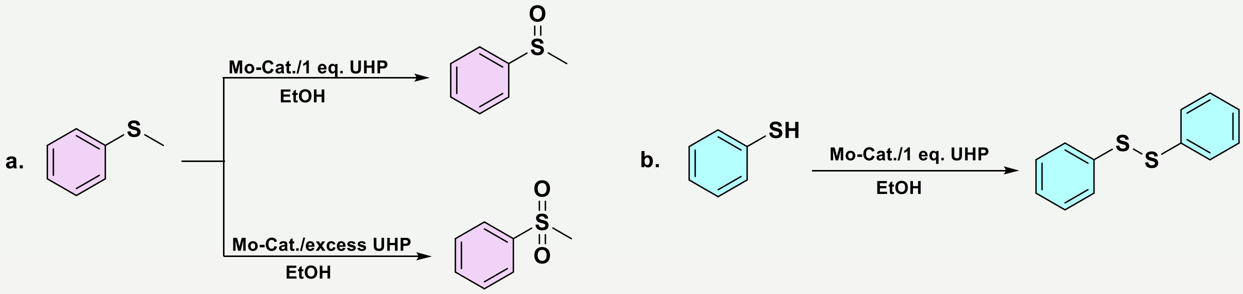
Catalytic application of metal complexes containing glucopyranosylamine-derived ligands are limited and we have explored few Cu(II) and Mo(VI) catalyzed organic transformations. Since, Mo(VI) complexes are well known for catalytic oxidation reactions, we are exploring it's application in selective oxidation of organic sulfides. The oxides of organic sulfides are important from biological as well as pharmaceutical points of view due to their wide application in drug development. Sulfoxides are used in esomeprazole (anti-peptic ulcer drug), aprikalim (anti-hypertensive drug), armodafinil (for sleep disorder), oxisurane (immunosuppressor) etc., while some of the sulfones-based drugs are Dapsone for leprosy, Casodex for prostate cancer etc.[1,2] We have succeeded in the selective synthesis of sulfoxides and sulfones using R-S-R/ and disulfides using R-SH (Scheme 1). The methodology is precise for sulfide and thiol oxidation irrespective of alkene, amine, aldehyde, and ketone groups in the same molecule. The catalyst has been reused five times without appreciable loss in its activity. In order to reduce the catalyst loading, the monotopic ligand has been replaced with ditopic ones and the catalytic activity of both mono and dinuclear complex has been compared. The quantity of catalyst loading has decreased in the latter case. Interesting the oxidation of thiol yielded disulfides, which plays important role in enhancing the pharmacological properties of peptides.[3]



Scheme 1: Catalytic oxidation of organic sulfides and thiols.

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IL-13

Efficient syntheses of porphyrin-based photosensitizers for near infrared photodynamic cancer therapy

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Porphyrins and metalloporphyrins are a distinct class of compounds utilized in various fields including electron transport, catalysis, optoelectronic devices, photodynamic therapy and building blocks for supramolecular assembly.[1] Given the interesting photophysical and electrochemical properties of metalloporphyrins, researchers have been continuing efforts to modify donor-acceptor system in porphyrin by using highly conjugated peripheral substituents on reactive *meso*- or β-positions.[2] For the modulation of photophysical properties of parent porphyrin, various extended π-systems with heteroaromatic moieties have been explored.[1] In some of the reported porphyrinoids, structural modifications at *meso*-position led to absorption region (~400-800 nm) with enhanced fluorescence profile (650-900 nm) and redox potential.[3] Particularly, heteroaromatic systems have attracted more attention in the construction of new *meso*-β π-extended porphyrins due to their, remarkable photophysical properties, electron rich affinity and high electron mobility toward the DNA.[4] Most importantly, such heteroaromatic-annulated systems possess highly active and proton bonding sites to be useful in porphyrin arrays and materials science.[5] In continuation of our efforts to identify photosensitizers with improved photophysical and electrochemical properties and demand for NIR dyes, we have prepared various *meso*,β-heterocycle-appended/fused porphyrins and studied their optical and electrochemical properties.[6] In addition, we have synthesized porphyrin conjugates endowed with remarkable photocytotoxicity against cancer cell lines in the presence of visible light. Design, synthesis, structural elucidation and photocytotoxicity studies of modified porphyrin-based macrocycles will be discussed during the presentation.

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IL-14

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Abstract Awaited

IL-15

Design and synthesis of natural product and heterocyclic compounds for its biological activity

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Catechins such as (−)-epigallocatechin-3-gallate, (+)-epicatechin, (−)-catechin, (−)-epicatechin and gallocatechin gallate and heterocyclic compounds viz quinazolinone, benzofuran, oxazolone, triazoles, oxadiazoles have been to possesses different biological activities, *viz* antimutagenic, antibacterial, analgesic, antitumor and cancer preventive. Novel natural products and heterocyclic compounds have been designed, synthesized and fully characterized by analytical data. Most of the synthesized compounds exhibited significant activities, among which, some of the compounds showed good antioxidant, and broad spectrum anti-proliferative effects. It also showed excellent antibacterial for both Gram negative, Gram positive bacteria and antifungal activity more than the standard drug. Molecular docking studies have also exhibited good binding affinity of compound with the receptor complementing the biological activity reported.

IL-16

Redox Active Fragments and Redox Cascades

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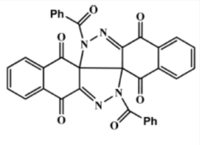
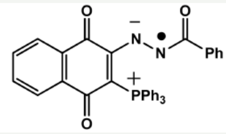
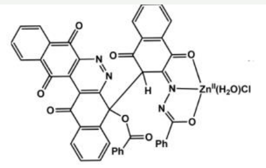
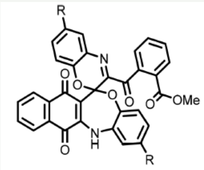
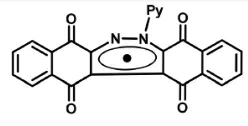
The nature follows cascade path for syntheses with higher atom economy having reduced chemical waste. Cascade reactions that lead to C−C, C−N, or C−X (X = O, P, S) bond formations furnishing functional molecules are worthy in chemical science. Isolation or detection of a chemical species that undergoes multi-component cascade reaction generating bioactive products not isolable from a schematic path has a significant effect on pharmacy. Recently, developing multi-step reactions using several enzymes in one pot, succeeded significantly. In last two decades several cascade reactions were established in organic syntheses. These are classified as nucleophilic/electrophilic, radical, pericyclic, or transition-metal-catalyzed cascades. However, in the vast coordination chemistry, no such reaction was exploited effectively so far, and the same was explored in our laboratory. In this search, diverse redox active fragments that promote cascade reactions are disclosed. The study reveals that the redox active 1,4-naphthoquinone derivatives in presence of 3d metal ions promote redox cascades producing bioactive diarylindazolo[3a,3-c]indazole, zwitterionic triphenylphosphonio-hydrazyl radical, pyridazine , spiro oxazine-oxazepine and carbazole derivatives.[1-3] Two 1,2-benzodiazinyl radicals, cinnolinyl radicals by name, were also successfully isolated by cascade routes using 1,4- naphthoquinone as a precursor.[4] Notably, the redox cascades of these derivatives in presence of 4d metal ions are different.[5]











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IL-17

Metal-nanocomposites: Synthesis and its application in Catalysis

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Application of metal nanoparticles in catalysis is of significant interest due to their unique electronic, optical, and catalytic properties and also exceptionally large surface area to volume ratio. Earth-abundant and less expensive metals have been attracted considerable attention as compared to the rare and expensive noble-metal catalysts. These metal nanoparticles show different quantum properties and activities from that of the corresponding bulk materials because of their different sizes and shapes.

Various metal nanoparticles like, Ag, Pd, Cu have been synthesised on support materials and their catalytic activities related to various organic reactions like, Heck, Suzuki, Sonogashira, Click reaction have been successfully demonstrated. Futhermore, the Ag-nanobicomposites materials were also found to be effective for the wastewater treatments and removal of dyes.

The synthesis and characterization of these (Ag, Pd, Cu) metal- nanocomposites and their applications in various catalytic reactions will be discussed.

IL-18

Metal-Catalyzed Strategies for Fostering Fused Diazaheterocycles as Promising Pharmacophores

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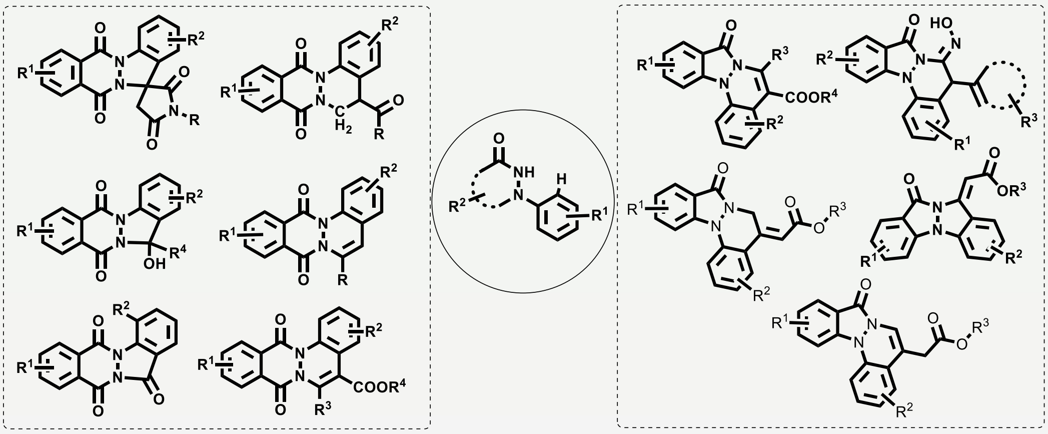
The past few decades have witnessed impressive advancements in the area of transition metal-catalyzed C-H activation strategies, exclusively contributing towards the construction of complex heterocyclic scaffolds centered on diazaheterocyclic molecular architectures. Among the known diazaheterocycles, indazole and phthalazine in their fused/functionalized forms have been recognized as valuable synthetic targets due to their wide range of applications in the field of material and medicinal chemistry. Thus, the demand of developing more efficient protocols for synthesizing fused-indazoles and fused-phthalazines in minimum number of steps from readily available precursors continues unabated. In this realm, we have successfully developed[1] eye-catching transition metal-catalyzed strategies for the synthesis of indazolo-fused indazolylidenes, hydroxy-dihydroindazolo[1,2-*b*]phthalazines, hydroxyimino functionalized indazolo[1,2-*a*]cinnolines & phthalazino[2,3-*a*]cinnolines, 6-arylphthalazino[2,3-*a*]cinnoline-8,13-diones, 5-acyl-5,6-dihydrophthalazino[2,3-*a*]cinnoline-8,13-diones, indazolo[1,2-*b*]phthalazine-triones, indazolo[1,2-*a*]cinnolines and spiro[indazolo[1,2-*b*]phthalazine-13,3'-pyrrolidine]-2′,5′,6,11-tetraones *via* directing group-assisted C-H functionalization, which shall be discussed.



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IL-19

Oxidant-Promoted, Palladium-catalyzed, Regioselective Synthesis of Bioactive Heterocycles via C–H Bond Activation: Chemistry on 1-Aryl-1*H*-indazoles and 2-Aryl-2*H*-indazoles

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Abstract: The transition-metal-catalyzed chelation-assisted approaches and cross-dehydrogenative coupling, often abbreviated as CDC, have been documented as the two most significant tools amidst various methodologies for the regioselective C-H bond activation. In this perspective, Pd-catalyzed chelation-assisted *ortho* activation of C-H bond has emerged as an interesting approach towards sustainable synthetic developments as the strategy offers several advantages such as greener route, high selectivity, no pre-functionalization of starting materials, operationally simple pathway etc. which furnished the desired molecular framework in organic synthesis.

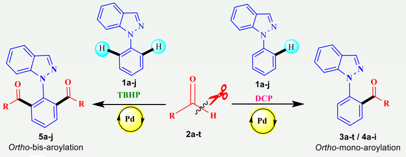

Figure 1. Oxidant-switched Pd-catalyzed Cross-dehydrogenative coupling strategy **direct mono-/bis-*ortho*-aroylation of substituted 1-phenyl-1*H*-Indazoles**.

The presence of various pharmaceutically important biological activities flaunted by 1-phenyl-(1*H/2H)*-indazoles such as JNK3 inhibitors, anti-inflammatory, antiviral, antimicrobial, anticancer etc. have further stimulated the emergence of novel method towards its C-H functionalization (Figure 1). Herein, we will discuss the development of **oxidant-switched Palladium-catalyzed regioselective** $C_{(sp^2)}$–H/$C_{(sp^2)}$–H **cross-dehydrogenative coupling (CDC) for direct mono-/bis-*ortho*-aroylation of substituted 1-phenyl-1*H*-Indazoles 1a-j with various substituted** aldehydes **2a-t** *via* $C_{(sp^2)}$–H bond activation which generated a miscellaneous variety of mono-substituted *ortho*-benzoyl/acyl-1-aryl-1*H*-indazoles **3a-t/4a-i** and bis-substituted *ortho*-benzoyl-1-aryl-1*H*-indazoles **5a-j** in upto 88% yields (Figure 1).

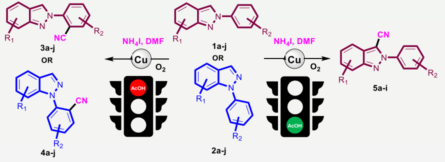

Figure 2. Cu-promoted regiodivergent, AcOH-switchable, distal and proximal direct cyanation of N-aryl-(1*H*/2*H*)-indazoles via C(sp^2)–H bond activation

In continuation, **we will also discuss the copper-promoted regiodivergent, AcOH-switchable, distal and proximal direct cyanation of N-aryl-(1*H*/2*H*)-indazoles *via* aerobic oxidative C(sp^2)–H bond activation which generated (C-2')-cyanated 2-aryl-2*H*-indazoles 3a-j, (C-2')-cyanated 1-aryl-1*H*-indazoles 4a-j [distal] or C-3 cyanated 2-aryl-2*H*-indazoles 5a-i [proximal] products in good to excellent yields. The cyanide (CN$^-$) ion surrogate was generated *via* the unification of dimethylformamide (DMF) and ammonium iodide (NH_4I). The utilization of molecular oxygen (aerobic oxidative strategy) as a clean and safe oxidant is liable for generous value addition to bioactive heterocycles. (Figure 2).**

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IL-20

Progress in Metallic Chemotherapeutic Agents, Structural Elucidation, In vivo and In vitro Investigations

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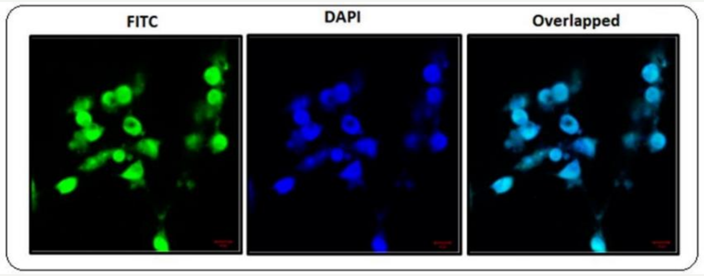
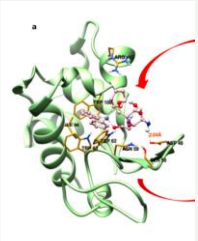
Molecular design of the metallic cancer drug is an interdisciplinary thrust area of bioinorganic, drug, and medicinal Chemistry research[1,2], the development of the new drug, delivery, and therapeutic strategies that could target cancer cells are in progress. New potential metallic-drug molecules were designed, synthesized, and characterized by various spectroscopic methods and further confirmed by X-ray crystallography. In vitro DNA binding studies of the compounds, docking studies and Gel electrophoretic assay demonstrates the ability of the compounds to bind with DNA through the hydrolytic/oxidative process. To understand the drug-protein interaction the affinity of compounds toward proteins was also investigated. The complexes showed high inhibitory activity against Topo-Iα, glutathione peroxidase, and IC_{50}, suggesting that complexes were efficient DNA cleaving agents. In vitro results of anticancer activity against the carcinoma cell lines revealed that complexes can kill the chosen cancer cells. The mode of cell death induced by complexes was apoptosis as revealed by EB staining, Hoechst 33258 staining. The drug delivery via graphene oxide loaded nano metallic drugs conjugate was investigated and revealed that the nano conjugate drug has a high potential to inhibit the cancer-promoting enzyme and kill the cancer cells via an apoptotic pathway at low concentration. The selected compounds were evaluated for cancer in vivo and found highly effective at low doses in comparison to the existing drugs.





Best fit molecular docked pose of metallic drug at the active site of lysozyme.

Fig. Confocal microscopic images of Du145 cells with metallic drug-GO seeded in chamber slides.

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IL-21

Design and Synthesis of Quinoline-based Dual Inhibitors of Topoisomerase and Histone Deacetylases as Anticancer Agents

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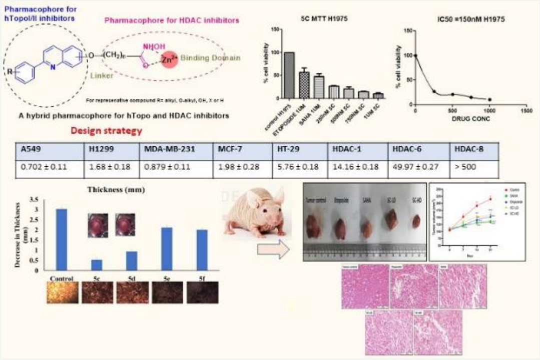
Abstract: Topoisomerases (Topos) are the second most abundant protein in the nucleus after histone deacetylases (HDAC), which play a pivotal role in regulating cellular processes.[1] Although a large number of anticancer drugs are known to inhibit these proteins, many of them have failed to yield the much-desired result.[2] In most cases, such failure can be attributed to the lack of selectivity, less efficacy, more side effects, and multi-drug resistance (MDR).[1] Further, combination therapies are associated with drawbacks, including differential pharmacokinetic profiling and drug-drug interactions.[3] Therefore, a single administration of a compound with the desired capability of dual/multi-inhibition of biological targets is more feasible in treating complex diseases like cancer.[4] Most known dual inhibitors of TopoI/II inhibitors are derived from existing drugs such as doxorubicin and camptothecin, which have multiple drug instability including limited solubility, and toxicity due to parent molecules from which they are derived.



A549	H1299	MDA-MB-231	MCF-7	HT-29	HDAC-1	HDAC-6	HDAC-8
0.702 ± 0.11	1.68 ± 0.18	0.879 ± 0.11	1.98 ± 0.28	5.76 ± 0.18	14.16 ± 0.18	49.97 ± 0.27	> 500

In continuation to our ongoing work in anticancer drug discovery,[5] we have designed, and synthesized novel quinoline-bridged hydroxamate-based dual inhibitors considering the pharmacophoric features of human topoisomerases and histone deacetylase and explored their mechanistic insights as anticancer agents.[6]

From the pool of synthetics, compound **5c** emerged as a dual inhibitor of hTopo1 and II, along with HDAC-1. The anticancer investigation on **5c** revealed its potential anticancer activity in 2D and 3D in vitro models, with no toxicity towards H9c2 cardiac cells. Further, It induced cancer cell death via apoptosis by ROS upsurge and in mitochondrial-dependent mode via halting the cell cycle at the G1 phase. 5c compound modulated the expression of key oncogenic targets and possessed good stability in human and mouse liver microsomes. Moreover, in vivo results indicated that the administration of the **5c** compound significantly reduced the growth of the tumor in the A549 cell-induced lung cancer xenograft nude mice compared to standard anticancer drugs SAHA and Etoposide.

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IL-22

Hypervalent Iodine Reagents as key Replacements of Transition Metals in Organic Synthesis

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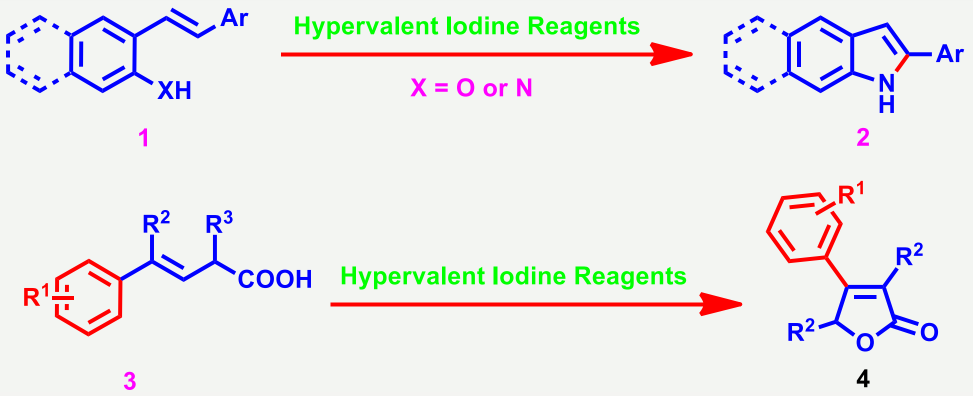
Abstract

In past few decades, hypervalent iodine reagents have been developed as highly valuable reagents in synthetic organic chemistry. Because of mild reaction conditions and environmentally friendly behaviors, these reagents are the key replacements of toxic heavy metals. Various hypervalent reagents have been developed as oxidants but their applications are not limited to oxidative functionalization and several iodine(III) reagents have been known for their electrophilic nature. Various synthetic transformations such as cyclization reactions, □-functionalizations of carbonyl compounds, atom-transfer reactions and oxidative rearrangements have been also achieved successfully. Recently, these reagents have been received a particular attention due to their applications in catalysis. Various synthetic transformations have been successfully achieved using both iodine(III) or iodine(V) reagents.



Scheme 1.

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IL-23

Ionic Liquids and Deep Eutectic Solvents as Green Solvent for Separation of Close Boiling Point Mixtures

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Research focusses on green solvent for the essence of eliminating environmental unfriendly solvents is still under intense research for industrial usages. Therefore, in the recent decades, a lot of solvent-free processes and more successful recycling protocols have been developed. The aim of green chemistry is to design environmentally friendly chemical processes and synthetic methodologies in order to eliminate and reduce the use of hazardous and toxic chemicals at any stage of production in the industries and laboratories. Hence, ionic liquids (ILs) and deep eutectic solvents (DESs) have been identified as potentially cost-effective and environmentally friendly replacements for traditional volatile organic solvents. In designing separation techniques, the activity coefficients at infinite dilution of solutes in the DESs/ILs are crucial. Hence, activity coefficients at infinite dilution for polar and non-polar organic solutes: solutes include alkanes, alkenes, alcohols, ketones, thiophene, heterocyclics, cycloalkanes, acetonitrile, tetrahydrofuran, cycloalkenes, aromatic hydrocarbon and water in DESs/ILs were evaluated using gas-liquid chromatography technique (GLC) at various temperatures. Partial molar excess enthalpies at infinite dilution were calculated from the temperature dependence of activity coefficients at infinite dilution. The selectivity and capacity values for separation of close boiling point mixtures at T = 323.15 K were calculated and compared to literature values for DESs, ionic liquids (ILs), and sulfolane to assess the suitability of the DESs/ILs for possible use as an entrainers. The potential of DESs/ILs to replace traditional solvents was observed because it had a high separation parameter (capacity and selectivity) for all chosen systems involving close boiling point mixtures.

Keywords: DESs, Activity coefficients at infinite dilution, Separation, GLC.

IL-24

Versatility of hetero-allenes: An easy access for the syntheses of biologically potent scaffolds

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Abstract:

In recent years, development of novel synthetic methodologies have been attracted a great deal of attention for organic chemists around the globe, for the synthesis of structurally diverse biologically potent molecules. The advantages associated with these synthetic methodologies are lesser synthetic steps, use of cheaper and safer new alternatives, involves overall lesser reaction time, milder reaction conditions, and afforded high yields. Extensive efforts have been made by organic chemists around the globe and thus developed several kinds of new and highly efficient methods for the generation of various kinds of structurally diverse molecules of biological significance.

In recent years, carbon dioxide/carbon disulfide/carbonyl sulfide has been employed as a cheap and safe alternative eliminating the use of harmful reagents such as CO and $COCl_2$. Recently, carbon dioxide/carbon disulfide/carbonyl sulfide has frequently been employed as a green reagent in its various conditions and forms for the syntheses of structurally diverse biologically potent scaffolds employing diversity of starting materials, reagents and catalytic systems. In the present talk, we will focus some of our novel and efficient methods for the synthesis of biologically potent scaffolds.

IL-25

The Role of primary and secondary sphere ligands on the C-H activation reactivity, quantum mechanical tunneling of Fe(IV)O complexes

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Bio-inspired Fe(IV)O complexes are very significant due to their effective catalysis in C-H activation.[1-2] There are various close interrelated reactivity factors of these complexes, e.g. the axial or equatorial ligand connectivity to the central metal, general ligand architecture, energy of the acceptor orbital, spin state, electrophilicity, quantum mechanical tunneling, etc.[3]

In the current presentation, we will discuss the role of axial ligands (primary) and a few secondary sphere ligands in C-H activation reactivity and quantum mechanical tunneling.[4-5] The observed facts will be generalized. The tunneling-corrected kinetic isotope effect will also be discussed to define the reactive spin state. The presented conclusion may further open the possibility for the design of metal-based optimum catalysts with systematic ligand/substituent tuning.

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IL-26

Discovery of Nurr1 agonist and development clinical candidate for the treatment of Parkinson disease

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In order to address the issue of drug resistance and improve the ADME properties of a drug molecule concept of molecular hybridization was put forward wherein two or more distinct pharmacophores are covalently linked into a single molecule. This approach may lead to a molecule with improved efficacy and may solve the problem of drug resistance and reduce the undesired side effects [1,2]. The development of such molecular frameworks with synthetic selectivity and economic viability is still a challenging task for the pharmaceutical industry. Drugs developed through this approach can be used for the cure of infectious diseases where treatment is limited to few drugs and the known drugs have limitations such as toxicity, pharmacokinetics, pharmacodynamic and drug resistance. The benefit of using molecular hybrid is to activate different or same targets by a single molecule, and increase the therapeutic efficacy and to improve the bioavailability. Molecular hybridization approach has resulted many drug candidates with improved activity profile and some of these compounds are in clinical trials. We have utilized this concept in designing antimalarial molecules and many molecules with aminiquinoline and pyrimidine phamacohpore showed low nano molar activity. Later a massive multi-institutional collaboration was started and over 700 new molecules were studies for Nurr1 activation, a potential target for Parkinson disease model and identified 15 hits out of which 3 compounds have cleared pre-clinical trials and technology has been transferred to NURRON pharmaceuticals for further development [3-18]. These molecules activate the Nurr1 enzyme which is essential for the survival of the dopamine neurons, stops the aggregation of α-synuclein protein in the brain, and promotes autophagy. Systematic studies demonstrated that these compounds can cures the Parkinson induced mice model at 5 mg/kg body weight without any toxicity.

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IL-27

Chemistry Of Heterocyclic Compounds & their Biological Importance

Anurag Tiwari

Thermo Fisher Scientific India Pvt. Ltd., Kolkata.

Abstract Awaited

IL-28

Expediting Research with Accuracy and Confidence

Mandar Bodas

Solution Consultants, Research Solutions-Life Sciences, Elsevier.

Abstract Awaited

IL-29

LC-MS in Advance Purification, Separation and Characterization.

Thermo Fisher Scientific India Pvt. Ltd., Kolkata.

Abstract Awaited

IL-30

Bench Top Non-Cryo NMR in Research

Sandip Jagtap

Labindia Analytical Instruments Pvt. Ltd., Kolkata

Abstract Awaited

IL-31

Exploration of THQ Derivatives as Potent mTOR Inhibitors for Lung Cancer

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Abstract

The present research work was started with a detailed literature review of cancer where it was observed that lung cancer is one of the most dangerous cancer among all the other types of cancer. Many genes get mutated in lung cancer but the involvement of EGFR, KRAS, PTEN, and PIK3 are more common. Unavailability of drugs or resistance to the available drugs is the major problem in the treatment of lung cancer. In the present research, mTOR was selected as an alternative target for the treatment of lung cancer which involves the PI3K/AKT/mTOR pathway. For the identification of the core scaffold, pharmacophore modeling followed by virtual screening, molecular docking, and *in-silico* ADMET studies were performed which gave tetrahydroquinoline (THQ) as a core scaffold. Simultaneously for the identification of the substituents required for the mTOR inhibition, a 3D-QSAR (CoMFA and CoMSIA) study and a knowledge-based drug designing approach was adopted.

For the synthesis of these desired THQ derivatives, Fmoc protection and deprotection chemistry were utilized for the selective nitration at the 6th position of the THQ which gave *N*-substituted 6-nitrotetrahydorquinoline. Further reduction was carried out with the aid of zinc/ammonium chloride resulting in the *N*-substituted 6-aminotetrahydorquinoline. The final desired compounds were synthesized by the derivatization of the amino group presented at the 6th position of *N*-substituted THQ derivatives. All these synthesized compounds were characterized by FTIR, ^{1}H, ^{13}C NMR, and Mass analysis, while the purity was checked with the HPLC.

All these compounds were screened for antiproliferative activity against the panel of the cancerous cell line along with cellular mTOR enzyme assay where 6 compounds were found potent. These compounds were further evaluated for the specialized *in-vitro* biological evaluation viz. colony forming assay, flow cytometric analysis, gene expression study, and western blot analysis. Based on these studies, compounds HB-UC-1 and HB-UC-5 were found best against lung cancer and mTOR. These two compounds were further taken for *in-vivo* biological evaluation. Initially, the effect of compounds HB-UC-1 and HB-UC-5 on the lifespan of cancer-bearing animals were evaluated for up to 30 days where these compounds gave promising outcomes. Further, these compounds were taken for testing in the bezo[a]pyrene-induced lung cancer animal model where the effectiveness of these compounds was reflected through the biochemical parameters and histopathological evaluation of the lung tissue.

The results of the whole study gave promising outcomes as a potent hit molecule that is under investigation and further modifications to get lead compound for the treatment of lung cancer.

IL-32

Synthesis of various functionalized carbocycles and heterocycles from cyanomethylarenes

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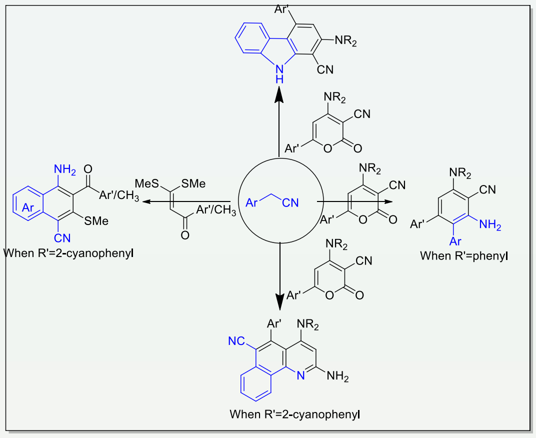
ABSTRACT:



Various functionalized cyanomethylarenes were used as precursor from several decades. Recently, Our research grouop have explored the functionalized cyanomethylarenes as a carbanion source for various reactions. Various functionalized naphthalenes was afforded in good to excellent yield by reactions of ketenedithioacetals with 2-cyanomethylbenzonitrile.[1,2] We studied 2-cyanomethylbenzonitrile, benzyl cyanide and o-and p-substituted benzyl cyanide and used them as a carbanion source to explore their chemistry. Furthermore, 2-cyanomethylbenzonitrile provides highly functionalized beno[*h*]quinolines by ring transformation with 2-pyranone.[3] 5,6-Dihydro-2*H*-benzo[*h*]chromenes react with cyanomethylbenzonitrile to afford 4,5-dihydro-1*H*-benz[*e*]indenes.[4] 1*H*-Naphtho[1,2-*d*]imidazole were also synthesized in three steps involving 2-(1-cyno-2,2-bis methylsulfanyl vinyl)-benzonitrile[1,5] as an intermediate obtained from 2-cyanomethylbenzonitrile. We have also used functionalized benzyl cyanide as carbanion source to carry out the ring transformation of 2-pyranone and various teraryls and enones has been achieved under different reaction conditions.

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Il-33

Peptide signatures for Cellular function of Proteins

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Abstract Awaited

IL-34

Diversity Oriented Synthesis by Multicomponent Cyclization Reactions

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Abstract: Design and development of cost and step economic methods for the synthesis of important bioactive heterocycles has remained and everlasting challenge in organic synthesis. Multicomponent cyclization reactions are considered as an important strategy for the pot and step economic synthesis of heterocycles. [1] We have developed several methods for the synthesis of fused and functionalized heterocycles using arylglyoxal based multicomponent cyclization reactions. During our study, we realized that these multicomponent cyclization reactions provide different products depending upon reaction conditions, solvents, catalysts and the types of the reactants involved. In this presentation some of our recent multicomponent cyclization reactions for the synthesis of diverse fused and functionalized furans, pyrroles and thiazoles from the readily available starting materials will be presented. [2]

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Il-35

Integrated Approach toward the Discovery of Drugs from Medicinal Plants

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The new drug discovery program is currently facing serious challenges due to decreasing in number of new drug approvals coupled with exorbitant rising cost. Search of new chemical entities or new leads by use of combinatorial chemistry has provided new hope, but even this scientific approach has failed to improve the success rate in new drug discovery. This circumstances, prompted the scientists to come out with a novel approach of integrated drug discovery, where drug discovery from plant sources can be synergized by using Ayurvedic wisdom. The initial steps of the discovery of new drug are to identification of new leads either through synthesis or isolated from natural resources. Medicinal plants constantly played significant roles in proving new drugs or new leads as well documented in the literatures. Bioassay-guided fractionation of the identified plant may lead to standardize the extract or isolating the bioactive compounds as new drugs. This integrated approach would lead to saving of cost and time, coupled with enhanced success rate in drug discovery. Few drugs developed from natural sources have undoubtedly revolutionized medicine, like antibiotics (e.g. penicillin, tetracycline, erythromycin), antiparasitics (e.g. avermectin), antimalarials (e.g. quinine, artemisinin), lipid control agents (e.g. lovastatin and analogs), immunosuppressants for organ transplants (e.g. cyclosporine, rapamycins), and anticancer drugs (e.g. paclitaxel, irinotecan) [1]. Keeping in view of the above facts and use of medicinal plants in discovery of new drugs or new chemical entities and our continuous work and efforts to identify the new therapeutic agents, recently, in our laboratory, we have isolated and identified the many bioactive lead molecules from plants by using various chromatigraphic and spectral techniques [2, 3]. In this presentation, the detail techniques involved in the isolations, characterizations and biological screening evaluations of the isolated plant-derived lead molecules in our laboratories will be discussed.

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Il-36

Why Intermolecular Nitric Oxide (NO) Transfer? Exploring the Factors and Mechanistic Aspects of NO Transfer Reaction

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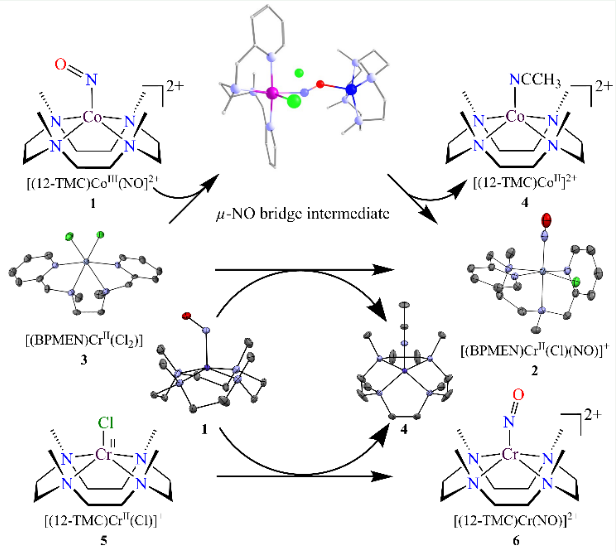
Abstract:

The metal-centers and the ligand frameworks greatly influence small molecule activation & their transfer reactions in biological or catalytic reactions.[1,2] Here, we discuss directed nitric oxide (NO) transfer chemistry in low-spin mononuclear $\{Co(NO)\}^8$, $[(12\text{-TMC})Co^{III}(NO^-)]^{2+}$ (**1-CoNO**, $S = 0$), and $\{Cr(NO)\}^5$, $([(BPMEN)Cr(NO)(Cl)]^+)$ (**4-CrNO**, $S = 1/2$), complexes. **1-CoNO** transfers its bound NO moiety to a high-spin $[(BPMEN)Cr^{II}(Cl_2)]$ (**2-Cr**, $S = 2$) and generates **4-CrNO** via an associative pathway; however, we did not observe the reverse reaction. Spectral titration for NO transfer reaction between **1-CoNO** and **2-Cr** confirmed 1:1 reaction stoichiometry. The experimental and theoretical observation supports the formation of μ-NO bridged intermediate species ($\{Cr\text{-}NO\text{-}Co\}^{4+}$). For the first time, we observed the formation of an intermediate prior to NO transfer. Mechanistic investigations using ^{15}N-labeled-^{15}NO and tracking the ^{15}N-atom established that the NO moiety in **4-CrNO** is derived from **1-CoNO**. Further, to investigate the factors deciding the NO transfer reactivity, we explored the NO transfer reaction between another high-spin Cr^{II}-complex, $[(12\text{-TMC})Cr^{II}(Cl)]^+$ (**5-Cr,** $S = 2$), and **1-CoNO**, showing the generation of the low-spin $[(12\text{-TMC})Cr(NO)(Cl)]^+$ (**6-CrNO**, $S = 1/2$); however, again there was no opposite reaction, i.e., from Cr-center to Co-center. Kinetic measurement suggests the NO transfer rate is 3.4 times faster in the latter case than the former. The above results advocate clearly that the NO transfer from Co-center generates thermally stable and low-spin & inert $\{Cr(NO)\}^5$ complexes (**4-CrNO** & **6-CrNO**) from high-spin & labile Cr-complexes (**2-Cr** & **5-Cr**), suggesting a metal-directed NO transfer (Cobalt to Chromium, not Chromium to Cobalt). These results explicitly highlight that the ligand can stabilize the intermediate and affect the NO transfer rate but net NO transfer is strongly influenced by the labile/inert behavior of the metal-centers and /or thermal stability rather than the ligand architecture.[3]



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IL-37

Palladium Catalysed Regioselective Monohalogenation of 1-methyl-3-phenylquinoxalin-2(1*H*)-ones via C-H activation under microwave radiations

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Microwave assisted, N-directed, Pd-catalyzed regioselective ortho-halogenation of 3-aryl ring of 1-alkyl/benzyl-3-phenylquinoxalin-2(1*H*)-one derivatives would be discussed using readily available N-halosuccinimides (NXS) as halogenating agents. The nitrogen atom of quinoxalin-2(1*H*)-one worked as an effective directing group and helped in achieving regioselective halogenated products in good yields. The reaction proceeded smoothly with wide substrate scope, high functional group tolerance and short reaction time. The post-functionalization scope of the synthesized molecules was also explored by carrying out Suzuki-Miyaura coupling reaction and Rosenmund-von Braun reaction, which resulted the products in good yields.

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IL-38

Development of Novel Synthetic Approaches for Establishing a variety of Luminescent mono metallic and bimetallic Complexes as Cancer Theranostics

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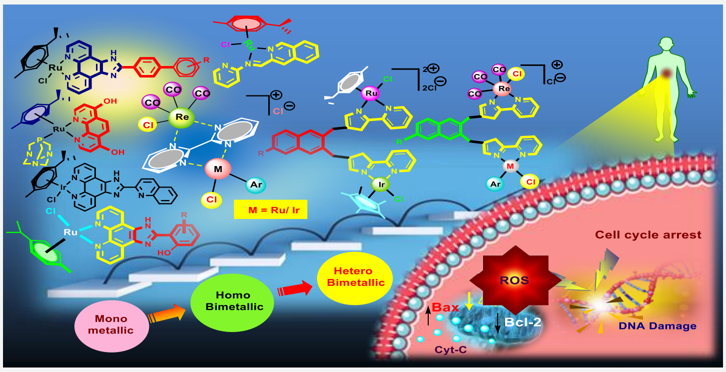
ABSTRACT

Chemotherapy is the most prevalent traditional cancer therapy but it lacks tumor specificity and thus it renders normal cells at risk. Therefore, considerable attention should be given on the design of new metal-based drugs by following approaches including (i) selectivity in cancer cell by non-covalent modes of DNA interaction (ii) development of various photo-toxic agents as these produce reactive oxygen species (ROS) at the photo-exposed cancer cells leaving the unexposed healthy cells minimally affected. (iii) “Theranostic”, which includes simultaneous diagnostic and therapeutic functions in a single system improving the outcome of a disease state. With respect to therapeutic regimes, improved treatment effect is achieved by effective localization at the tumor specific sites of the therapeutic agents whereas from diagnostic aspect imaging agents along with therapeutic agents combined with biomarkers (tumor specific markers) are carried from one system to another enabling them to differentiate the tumor cells from normal cells. In continuation of our present work on anticancer organoruthenium, organoiridium and organorhenium complexes, we have introduced the convenient and effective synthetic approaches for designing the monometallic and bimetallic Ru(II)/Ir(III)/Re(I) complexes which can address all three approaches. The operational simplicity, good yield, ease of isolation of the products and high chemoselectivity will be the main advantages of these methods.



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IL-39

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Abstract Awaited

Il-40

Synthesis of Isatin and 1,4-Dihydropyridne Scaffolds as Anti-Breast Cancer Agents and Their Applications as Chemosensors

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The exploration of novel N-containing heterocycles having potential biological and pharmacological properties have attracted immense interest in present era. Isatin (1*H*-indole-2,3-dione) is a synthetically versatile substrate that can be used to synthesize a large variety of polyfunctional heterocyclic compounds such as quinolones and indoles. Another promising heterocycle, 1,2,3-triazole is the most widely explored five-membered heterocyclic scaffold that has attracted scientific fraternity over the past few decades and its applications have also been extended to widespread diseases. 1,4- and 1,2-Dihydropyridines account for another important scaffold in the field of medicinal chemistry. The interesting biological profile of these scaffolds prompted us to synthesize some novel triazole tethered isatin and triazole tethered isatin-dihydropyridine hybrids. These synthesized hybrids were well characterized and evaluated against a panel of human cancer cell lines viz. HeLa, Huh-7, PC-3, IMR-32, MDA-MB-231 and MCF-7 using doxorubicin as standard and tamoxifen as standard drugs.

A copper catalysed click chemistry (CuAAC) approach has been used to synthesize 1,2,3-triazole linked isatin, dihydropyridine or Rodamine fluorescent and colorimetric chemosensors for the detection of biologically important metal ions. The sugar and pyrene appended bis-triazolylated-1,4-dihydropyridine based probes**,** acted as a turn-off fluorescent sensors towards Fe^{2+} and Cu^{2+}, respectively. However, isatin-triazole functionalized rhodamine based probe**,** exhibited a selective binding towards Cu^{2+} and Fe^{3+} through a turn-on fluorescence response. These colorimetric or florescent chemosensors find applications in the detection of metal ions, amino acids and anions in water, real sample and in body tissues (cell imaging).

Il-41

Extracting Green Hydrogen as Clean Fuel from Seawater by Electrocatalytic Water Splitting

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Abstract Awaited

IL-42

“Green” and Click-Chemistry Approaches: Opportunity for Simplification and Innovation Towards Step-Economical Synthesis of Natural Polyphenols & Thiophenols-Based Small Molecules of Biological and Commercial Importance

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Small molecules of natural origin including polyphenolics and thiophenol based heterocyclic compounds have drawn great interest from the scientific community as they are associated with wide range of biological activities including anticancer, antimalarial, antibacterial, antifungal and anti-inflammatory etc. However, exploration of these bioactive molecules is severely hindered by their insufficient percentage in their natural resources, difficult isolation procedure, limiting trials for wider applications besides their tedious multistep synthesis involving protection-deprotection strategy. The shortcomings of the prevalent methodologies have provided a fresh stimulus to develop new strategies based on “Green” and Click Chemistry with minimum number of steps, readily available starting materials and reagents, simple product separation and purification, high to complete atom economy, waste minimization or no waste, compatible with aqueous environment or no solvent or green solvents and high yield with few to no by-products besides being devoid of protection-deprotection steps. Our groups from noticeable time have been working on such green methodologies for extraction and purification of natural molecules as well as design and synthesis of various polyphenolic and thiophenolic based bioactive molecules like FEMA-GRAS approved 4-vinylphenols of commercial importance, stilbenoids (e.g. natural resveratrol, Pterostilbene), hybrid molecules (e.g salvianolic acid F) and 3-sulphenylated indole with their biological evaluation. Moreover, the details of microwave- and ionic liquid-promoted step-economical synthesis of such natural and non-natural molecules of commercial importance will be discussed during presentation.

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IL-43

Nanomaterial a Versatile Innovation as a Electrochemical sensor, Catalyst & Electrode material.

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Abstract

Developing matter at the nanoscale enables the development of new materials, tools, and systems with unique features and capabilities which is known as nanotechnology. A new scientific branch of materials, chemistry, and physics that places an emphasis on the rational synthesis and research of nanoscale materials has just evolved as a result of the recent growth of nanotechnology. Nanomaterial act as simple, inexpensive, highly sensitive and selective and therefore it can be used as Electrochemical sensor, Heterogeneous Catalyst, Super capacitors, Electrode material, Wound Healing material, used as a pollutant removal(Removal of Heavy Metal Ions from water soures as well as Waste water Treatment), Energy source and Photo catalyst. With increasing environmental concerns worldwide, Nano-materials have become more important and useful innovations for above mention applications.

Keywords- Nanotechnology, Heterogeneous Catalyst, electrode material, photo catalyst,

IL-44

1,3-Site-Selective Functionalization of Phenols to Multi-functionalArenes via Oxidation-NGP Strategy

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Functionalized arenes are one of the most abundant and indispensable building blocks in various functional organic materials including pharmaceuticals, agrochemicals, polymers, and organic materials, that has significant impact in science, technology and society. Given the importance of these building blocks as unique and most transformative molecule to diverse structures, chemists intrigued towards their step- and atom-economic synthesis and functionalization.[1] Anilines, amides, and organophosphoranes are particularly interesting in terms of their wide applications andstriving in step-economical synthesis. Furthermore, site-selective multi- functionalization of arenes are relatively thought-provoking process, which usually entails multi step sequences with consequent multiple purification steps.

p-Quinols serve as electrophilic aryl group surrogates with multi-facet reactivity with nucleophiles. Our group is engaged in exploring this reactivity for site-selective 1,3- dual functionalization with ambiphilic molecules through Neighboring Group Participation (NGP). This strategy provides the rapid synthesis 3-amino- benzamides, 3-arylphosphonates[2] and □-(amino)aryl carbonyls[3] via *p*-quinols. This method was further elaborated for the switch of reactivity to □-(sp^3)arylation of amines.[4]

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IL-45

PHARMACEUTICALS IN THE ENVIRONMENT: A problematic requiring attention of chemists, biologists, and pharmaceutical scientists

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The presence of pharmaceuticals in the environment is a matter of concern, keeping into view that they are potent chemicals. The source of contamination may be the discharge from pharmaceutical industry, hospital affluents, regulatory disposal of counterfeits, household disposal of expired medicines, etc. In India, the rampart use of drugs and hormones for increasing yields of milk and food and even use of drugs for abuse can also be considered as additional factors in loading of the environment. Residues of un-metabolized drugs are excreted in urine and faeces, and topically applied medications are washed from skin during bathing. In future, there is likelihood of increase in loading of environment with pharmaceuticals with enhancement in number of companies, hospitals, patients and improvement of general affordability of the latter to buy medicines. Although there are no known short term effects reported on humans, long term effects have not been ruled out. Therefore, regulatory bodies world-wide are striving hard to attend to this issue, though in India and other developing countries, no stringent regulations have been implemented yet. In recent years, reliable protocols have been established for residue analysis of these pollutants down to picogram levels. Using the same, the author and his team was able to establish the presence of diclofenac in ground water used for drinking in several villages surrounding NIPER, SAS Nagar. The presentation will cover the above-given aspects to sensitize on the issue, and propose the same as a newer research area for chemists, biologists, and pharmaceutical scientists.

IL-46

THE ROLE OF RADIOMETAL ISOTOPES: CONCEPT FOR THERANOSTIC RADIOPHARMACEUTICALS

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The future of Radiometal-Based Radiopharmaceuticals and theranostics appears to be necessary to identify the most promising strategies to tackle upcoming challenge in Health care. It is interesting to note that although a plethora of potentially medically useful metal radionuclides has been suggested over the last decades, only a few have made their way towards frequent application or even into clinical routine studies. We are focused on such of them for example 64Cu-Copper, 89Zr-Zirconium, and 68Ga-Gallium labelled radio-pharmaceuticals. Our research primarily focused on their production and incorporation of them to either bio-molecules, metal chelator conjugated with bio-molecules or peptides

IL-47

Ru(II) complexes of anthracene linked pyrazolyl pyridine and benzimidazolyl pyridine: Absorption and Emission spectroscopy

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The tunability of the color of absorption/ emission and the lifetime of the excited state along with the relative stability of such complexes over many cycles of excitation-emission have made the transition metal complexes particularly attractive. [1-4]. Lifetime of MLCT based triplet states, which are the lowest excited state of most frequently used Ru(II)-diimine types of sensitizer complexes, are often limited by the relaxation of the spin restriction of the triplet excited state decay to the singlet ground state, because of the relatively large spin-orbit coupling of Ru(II). Meyer et al. One way of circumventing this problem is to append to the diimine ligands an organic fluorophore like anthracene (An), whose triplet excited state is lower in energy than the ^{3}MLCT state of the excited Ru(II) dimine complex, so that facile energy transfer from the ^{3}MLCT state ultimately leads to formation of ^{3}An state in less than 5 ns [5].

Herein we describe the synthesis, characterization, and spectroscopic properties of Ru(II) complexes of 1-(9-anthrayl methelene)pyrazolyl pyridine (L^1) and 1-(9-anthrayl methelene)benzimidazolyl pyridine (L^2). Complexes 1 - 4 has been designed on the basis of varrying number of anthracene appended polypyridyl ligands. Luminiscence study shows that molecules with higher number of anthracene moieties yields higher quantum yield.

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IL-48

Expanding the Medicinal Chemistry Toolbox: From Method Development to Delivery of Drug Like Molecules

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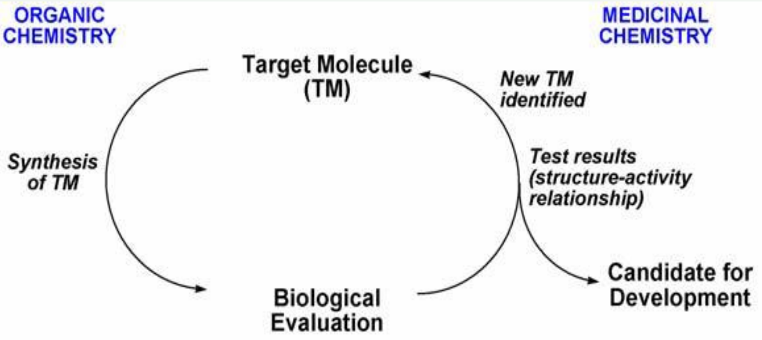
Abstract:
The pharmaceutical industry remains solely reliant on synthetic methodology to prepare drugs or drug like molecules for their discovery/process program. The expansion of synthetic methodology in recent years has greatly facilitated the preparation of molecules that would once have been considered an insurmountable synthetic challenge. In turn, the pharmaceutical industry, where large numbers of molecules are prepared and tested for their therapeutic use became the principal end-users and beneficiaries of this enlarged toolkit. Designing and discussing of various synthetic tools for the synthesis of pharmaceutically important heterocycles and generation of new chemotypes with translational potential will form the basic premise of my presentation.[1]



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IL-49

one-pot reactions for 2-pyridone and pyrano[2,3-c]pyrazole scaffolds enabling *In-vitro* anti-glioma activity

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Abstract

2-pyridone and and pyrano[2,3-c]pyrazoles were synthesized via one-pot reactions using greener routes and screened for their kinases and anticancer activity. A assembly of 26 compounds was assessed against different solid tumor cell lines, with compound 4j showing promising glioma growth inhibitory properties and was screened against 139 purified kinases and exhibited low micromolar activity against kinase AKT2/PKBb. AKT signaling is one of the main oncogenic paths in glioma and is repeatedly targeted for novel therapeutics. 4j exhibited significantly less cytotoxicity against non-cancerous cells even at fourfold–fivefold the concentration. While compound 5o showed anti-cancer properties against liver, breast, and lung cancers as well as primary patient-derived glioblastoma cell lines. Furthermore, 5o in combination with specific clinically relevant small molecule inhibitors induced enhanced cytotoxicity in glioblastoma cells.

Herein we establish a novel biochemical kinase inhibitory function for N-(4-chlorophenyl) substituted pyrano[2,3-c]pyrazoles and further report their anti-glioma activity in vitro for the first time.

IL-50

Synthesis of five- and six-membered heterocycles and their bioactivities

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Heterocyclic compounds are pregnant with multifaceted potentialities, such as pharmaceuticals, natural compounds, drugs, and agrochemicals. Besides their fundamental role in drug discovery, they are also used as sanitizers, developers, antioxidants, corrosion inhibitors, copolymers, and dyestuff. Therefore, heterocyclic compounds are indispensable parts of our daily life.

Various powerful methodologies for their synthesis have been developed in recent decades. Among different useful methodologies, transition metal-catalyzed heteroannulation is explored as a valuable and convenient method for forming five- and six-membered heterocycles. Here, I will discuss the use of palladium to construct various heterocyclic compounds. The presentation will focus mainly on two types of heterocycles; the first is "sultam" i.e., cyclic sulfonamide and the second is "sultone" i.e. cyclic sulfonates through some recent examples from our research group.[1-4] Some review articles are also there on the synthesis of heterocycles and catalysis, in our research group. [5-8] The first part of my lecture will focus on the recent development of our group on the Pd-catalyzed synthesis of five- and six-membered heterocycles. The second part will concentrate on the biological importance of the synthesized heterocycles.[9,10] The details will be presented at the conference.

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IL-51

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Abstract Awaited

IL-52

Electronic Structure and Electron Transfer in Transition Metal Complexes with Non-innocent (Redox-active) Ligands

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The study of metal-coordinated radicals has gained immense interest from perspectives of bio-inorganic chemistry, especially as model systems of various biologically active metalloproteins involved in multifaceted redox reactions in the body. One conspicuous example of such a metalloprotein is Galactose Oxidase. In recent years considerable interest is also directed to the understanding of electronic structures of transition metal complexes with redox-active/non-innocent ligands, due to their wide-spread presence in biological systems. The redox level of a non-innocent ligand (or ligands), coordinated to transition metal ions, cannot be unambiguously described by the chemical formula alone. In fact, the physical oxidation state differs from the formal oxidation state if an open shell organic radical is coordinated to transition metal ions [1-5]. From both these perspectives we have initiated a program to synthesize and to determine the molecular and electronic structure of such metal-coordinated radical complexes using non-innocent ligands. In this continuing attempt, we have used a series of spectroscopic and electrochemical techniques, and finally performed the electronic structural calculations using Density Functional Theory (DFT) at the B3LYP level and have attempted to assign the redox level of both the metal ion and the ligand. Specifically, we have synthesized non-innocent ligand system containing azo-appended *o*-aminophenolate functionality and transition metal complexes. In this presentation an overview of our activity in this field will be highlighted.

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IL-53

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Abstract Awaited

IL-54

Pre-Clinical Phase : DSST – In-silico Designing, Synthesis, Screening and Toxicity for NCE

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Abstract

In-silico designing of the new molecules using Schrodinger's software. Selection of molecules using various computational tools such ADMET, Docking, Pharmacophore, QSAR etc... Selected molecules are synthesized by the Green Chemistry method, purified and well characterized. Screening synthesized molecules for anticancer, antituberculosis, antimalarial activities and they are studied for the toxicity study too. We are working on per-clinical phase by DSST approach getting support of Schrodinger's software. The phase 0 work after taking proper approval in future may enter in Phase I.

IL-55

Tunable Plasmonic and Luminescent Nanocrystals : Soft Chemical Synthesis and Theranostic and Photocatalytic Applications

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Nanomaterials have touched every aspect of human life, however, most of their syntheses utilizes capping agents, reducing agents and solvents that are damaging to the environment. There is a need to make the processes greener and sustainable. The talk describes the aqueous syntheses routes for plasmonic and luminescent nanomaterials using mild reagents and eco-friendly conditions. In the first part, synthesis of hollow plasmonic nanoshells of silver is described which have tunable size, shape and structure. Application of such nansostructures in solar-catalysis and chemo-photothermal therapy will also be discussed. The choice of silver stems from the fact that it has highest quality factor for surface plasmons and greater photothermal efficiency in the spectral region of 400-1200 nm. Thus, it presents an opportunity to study the plasmonic properties over wide wavelength region and harness them for suitable applications.

Hollow silver nanoshells (HAgNS) with tunable plasmon bands were synthesized by employing a combination of mild reductant (hydrazine hydrate) and a mild stabilizer (sodium citrate). The plasmon peak was tuned in a wide range from 460 nm to 630 nm. In the second part, we also developed a method using folic acid as stabilizer. A peculiar folate-directed shape transformation from solid nanospheres to hollow silver nanocubes (HAgNCs) has also been discovered and temporal evolution was spectroscopically followed. Molar extinction coefficient (eSPR) at the plasmon peak was found to increase exponentially with the size.

The cube-shaped hollow silver nanoshells were found to be very good solar photocatalyst in the entire visible range at sub-picomolar level. These hollow silver nanocubes Furthermore, the Anisotropic Silver NCs vis-à-vis spherical have been found to act as an excellent SERS tool for the detection of metal ion contaminants such as of As (III), Cr(III) and Cr(VI).

Among the soft approaches for luminescent NCs, A supersaturation-controlled synthesis of ZnTe QDs was developed and their non-linear optical properties have been investigated by the Z-scan technique using a low power He-Ne laser (15mW, 632.8 nm) in a non-resonant condition. The ZnTe QDs having an average size of 0.8 nm and 1.7 nm followed the three-photon absorption model. The QDs were well-suited for the fabrication of all-optical switching devices. The self-assembled nanostructures also offer themselves as an attractive alternative to conventional materials in making waveguides for SCG application.

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IL-56

Carbocyclic nucleosides: Search for novel synthetic methodologies

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The search for novel carbocyclic nucleosides has been an intensive area of research, aiming at more efficacious antiviral agents. Rhodium-catalyzed reductive cyclization of 1,6-enyne cyclization has provided a unique 4’methyl-6’-substituted carbocyclic intermediate, which has been further explored as a close resemblance with Aristeromycin analogs. A systematic study to explore its potential and synthesize a series of carbocyclic nucleosides and to evaluate as potential antiviral agents.

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IL-57

Targeting skeletal muscle based NST towards countering metabolic diseases: Identifying mechanisms and molecules

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Metabolic syndromes including obesity and type II diabetes are becoming more and more common worldwide. It is widely accepted that this trend is due to dysregulation in the energy homeostasis of an individual. In our body, energy enters in the form of food and drinks. If the energy is not exhausted, body tries to store the unspent energy and this activates several metabolic remodeling of various organs, which is a major cause of initiating the program leading to the metabolic disorders. However, mammalians have ability to resist excessive weight gain due to energy surplus which has been termed as “Diet Induced Thermogenesis or DIT”. Ever since the discovery of DIT in 1970s, researchers have been focusing to delineate mechanisms that contribute to this process. Early studies established the role of uncoupling protein 1 (UCP1) in the inner mitochondrial membrane of brown adipose tissue (BAT) in DIT. BAT is the major organ of cold-induced nonshivering thermogenesis (NST) in eutherian mammals and it is suggested that sites of NST can be targeted to get benefit of activating DIT. We have shown that the other site of NST in mammals is the skeletal muscle. Now, there is a hot debate in the field as to which of these mechanisms of DIT can be the best to target pharmacologically for countering obesity (and/or diabetes) in humans. Muscle NST being based on futile cycling of calcium ions, seems to be a safer route to increase energy expenditure and reduce energy surplus thereby countering obesity. Therefore, it is necessary to carefully define the details of mechanism involved in activation and maintenance of muscle NST.

IL-58

Substrate induced catalyst formation under non-equilibrium conditions

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Abstract:
There remain critical gaps in our understanding of the emergence of functional biopolymers in the origins of Earth’s biosphere. For instance, extant proteins, evolved over millions of years, carry out an impressive array of responsibilities, from catalysis and molecular recognition to motility and compartmentalization. One of the major goals of our lab is to investigate the possible origins of advanced enzymatic functions from folds of short peptide based paracrystalline phases. Further, we are excited about understanding the non-equilibrium structures of living systems.[1-6] I will show our recent discoveries of simple chemical systems that can be substrate-driven to access higher energy self-assembled states, just as seen in natural microtubules. Further, I will attempt to sketch our aims of developing self-assembled autonomous materials that can show temporal control of functions.[5,7-10]

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IL-59

Identification of Siderophores and Their Sensory Applications

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ABSTRACT: India has an exclusive economic zone along the vast seashore covering 7500 km. The living and non-living resources of this zone with rich biodiversity, bioactive substances, and microbial resources measure about two third of the total land mass of the country. Enormous research opportunities on Indian marine resources have largely remain unexplored. For example, how do open-ocean microorganisms acquire metal ions for their nutrition? What are the chemical nature of various metal chelators whose existence have been well demonstrated in the literature? Is the chemistry of several metals in surface seawater controlled by the metallophores that are secreted by the prokaryotes? Because of nutritional requirements, microorganisms/fungi/plants sequester metal ions via a range of mechanisms. A classic system of “microbial-iron” interaction involves low molecular weight metal-chelating molecules called “siderophores”. These ionophores are polar and hydrophilic in nature. In this presentation, a brief overview on the chemistry of siderophores will be provided followed by the discussion on the isolation and structural characterization of siderophores. Various biotechnological applications of the siderophores particularly, sensory applications will also be discussed in this presentation.

IL-60

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Abstract Awaited

IL-61

Stereoselective Synthesis of Natural Product Inspired Glycohydrids as Anticancer Agents

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Abstract Awaited

IL-62

High-throughput Identification of Novel Anticancer Molecules from *Roscoea purpurea*

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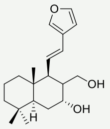
Abstract:
In our ongoing research program to discover bioactive natural products from natural resource especially from high altitude with profound biological activities, our interest was focused on the *Roscoea purpurea* (rhizomes) commonly known as "kakoli". *Roscoea purpurea* is an essential ingredient of an important Ayurvedic preparation known as *Astavarga*, which is a group of eight medicinal plants claimed to be useful in promoting body fat, healing fractures, seminal weakness, fever, abnormal thirst, diabetic conditions and as a cure for vata, pitta, rakta doshas.[1] *Astavarga* plants are considered as very good *Rasayana* with rejuvenating and health-promoting properties, and are known to strengthen the immune system and have immense cell regeneration capacity.[2] *Astavarga* plants are also reported to restore health immediately and work as antioxidants in the body.[3-5] Amongst eight Astavarga plants *Roscoea purpurea* is one of the essential ingredients of several herbal formulations like tonic and Chyawanprash. Traditionally it is used for the treatment of diabetic, hypertension, diarrhea, fever, inflammation etc. In Nepal, the tubers are boiled for edible purpose and also used in traditional veterinary medicine.[6] We were mainly interested in the traditional use of the rhizomes of *Roscoea purpurea* as immuno-potentiating agent. In the view of its importance in traditional medicinal system, no substantial phytochemical and pharmacological works have been carried out. Previous phytochemical investigations on *R. purpurea* have described the isolation of two principal groups of compounds, steroids and phenolic derivatives.[7-9] To date, only few compounds have been identified and quantified through HPLC analysis from tubers of this plant by Singh and co workers,[7-9] and they are presumed to be associated with its potent antioxidant activity.[10-11]



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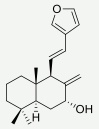

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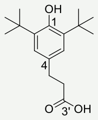

3

Ethanolic extract of the plant have shown *in-vitro* anti cancer and anti-oxidant activities. In this study, a fraction of the crude extract guided by the anti-cancer bioactivity led to the isolation of potent anticancer compounds **1-3** along with several known compounds. The structures of isolated compounds were elucidated by detailed spectroscopic 1D/2D analysis. In this presentation, we will talk about isolation, structure elucidation and anticancer activity of compounds **1-3**. We will also discuss different methods used to prove the authenticity of natural origin of **3,** a rare 3-(3,5-di-*tert*-butyl-4-hydroxyphenyl) propanoic acid commonly known as Fenozan acid (FZA).

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IL-63

Catalysis, Sensing and Phytofabrication of metallic nanoparticles: From Green Synthesis to Environmental Remediation

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The green synthesis of nanoscale materials is of special interest to researchers all over the world. We describe a simple, robust, inexpensive, and environmentally friendly approach to the synthesis of gold, silver, copper and iron oxide nanoparticles using a variety of biomolecules/phytochemicals as potential reducers and stabilizers. The green approach to the controlled synthesis of nanoparticles with different morphologies is based on the use of plant extracts. In this lecture, current plant-mediated strategies for preparing nanoparticles of gold, silver, and iron are briefly described, and morphologically dependent nanoparticles for the antioxidant activity, H_2O_2 sensing, catalytic activity for the remediation of organic pollutants are highlighted. Overall, the approach presented in the article supports environmental protection and is a promising alternative to other synthesis techniques.

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IL-64

"Safety Evaluations of Herbal Preparations in Experimental Animals"

Prof. R. K. Singh

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Abstract:-

Regulatory toxicity studies have become mandatory for herbal preparations in experimental animals like mice, rats, rabbits and monkeys. These studies are acute and subacute toxicity studies, reproductive toxicity studies, genotoxicity and carcinogenicity studies. In most of the countries of the world, O.E.C.D. Guidelines (2005) are being followed for the above studies.

The comprehensive toxicology studies on herbal antimalarial and hepatoprotective compounds were carried out by my research group in experimental animals in which no adverse effects were found.

IL-65

Bioentrepreneurship - Platform beyond business!

Dr Nivedita Jena

Scope of Biotech and Current startup Ecosystem
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Abstract

The biotechnology “startups” and entrepreneurship world offers exciting new avenues for driving state-of-the-art research from the lab to the market. The realm and the role of the bioscience sector are rapidly changing, creating new opportunities for small startups in this area. The Indian stratup ecosystem is growing, and the government has made significant headway in creating ample opportunities for researchers and scientists to take their research to commercialization. The number of startups in India has grown rapidly over the last few years, making an impact by improving people’s health through science and innovation. Enablers like DBT-BIRAC, NITI Aayog, Meity, and MSME have contributed immensely to this feat. The other enablers for the increase in small startups/companies are large pharma companies. Large pharmaceutical companies downsize and outsource their R & D work to smaller companies. The two strategies employed by large companies are 1. Acquiring smaller or startup biotechnology companies provides support for their development efforts. 2. Collaborate with academics for their research efforts. This strategy helps in more efficient and less expensive for the companies. These strategies have created ample opportunities in these areas. This talk will focus on several initiatives taken up by the government (BIRAC schemes and schemes from DST) and entrepreneurship opportunities and trendsavailable in India for all scientists to collaborate and start a new venture that can create an impact and benefit society with technology.

SHORT GUN

SG-1

Activated porous carbon materials /graphene /nanoribbons synthesis for energy production and storage applications

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Carbon materials based electronics that are flexible compare to rigid counterparts became potentially applicable for next generation displays, lightings or energy storage and conversion devices including solar cells or battery.[1] Practically flexible electronics possible if indium-tin-oxide (ITO) electrode is especially replaced by some organic materials which are transparent and conducting as well as exhibit unique mechanical, electronic properties with excellent optical transmittance behavior.[2] However, porous carbon materials such as covalent organic frameworks (COFs), conjugated microporous polymers (CMPs), covalent organic polymers (COPs), and holey graphene materials have emerged in the last decade with outstanding applications in energy production and storage devices applications such as hydrogen fuel production (Figure 1),[3-7] solar cells (SCs), field effect transistors (FETs), light-emitting diodes (LEDs) and supercapacitors applications *etc*. Organic electronics are generally based on conducting polymers, but recently it has been observed that semiconducting nature of porous carbon materials such as warped poly aromatic hydrocarbons (PAHs),[8-9] defective graphenes (defects arise either by warped structure and ordered pore structure or by doping), graphene nanoribbons (GNRs), COFs, CMPs make them potential candidates for future electronics.

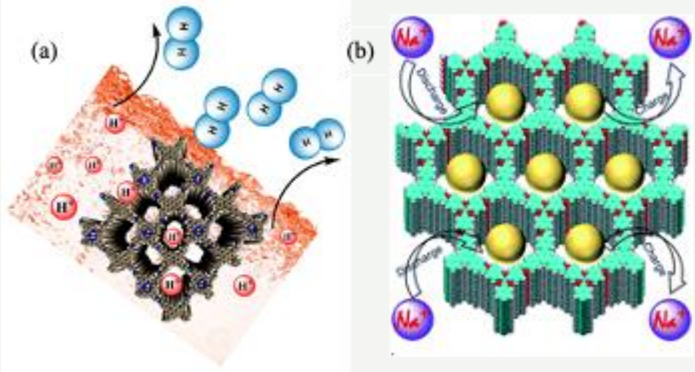

Figure 1: (a) and (b) Porous COF materials for hydrogen fuel and storage battery application respectively

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SG-2

Photo-mechanical molecular crystals: a future machinery tool

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Nature provides numerous examples of light-powered devices that can autonomously change their shape, size or display static/ dynamic motion in presence of natural light. Mimicking such function in the laboratory, i.e developing light powered autonomous micro/macro-machines using soft organic/metal organic molecular material represents one of the most difficult challenges in today's research and demands huge imagination, skills and tedious efforts from the involved researchers. Smart organic crystalline materials that are capable of displaying macroscopic responses such as shape deformation, size alteration or motion under light illumination have emerged as potential candidates for this purpose. The design of such molecules is accomplished by incorporating a photo-active unit that can absorb photons to initiate photoresponse and a suitable supramolecular synthon for non-covalent interactions for the propagation. On the simplest mechanistic view, the molecular motion triggered by light is cooperatively amplified to supramolecular to macroscopic scale with the help of intermolecular cooperative mechanism involving reconfigurable non-covalent interactions. While few such molecular crystals have been reported to exhibit fascinating macroscopic mechanical responses, the quest for developing new molecular systems having superior or novel mechanical responses is a never-ending process in material chemistry research. In this invited talk, we shall discuss about some of the novel light responsive materials that have recently been developed in our laboratory.

SG-3

Storage and stabilization of biomacromolecules in a nanotubular ionic covalent organic framework

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Biomacromolecules like Ribo-nucleic acids (RNA) are widely studied by biologists and chemists for understanding their role in cell chemistry and genetics. But these molecules are prone to rapid degradation in the extracellular environment. Traditionally, these are preserved by storing them at -20 ^{o}C to -80 ^{o}C. Investigating methods for storing biomacromolecules at room temperature has emerged as an interesting challenge. Recent studies show that ionic liquids (ILs) can act as an efficient solvent for storing various enzymes, biopolymers and proteins [1]. A mechanistic study by Tulsiyan et al. revealed that biomacromolecules are stabilized in choline amino acid-based ILs via an interaction with the cationic charge of the IL [2]. But ILs are generally toxic and moreover, high vapor pressure of ILs makes recovery of biomacromolecules from a solution of ILs a cumbersome process. A more appropriate platform for the storage of these biomolecules will be inside ionic porous solid materials. Covalent organic frameworks (COFs) are a class of crystalline, porous organic materials constructed by connecting molecular organic building blocks through dynamic linkages. In this work, we have prepared an imine-linked ionic COF with nanotubular morphology. Biomacromolecules are encapsulated inside the nanotubular COF and stabilized via a favorable interaction with the cationic charge. The loading activity of the ionic COF is compared with another non-ionic COF with a similar pore size. A higher loading capacity and extended stabilization period of the biomacromolecules were observed with the ionic nanotubular COF.

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SG-4

A riveting combination of various computational approaches to design, optimize and predict the bioactivity of highly selective and potent PKM2 modulators

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Pyruvate Kinase M2 (PKM2) plays a critical role in cancer metastasis by switching to an inactive dimer that causes the accumulation of glycolytic metabolites promoting tumorigenesis. Dimeric PKM2 has also been observed to undergo nuclear translocation promoting transcription of various oncogenes. The evident dearth of anticancer modulators targeting PKM2 in tumors has gained importance among researchers to design potent activators/inhibitors that could offer a potential therapeutic strategy to control cancer progression.

Herein, we have attempted to address the persisting dearth of PKM2 modulators using various computational approaches. In the first approach, boronic acid-based potent PKM2 activators were designed using the scaffold hopping strategy. Thorough MD simulations analysis performed on a few selected compounds revealed a modulator which was capable of stabilizing the center of the dimeric interface that promotes PKM2 tetramerization. In the second approach, the link and grow strategy was incorporated to design novel imidazopyrimidines-based anticancer modulators. The most potent modulator selected for MD simulations demonstrated their potential to form and stabilized the functional relevant tetrameric conformation. In the third approach, knowledge-based drug discovery was employed to design a virtual library of palindromic and non-palindromic PKM2 activators by incorporating the knowledge of functional groups, rings, and any interesting structural feature present in the data set of experimentally known PKM2 activators All the virtually designed compounds were observed to confer high-binding affinities ranging from -15.0 to -9.1 kcal/mol to the receptor protein. These activators also demonstrated optimum pharmacokinetic and toxicity profiles. Importantly, these activators were conclusively observed to stabilize the required tetrameric conformation in the dynamic environment, suggesting that they have the potential to restore the normal glycolytic pathway. Finally, to overcome the existing limitations in synthesis and biological evaluation of potential drug candidates, we have designed an AI-based model by utilizing molecular descriptors and testing various machine-learning algorithms. This model was used for predicting the bioactivity of novel computationally designed PKM2 modulators.

SG-5

Cobalt bis(terpyridine) complex as an efficient photosensitiser for photocatalytic hydrogen evolution

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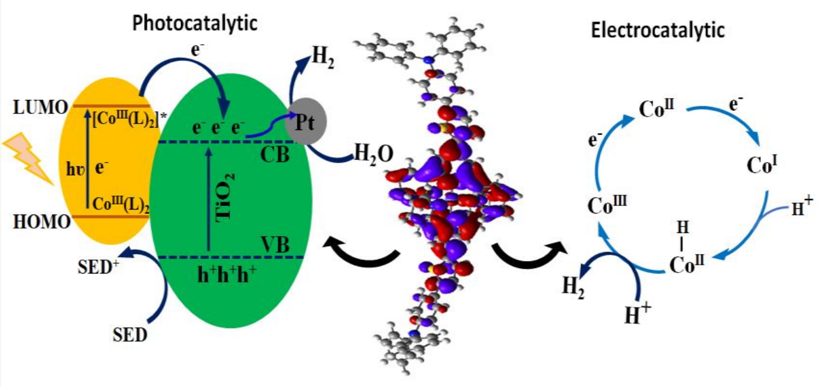
Photocatalytic hydrogen evolution is considered to be the holy grail of artificial photosynthesis. Here, we demonstrate a novel cobalt bis-(terpyridine) complex that functions as a photosensitizer for hydrogen production over platinized TiO_2 catalyst under visible light in the presence of sacrificial electron donor (SED) i.e. methanol. The Co bis-(terpyridine) complex-Pt/TiO_2 photocatalyst exhibited excellent activity for hydrogen evolution (2859 $\mu molg^{-1}$) with a high turnover number (5718) and apparent quantum yield (AQY) of 5.34% compared to the corresponding bare Pt/TiO_2. Moreover, the catalyst shows electrocatalytic activity for the reduction of protons in acetonitrile solvent using trifluoroacetic acid (TFA) at 0.63 V with a turn-over frequency of 18.64 s^{-1} with an 8:1 ratio of the acid to the catalyst. The additional donating group 4'-(5-(4-diphenylamino)phenylthiophen-2-yl)-2,2':6',2"-terpyridine π-conjugated bridge unit provide an excellent surface protection through steric hindrance leading to a good photocatalytic performance. This work will lead to the development of newer integrated photocatalysts for visible light assisted hydrogen evolution.



SG-6

Exploring The Application of Pirfenidone-Fumaric acid Cocrystal in Developing a Sustained Release Formulation by Comparative Bioavailability Study: From Bench-side to Bedside

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Pirfenidone (PFD) is the first pharmacological agent approved by the US Food and Drug Administration (FDA) in 2014 for the treatment of idiopathic pulmonary fibrosis (IPF). The recommended daily dosage of PFD in patients with IPF is very high (2403mg/day) and must be mitigated through additives. In this work, the cocrystallization of pirfenidone with Fumaric acid (FA) is explored as an alternative approach to reducing its solubility and the new crystalline solid is thoroughly characterized by single crystal X-ray diffraction (SCXRD), powder X-ray diffraction analysis (PXRD), fourier transform infrared (FTIR) spectroscopy, differential scanning calorimetry (DSC), and thermogravimetric analysis (TGA). Equilibrium solubility and intrinsic dissolution rates (IDR) are studied for the cocrystal and compared to that of the parent drug. PFD-FA cocrystal exhibits drastically lower aqueous solubility and dissolution rates, rationalized based on both lattice energy calculations and consideration of intermolecular interactions in the solid state. Furthermore, sustained-release (SR) formulations of the PFD-FA cocrystal of two different strengths such as 200 and 600 mg are prepared and its comparative bioavailability in healthy human volunteers is studied against the reference formulation PIRFENEX (200 mg). A single-dose pharmacokinetic study (200 mg IR vs 200 mg SR) demonstrates that the test formulation exhibits lower C_{max} and T_{max} in comparison to the reference formulation, which shows that the cocrystal behaves like an SR formulation. Further in the multiple-dose comparative bioavailability study (200 mg IR thrice daily vs 600 mg SR once daily), the test formulation is found bioequivalent to the reference formulation. This work suggests that cocrystallization offers a promising strategy to reduce the solubility of PFD and opens the door for potential new dosage forms of this important pharmaceutical.

SG-7

Understanding Biomolecular Recognition in Human Interleukin for Therapeutic Intervention

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Human interleukin-6 (hIL-6) is a multifunctional cytokine that regulates both innate and adaptive immunity along with inflammatory responses, metabolic processes, regenerative processes, and cancer. hIL-6 is responsible for the transition from chronic to persistent state of a plethora of diseases such as ulcerative colitis, Castleman's disease, Crohn's disease, rheumatoid arthritis, diabetic nephropathy, acute kidney disorder, myeloma, and COVID-19. Despite its involvement in several diseases, the assembly mechanism of the signaling complex formation of hIL-6 is not well understood. The formation of signaling complex of hIL-6 is a multi-step process. The first step in the signaling cascade involves binding of hIL-6 to IL-6R□ which then binds to ubiquitously expressed gp130 to form the ternary complex. This complex then homodimerizes to form the hexamer signaling complex. There is a potential to design and develop novel small molecule IL-6 antagonists from the insights obtained from understanding the structural basis for IL-6/IL-6Rα interactions. We use molecular dynamics simulation to understand the binding of hIL-6 to IL-6R□ that forms the crucial step in the signaling cascade of hIL-6 as hIL-6 cannot bind to gp130 directly. Our study reveals that the binding of hIL-6 with IL-6R□ induces structural and dynamic rearrangements in hIL-6 which subsequently facilitate the binding of hIL-6/IL-6R□ to gp130. The formation of hIL-6/IL-6R□ complex disrupts the intra-protein contacts in hIL-6 leading to an increase in flexibility of residues 48-58 of the flexible AB loop region along with rigidification of residues 59 to 78 in the same loop due to the formation of surface contacts with the receptor. The binary complex is primarily stabilized by two pairs of salt bridges, Arg181 (hIL-6)- Glu182 (IL-6Rα) and Arg184 (hIL-6)- Glu183 (IL-6Rα) as well as hydrophobic and aromatic stacking interactions mediated essentially by Phe residues in both proteins. An interplay of electrostatic, hydrophobic, hydrogen bonding, and aromatic stacking interactions facilitates the formation of the hIL-6/IL-6Rα complex. The understanding of interactions that drive the formation of hIL-6/IL- 6Rα complex is important in finding potential antagonists that can inhibit the formation of the complex and curb the downstream effects of hIL-6.

SG-8

Simplified & Affordable Arsenic Filter (SAAF):A solution to prevent arsenic poisoning

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ABSTRACT:

Drinking water containing arsenic more than the WHO MCL (10 ppb) is deemed to be unsafe. Although technologies exist to remediate arsenic in groundwater, most of them are either too expensive or involve complex technicalities which make their operation difficult in resource poor communities of developing countries. To address this problem; A cost-effective household gravity-based water purifier was developed for effective filtering of arsenic from water. The device comprises layers of naturally available iron ore fines (IOF) and manganese ore (MO) as adsorbent media combined with sand, gravels, and silver impregnated activated charcoal; where a layer of IOF is sandwiched between two layers of MO. This configuration provides synergistic effect of higher oxidation potential of MO to oxidize non-ionic As(III) to ionic As(V) and enhanced As(V) sequestration properties IOF. This filter unit is also capable to remove high concentration of iron which is usually present in the arsenic contaminated ground water. This device can deliver 210-240 L(flow rate of 10-12L/h) safe drinking water as per the BIS and WHO drinking water standard. Moreover, the purifier is of low-cost, user-friendly and does not require skilled man-power for its operation.

Keywords:*Arsenic, adsorption, water filter,iron ore fines (IOF), manganese ores (MO)*

SG-9

Copper-Catalyzed hydroboration of 1,3-Diynes as a Platform for Iterative Functionalization

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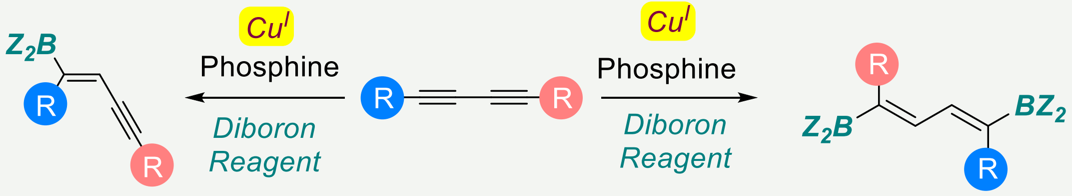
Over the past few decades, synthetic approaches to small molecules bearing diverse functionalities have witnessed an overwhelming transformation. Targets with high structural complexity can be easily assembled using small, modular building blocks similar to a 'Lego' construction using Iterative chemistry.[1-3] Organoboron compounds have been in the spotlight as versatile building blocks in natural product synthesis.[4] In this work, we present glovebox-free regioselective hydroboration of 1,3-diynes using bench stable boron source and Cu(I)/phosphine catalysis to access stable enynylboronates in a single operation. A variety of symmetrical and unsymmetrical 1,3-diynes were tolerated under these reaction conditions to produce enynylboronates in excellent yields and regioselectivities (up to >95:5). Under similar reaction conditions, one-pot dihydroboration of 1,3-diynes was also achieved to access a wide variety of bench stable dienylboronate esters in good yields and regioselectivities. Downstream transformations with enynylboronates and dienylboronates offered a range of value-added skeletons. DFT studies supported the proposed mechanism for the formation of hydroboration and dihydroboration products.



♦ Iterative Coupling Ready ♦ High Regioselectivity ♦ Glovebox Free
♦ Broad Substrate Scope ♦ Optical properties

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SG-10

Mechanochemistry: An Opportunity to do Engineering in Metal Organic Frameworks (MOFs)

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Mechanochemical synthesis exhibits enormous potential for the clean, economic and environmental-friendly efficient route for the chemical and structural transformation of molecules and materials. Over the years, mechanochemical grinding method has been used in important organic conversions such as asymmetric organocatalytic aldol reactions, Knoevenagel condensations, oxidative amidation of aldehydes etc. Recently the mechanochemical synthesis via neat grinding, liquid-assisted grinding (LAG) have shown significant potential for the construction of extended frameworks.

My work based on an attempt to design and synthesis of new phase pure MOF materials by solid state grinding or ball mill method. These types of mechano synthesized Phase pure MOF material is very rare and not possible to synthesize by traditional solvent based synthesis where the mixture of isomeric forms have been isolated. Time dependent kinetics study during the mechanosynthesis process revealed the formation of new metastable phases with the function of grinding time which is confirmed by powder X-ray diffractions. Less crystallinity, short of long range order and creation of defects in the structure of these mechanochemically synthesized MOFs afforded enhanced electrocatalytic activity towards oxygen evolution reaction (OER) in Fuel cell. Additionally, I will explain about the solvent-free mechanical milling process for two distinct MOF crystals induced the formation of a solid solution, which is also not feasible by conventional solution-based synthesis. This is the unique way to discover new phase of materials by mechanochemical synthesis which are unexplored yet in Metal-organic based materials.

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SG-11

Discovery of a potent first-in-class inhibitor of Aurora B Kinase for triple negative breast cancer

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The drug discovery and development efforts in the last couple of decades targeting Aurora Kinase B establish the crucial role of this kinase in several cancers. Unfortunately, these efforts did not result in any clinical success. The findings in recent years are particularly important as the role of Aurora B and its inhibitors in some major challenges in today’s oncology, like triple-negative breast cancer and EGFR therapy resistant lung cancers is identified. In this work, a based on screening a fragment library, a quinazoline-based Aurora B inhibitor was discovered. Following a series of medicinal chemistry cycles, the structure-activity relationship was established and a lead compound, SP-96 was identified with sub-nanomolar potency. Enzyme kinetics studies revealed SP-96 as a non-ATP-competitive inhibitor. The compound also shows growth inhibition of MDA-MB- 469, a triple-negative breast cancer cell line.

SG-12

Fortification in India: Current trend and future prospect

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Indian food habits are mostly concentrated on cereal-based product. They are deficient in micronutrients and merely fulfil the daily requirement of many essential nutrients. Thus, the bottom-line population of the income pyramid suffers from several public health problems related to nutrient or combined nutrient deficiencies. This includes iron (and other nutrients) deficiency anaemia, stunting, low-quality pregnancy leading to low birth weight, and vitamin A, folate, vitamin B12, zinc, omega-3 PUFA and vitamin D deficiency. Since neither the macro nor small nutrient deficiency disease happens in isolation, it requires combined intervention rather than treatments. To improve daily micronutrient status, food-to-food fortification or supplements have been recommended to remedy this global nutritional disorder. According to the recent NFHS 5 report, at least 67 percent of children (6-59 months) have anaemia compared to 58.6 percent in the last survey conducted in 2015-16. Among adults, 57 per cent of women and 25 percent of men (in the 15-49 group) have anaemia, and among women, its prevalence has increased from 53 percent in 2015-16 to 57 per cent in 2019-21. In men, it has risen from 23 percent to 25 percent. Thus, a low-cost indigenous technological solution is critical to combat micronutrient deficiencies. This lecture will present the current status and encompass the future prospec of micronutrient fortification.

ORAL

OL-1

An Ultra-highly Stretchable, Adhesive Transparent, Flexible, Pressure and Electro sensitive Hydrogel for Motion Sensing

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A multi-stimuli sensitive hydrogel has been produced through the grafting of acrylamide and *N*-hydroxy methyl acrylamide onto β-Cyclodextrin skeleton.[1] The developed hydrogel β-CD-*g*-(pAAm/pHMAm) displayed several remarkable features including ultra-high stretchability (>6000%), flexibility, stab resistivity, self-recoverability, electro-responsiveness, pressure-responsiveness, adhesiveness and high transparency (>90%). In addition, the gel exhibit biocompatibility, UV resistance as well as thermoresponsive shape memory properties. Based on these striking characteristics of the hydrogel, a flexible transparent pressure sensor for the real time monitoring of human motion have been fabricated. Besides, the sensor based on the gel exhibited high sensitivity (0.051 kPa^{-1} for 0–3.3 kPa) due to its nanofibrillar surface morphology. The flexible sensor exhibits very rapid response time (130 ms-210 ms) with acceptable stability (5000 cycles). Remarkably, the sensor can quickly sense both robust (index finger and wrist motions) as well as the tiny (swallowing, phonation) physiological actions.

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OL-2

Development of potent and selective Malic enzyme 3 inhibitors for the treatment of pancreatic cancer

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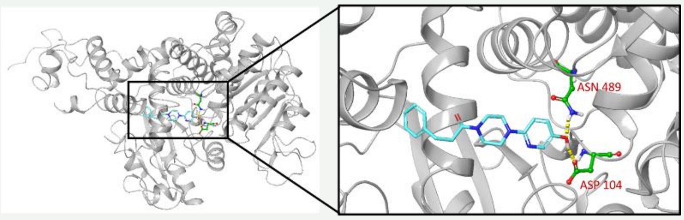
Abstract:

It is well documented that overexpression of Malic enzyme (ME) isoforms correlates with poor prognosis in diverse cancers [1-7]. ME plays a critical role in tumor development by catalyzing oxidative decarboxylation of L-malate into pyruvate and simultaneously reducing NADP+ to NADPH. While pyruvate production helps in generation of cellular building blocks, NADPH is required for maintaining redox homeostasis and energy production [8].



in silico binding mode of lead molecule with ME3 enzyme

In pancreatic ductal adenocarcinoma (PDAC), tumor suppressor gene SMAD4 is deleted along with its neighboring gene ME2. Dey *et. al.*, through compelling in vitro and in vivo experiments, demonstrated that in this genetic event ME3 takes over the role of ME2 [8]. Hence, targeting ME3 could be a potential therapeutic strategy for PDAC patients with SMAD4 and ME2 deletions. Hitherto no selective small molecule inhibitor of ME3 has been reported in the context of PDAC. Through molecular docking studies and exploration of structure activity relationships, potent and selective ME3 inhibitors were designed and synthesized. These compounds were capable of engaging with ME3 in cell lysates and exhibited growth inhibition of ME2$^{-/-}$ PDAC cells viz. BxPC-3.

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OL-3

In Vitro Evaluation of Cytotoxicity and Anti-Metastatic Properties of Novel Arene Ruthenium(II)-Tetrazolato Compounds on Human Cancer Cell Lines

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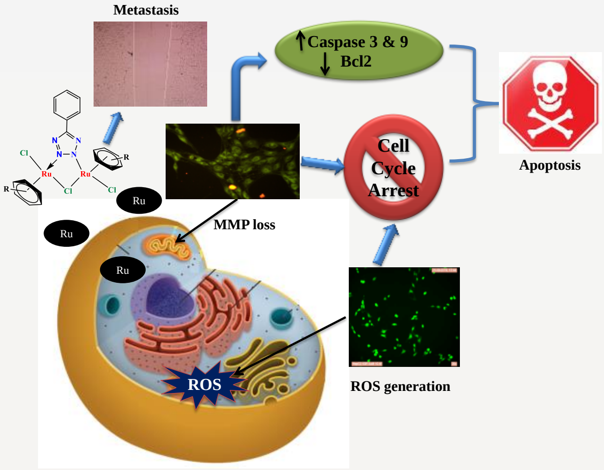
Abstract

Two new arene Ruthenium(II) complexes with chemical formula $[Ru_2(\eta^6\text{-}p\text{-cymene})_2(\mu\text{-L1})(\mu\text{-Cl})Cl_2]$ **[Ru]-1** and $[Ru(\eta^6\text{-}p\text{-cymene})(L2)Cl_2]$ **[Ru]-2** (**L1** = 5-phenyl-2H-tetrazole and **L2** = 2-(2H-tetrazol-5-yl)pyridine) were synthesized. Both the complexes were structurally characterized using single-crystal X-ray diffraction and other analytical techniques. The X-ray crystal structures of both the complexes revealed the coordination of tetrazolate ligands to two Ru(II) centres in bridging mode in **[Ru]-1,** while one Ru(II) centre in **[Ru]-2** in chelating fashion, with overall pseudo-octahedral geometry. The resulted complexes were screened for their cytotoxic activity against three different cancer cell lines, HCT116 (Colon cancer), HepG2 (Liver cancer) and MCF7 (breast cancer) under *in vitro* conditions. Interestingly, **[Ru]-1** showed much higher cytotoxicity with respect to **[Ru]-2** against all the screened cancer cell lines and even better than cisplatin. For exploring the mechanism of action of **[Ru]-1**, reactive oxygen species (ROS) production, alterations in mitochondrial membrane potential and gene expression profiling of apoptosis related genes (Bcl2, caspase-3 and caspase-9) were also evaluated. The cancerous cells treated with **[Ru]-1** showed an increase in intracellular ROS levels, disruption of mitochondrial membrane potential, up-regulation of proapoptotic caspase-3 and caspase-9 and down-regulation of antiapoptotic Bcl2. The results concluded that **[Ru]-1** induced apoptosis through oxidative stress mediated activation of intrinsic pathway by generating intracellular ROS, loss of MMP and alteration of expression of apoptosis related genes. In addition, antimetastatic activity of **[Ru]-1** was observed by wound healing assay showing anti-migratory property. The dual properties, antimetastatic activity and high cytotoxicity make **[Ru]-1** potent platform for the development of new anticancer agents.

Keywords: Arene Ru(II) complexes; Tetrazole ligands; Antimetastasis; Genome profiling; Cytotoxicity



OL-4

An Insight into Binding of Chrysophanol and Aloe-emodin to G-Quadruplex DNAs (HTel-22 and wHTel-26) using Spectroscopic and Molecular Docking Techniques

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ABSTRACT

Reports suggest telomeres, an attractive target for anticancer agents due to its role in cancer progression. The G-quadruplex stabilization by binding of small ligands in these telomeric units can disrupt telomere length limiting cancer cell proliferation. The present study deals with the interaction of anthraquinone compounds i.e. chrysophanol and aloe-emodin with Human Telomeric DNA (22-mer sequence) HTel-22: [d-{AGGG$(TTAGGG)_3$}] in Na^+ and Wild Type Human Telomeric DNA (26-mer sequence) wHTel-26: [d-{TT$(TTAGGG)_4$}] in K^+ using absorbance, fluorescence, circular dichroism spectroscopic and molecular docking techniques. The formation of G-quadruplex DNA was confirmed by signature peaks in CD spectra at 295 and 245 nm maxima, 265 nm minima for HTel-22 and maxima at 290 nm, shoulder at 265 nm and minima at 238 nm for wHTel-26. In absorbance spectra of chrysophanol and aloe-emodin with both quadruplex DNA sequences, the maximum shift in wavelength ($\Delta\lambda_{max}$) of 30 nm and 3-5 nm was observed suggesting the possibility of classical intercalation and external binding respectively. The binding affinities for both drugs have been observed in the binding range of 10^4 to 10^5 M^{-1} with the significant decrease in absorbance and fluorescence quenching spectra. Molecular docking studies revealed the involvement of common functional groups such as 8-OH, 1-OH, 9-CO and 10-CO in the structure of both chrysophanol and aloe-emodin. Additionally, the 3-CH_2OH group of aloe-emodin has also been involved in the interaction. The present knowledge on binding mode will be helpful in preparing alternate derivatives of anthraquinone which can act as a more potent telomerase inhibitor.

OL-5

ANTIPLATELET ACTIVITY OF AN ANTICOAGULANT PLA$_2$ FROM *Daboia russelii* VENOM

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Cardiovascular disease (CVD) is the largest single cause of mortality worldwide [1]. They have been associated with dysfunctional coagulation pathway or its components which subsequently results in heart attacks or strokes. The present management for CVDs mainly include pharmacotherapy and surgical procedure [2], [3]. Snake venom, which is a complex mixture of proteins targets the haemostatic system of prey/victim and the proteins targeting this system has been exploited for development of drugs. Several drugs used in the current treatment such as Eptifibatide and Tirofiban include bioactive components from snake venoms [4]. Symptoms observed during *Daboia russelii* envenomation such as persistent and profuse bleeding at the bite site is due to venom protein's interference in the blood coagulation cascade and platelet aggregation pathway after snake bite. Venom proteins affect platelet function by binding or degrading platelet receptors and modulating the activities of the agonists [5].

In this study, using a combination of Gel filtration chromatography and Reverse phase HPLC, an anticoagulant PLA$_2$, Daboxin P was isolated from *Daboia russelii* venom. Its effect on platelet aggregation induced by various agonists was studied and it was found that inhibition of thrombin induced platelet aggregation was the highest. In order to understand whether Daboxin P binds thrombin or its receptor, in silico interaction studies were performed and it was observed that the site of interaction of Daboxin P on the surface of thrombin is similar to the site of interaction of thrombin receptors, PAR1 and PAR4. The result of this experiment was further supported by biochemical and biophysical interaction studies.

Thus, the present study is an attempt to understand the anti-platelet effect of an anticoagulant PLA$_2$ enzyme from *Daboia russelii* venom and to understand its mechanism of action.

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OL-6

Unveiling the synthesis of isoxazolidines from intramolecular [3+2] nitrone cycloadditions in terms of molecular electron density theory

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Isoxazolidines represent an important class of five membered heterocycles with diverse range of biological properties[1]. The [3+2] cycloaddition (32CA) reactions of nitrones are among the classic synthetic strategies to generate chemo-, regio- and stereochemically defined isoxazolidines [1]. In 2016, Domingo [2] proposed the molecular electron density theory (MEDT) to identify the decisive role of electron density changes on molecular reactivity which has been successfully applied to analyze several (32CA) reactions [3-7]. The present MEDT study analyzes the regio- and stereoselective synthesis of isoxazolidines from intramolecular nitrone cycloadditions (Figure 1) by locating the transition states (Figure 2), electron localization function, conceptual density functional theory (CDFT) indices, and intermolecular interactions.

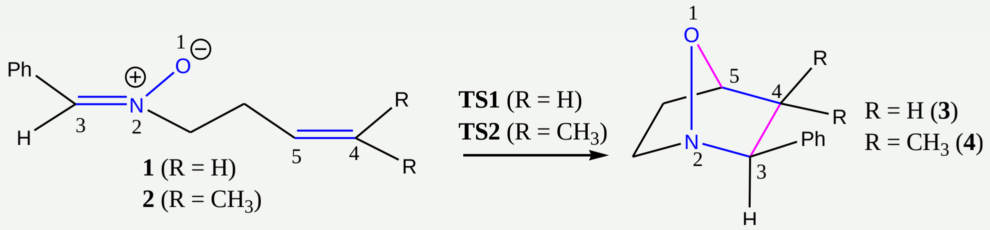

Figure 1. Intramolecular 32CA reactions of **1** and **2** to generate isoxazolidines **3** and **4**

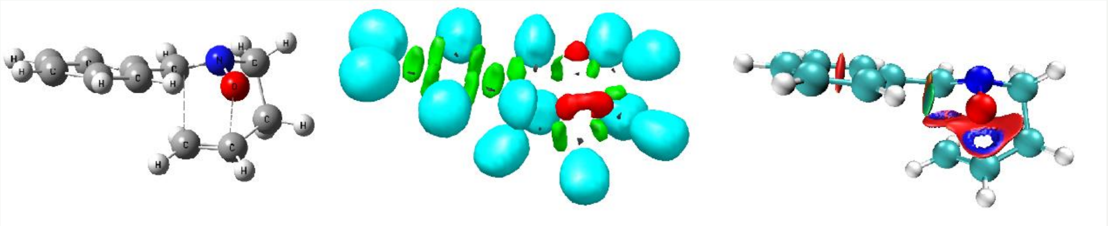

Figure 2. MPWB1K/6-311G(d,p) optimized geometry, ELF domain and NCI isosurface of **TS1**

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OL-7

Synthesis, Characterization and Application of Graphene/Zr Composite Supported on Activated Carbon for Efficient Removal of Fluoride from Drinking Water

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Abstract

Fluoride (F) is a serious public health issue in many regions of the world because of elevated concentration in water resources. Defluoridation of drinking water requires cost-effective adsorbents. The G/Zr/AC, which had been synthesized and characterized via transmission and field emission scanning electron microscopy, N_2 physisorption, energy dispersive X-ray spectrometry, Fourier transform-infrared spectroscopy, and X-ray diffraction. In addition, the point of zero charge was determined. The G/Zr/AC sorbent removal of fluoride from water was investigated in batch system under various conditions. The results showed that at low pH values, the G/Zr/AC Composite was more effective at adsorbing fluoride, with a maximum adsorption of 74.6 %.Among the conditions of temperature and agitation evaluated, the best results were achieved at 30 °C and 200 rpm, with removal percentages equal to 60.6% and 67.4%, respectively. The system proved equilibrium after four hours of operation. While the equilibrium data were best represented by the Langmuir isotherm (linear/non-linear) with maximal adsorption capacity equal to 81.47 mg/g, the pseudo second order kinetic model best described the kinetic data. In other words, the findings we got prove that the material produced is highly absorbent and can be used in the removal of fluoride from drinking water.

Keywords:
Adsorption, fluoride, Graphene, Zirconium, Activated carbon, drinking water

OL-8

Hetero-coordination assisted self-assembly of Mo(VI)-glycoconjugate complex into polymeric single-crystal and its catalytic application: a combined experimental and computational studies.

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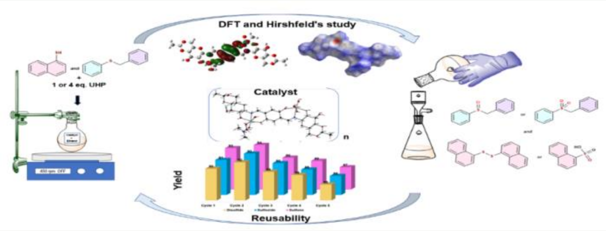
Pentacoordinate molybdenum or MoO_2(tridentate).D (D = monodentate ligand) complex tends to form polymeric or dimeric complexes due to the labile sixth coordination site. Previous reports show that polymeric or dimeric MoO_2 complexes generally formed due to self-assembly of discrete units via Mo=O---Mo interaction [1] or by using a bridging [2,3] ligand. Only a few occurrences involve dinuclear complexes [4] all other publications deal with mononuclear complexes. Herein, the reaction of $MoO_2(acac)_2$ with a glycoconjugate-based ditopic tridentate ligand leads to the formation of dinuclear molybdenum complex having accessible sixth coordination site. In solution phase, the complex found as discrete system with different solvent molecules, i.e., water, ethanol, methanol, DMSO, etc., in the sixth coordination site, providing the potential to bind with the substrate during catalysis. The ligand and MoO_2 complex are characterized by different experimental techniques like NMR, FTIR, UV-Vis, TGA, DSC, XPS, and HRMS. Recrystallization of dinuclear complex from DMF at low temperature afford polynuclear molybdenum complex having different coordination spheres about both the metal centres. Further, an efficient method for synthesizing sulfoxide, sulfones, and disulfides has been developed using Mo(VI) complex as catalyst and urea hydrogen peroxide as the oxygen source. The present method is precise for sulfide and thiol oxidation irrespective of alkene, amine, aldehyde, and ketone groups in the same molecule, with good to excellent isolated yield without tedious work-up. The catalyst has been reused five times without much loss in its activity. DFT and Hirshfeld's study on the MoO_2 complex explains the electronic spectrum properties and different interactions.



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OL-9

Development of Imidazopyrimidine-based compounds towards tumor pyruvate kinase-M2 modulation*

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Discovery of novel and potent lead molecules for the specific therapeutic targets by de novo drug design is still in infancy. In this presentation, link and grow strategy assisted unprecedented development of imidazopyri(mi)dine-based tumor pyruvate kinase M2 (PKM2) modulators will be discussed. The strategy led to development of a potent PKM2 activator IMID-2 with an AC50 of 90 nM. IMID-2 exhibited considerable cancer cell-selectivity against MCF-7 cells and membrane-permeability. ^{1}HNMR metabolomics studies also revealed that lactate concentrations in MCF-7 cells declined following insult with IMID-2. IMID-2 binds to a previously reported site at PKM2 adjacent to the interface of two monomers. In molecular dynamics (MD) simulation studies, it was observed that IMID-2 stabilizes the PKM2 at the dimeric interface, assisting in the formation of a biologically active tetramer conformation.

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OL-10

Ultrasound-promoted and [BMIM]BF$_4$ assisted green synthesis of functionalized pyrazolo quinoline core via one-pot multicomponent reaction, DFT study and pharmacological evaluation

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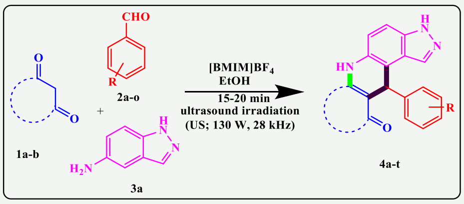
In recent trends in modern organic synthetic chemistry, multi-component reactions (MCRs) play a significant role in the construction of diverse complex entities. Many green approaches are widely used for the synthesis of biologically significant heterocyclic scaffolds and drug intermediates using three or more reactants with high selectivity, high efficiency, high atom economy, and step economy [1-5]. In the literature, various methods were reported for the synthesis of pyrazolo quinolones [6-8]. Most of them employ Lewis acids, salts, and metal-based catalysts as well as issues like prolonged reaction time and low yield are common.

An ultrasound-assisted green protocol is developed for one-pot synthesis of a new series of pharmaceutically relevant pyrazolo quinoline derivatives (**4a-t**) (Scheme 1). Pyrazolo quinoline derivatives (**4a-t**) were synthesized via a three-component tandem reaction of 1,3-dicarbonyls (**1a-b**), substituted aromatic aldehydes (**2a-o**), and 5-amino indazole (**3a**) in the presence of [BMIM]BF$_4$ ionic liquid in ethanol at ambient conditions. The main purpose of the present work was selective functionalization of pyrazolo quinoline (**4a-t**) core excluding another potential parallel reaction under environmentally benign reaction conditions. The salient features of the present protocol are amphiphilic behavior of ionic liquid, reusability of the [BMIM]BF$_4$ ionic liquid and mild reaction conditions. All the synthesized compounds were characterized by spectroscopic techniques like ^{1}H NMR, ^{13}C NMR and MS. The compounds were evaluated for their anti-inflammatory and antioxidant activity. The DFT study was also executed.



Scheme 2. Ultrasound-assisted environmental benign one-pot synthesis of novel pyrazolo quinolines (**4a-t**).

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OL-11

Quinoline based fluorescent chemosensor for selective detection of hydrazine and diethyl cyanophosphonate in aqueous medium

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Hydrazine (N_2H_4) is a chemical molecule having wide range of applications starting from its use in chemical reactions for the synthesis of pesticides, pharma and dye industry, rocket fuel etc[1,2]. Along with its wide range of applications it is also becoming a reason of environmental and health concerns, as a result wide ranging detection tools have been developed for the detection of hydrazine[3]. In this work we have designed, synthesized and evaluated a solvatochromic fluorescent probe (MQM) that is capable for the rapid and selective detection of hydrazine with a limit of detection (0.58 µM). The synthesized probe is capable of real-time detection of hydrazine in water, air, soil without any further processing of the sample for analysis and can also be used for the detection of hydrazine in biological samples. The most important application is the probe can be translated into a paper strip based portable analytical tool that can be used for rapid on-site detection of hydrazine without use of any sophisticated analytical instruments. The cost-effective translation of this probe is feasible due to its simple synthetic route and can be transformed into a paper strip based analytical tool can be easily prepared by coating the probe on paper strips and can be used for analysis. Further, the product of reaction between MQM with hydrazine was found selective for the detection of diethyl cyanophosphonate.

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OL-12

A natural antioxidant for the skin: *Salvianolic acid B enriched Red Sage extract.*

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Abstract: *Salvia miltiorrhiza* or the red sage is a herb which is extensively used in traditional Chinese medicine. Danshen is the dried roots of *Salvia miltiorrhiza* and is rich in hydrophilic polyphenolic acids-Salvianolic acids and hydrophobic abietane diterpenoids-Tanshinones. The polyphenolic acids in *Salvia miltiorrhiza* activate the Nrf2 (Nuclear Erythroid factor-2) and inhibit the oxidative stress Guo-Hui Li et. al. [1], Cheng-Yu Chen et. al. [2]. Exposure to increasing pollution levels in the environment triggers skin disorders such as acne, atopic dermatitis, hyperpigmentation, psoriasis and skin cancer. Polyphenolics bridge the gap for natural antioxidants by acting as topical antioxidants and protect the skin by decreasing the UV absorption and neutralize the free radicals produced by the pollutants. Salvianolic acid B protects the human dermal fibroblasts from UVB induced photoaging Zhengwang Sun et. al.[3].

The antioxidant mechanism of the biomarkers Salvianolic acid B, Danshensu and Tanshinone II A was elucidated by B3YLP-6/311G* model in gas/aqueous phase. The main biomarkers of *Salvia miltiorrhiza*-Salvianolic acid B, Danshensu and Tanshinone II A exert the antioxidant activity by hydrogen atom transfer mechanism. Among three compounds, Salvianolic Acid B is highly active as a free radical scavenger with a BDE (Bond dissociation energy) = ~ 75.73 kcal/mol while Tanshinone II A is observed to be least active with BDE = ~ 103.54 kcal/mol. The predictive antioxidant activity based on BDE= Salvianolic Acid B > Danshensu > Tanshinone II A.

The in-vitro antioxidant activity of the enriched extract of *Salvia miltiorrhiza* and the key biomarkers-Salvianolic acid B (**1**), Danshensu (Salvianic Acid A) (**2**) and Tanshinone II A (**3**) were evaluated for Hydroxy radical absorbance capacity (HORAC) and Oxygen radical absorbance capacity (ORAC). The HORAC activity of salvianolic acid B and the salvia extract was 2,34,244µmol gallic acid equivalent/g and 2,48,016µmol gallic acid equivalent/g respectively. The ORAC activity of salvianolic acid B and salvia extract was 11,976 µmol TROLOX equivalent/g and 11,664 µmol TROLOX equivalent/g respectively. The in-vitro antioxidant activity results are in line with the DFT calculations of the biomarkers.

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OL-13

A unique Ratiometric Fluorescent Probe for Mitochondrial pH Mapping during Mitophagy

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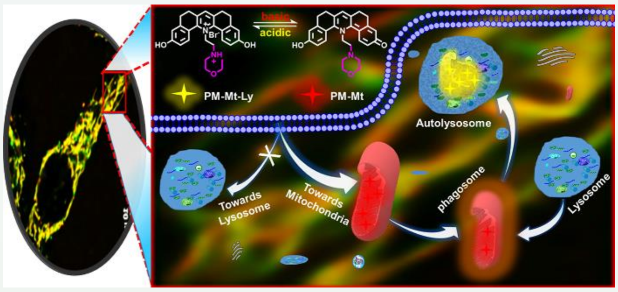

Abstract: Casey *et al.* describe that mitochondrial functions are heavily influenced by acid–base homeostasis [1]. Therefore, elucidation of the mitochondrial pH and its alterations during mitochondrial damage is an interesting question that needs to be addressed in living cells. A small molecular fluorescent probe is at the forefront to monitor pH and associated homeostasis due to several advantages, including simple, high-resolution, and non-invasive. Herein, we designed a unique small molecular morpholine conjugated fluorescent probe, **PM-Mor-OH**, based on the derivative of "IndiFluors," which was reported earlier by Munan *et al.* [2]. The lipophilic morpholine ligand has been extensively used to target lysosomes, but our probe unusually targets mitochondria. The morpholine ligand also plays a pivotal role in modulating the emission ratio ($\lambda_{green}/_{red}$) with internal pH variations (ΔpHi) via photo-induced electron transfer (PET). **PM-Mor-OH** exhibited "ratiometric" emission at a single excitation wavelength (λ_{ex}. 488 nm). Furthermore, the time-dependent density functional theory (TD-DFT) explained the bathochromic emission shift in basic pH due to intramolecular charge transfer (ICT). This probe was successfully applied to quantify the mitochondrial pH ratiometrically when treated with mitophagy-induced rapamycin drugs, A53T α-synuclein misfolded protein, and starvation conditions. In addition, the probe can monitor mCherry Parkin's translocation from cytoplasm to damaged mitochondria. The probe is suitable for monitoring ΔpHi when lysosomes fused with damaged mitochondria, known as mitophagy. Thus, **PM-Mito-OH** is a valuable probe for visualizing mitophagy and can be an appropriate chemical tool for diagnosing mitochondrial diseases.

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OL-14

Destabilization of *Staphylococcus aureus* biofilm by DNase/or Tween-80 adsorbed antibiotics loaded solid lipid nanoparticles

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Due to the emergence of the resistant against antibiotics caused due to biofilm formation by bacteria are very difficult to treat. *Staphylococcus aureus* is a gram positive, round shaped bacterium found on upper respiratory tract and on the skin and cause many respiratory and skin disease like pneumonia, abscesses etc. To overcome this challenge, gentamycin loaded and DNase coated solid-lipid nanoparticles were prepared. In this study we used Deoxyribonucleas I (DNase) and Tween-80 to destabilize biofilm formed by *S. aureus* in in-vitro conditions. The aim of proposed study was to explore application of DNase/or tween-80 adsorbed on to antibiotic loaded solid lipid nanoparticles (SLN) as destabiliser to destabilize biofilm formed by bacterium. Tween-80 and DNase adsorbed on Solid Lipid Nanoparticles (SLN) were evaluated against *S. aureus* biofilm to access biofilm destabilising property by scanning electron microscopy (SEM), bright field microscopy imaging and crystal violet staining method. In this study it was found that tween-80 and DNase destabilized biofilm efficiently. This study shown that tween-80 and DNase can be used as adjunct therapy along with antibiotics to combat against antibiotics resistance imposed due to biofilm formation.

Key words: *S. aureus*, Biofilm, Tween- 80, GRAS, DNase, SLN, Antibacterial, Anti-microbial resistance, Anti-biofilm

OL-15

Towards the Development of a Point-of-Care Diagnostic Kit for Hyperhomocysteinemia: Clinical Validation of Cardiac Patients' Samples

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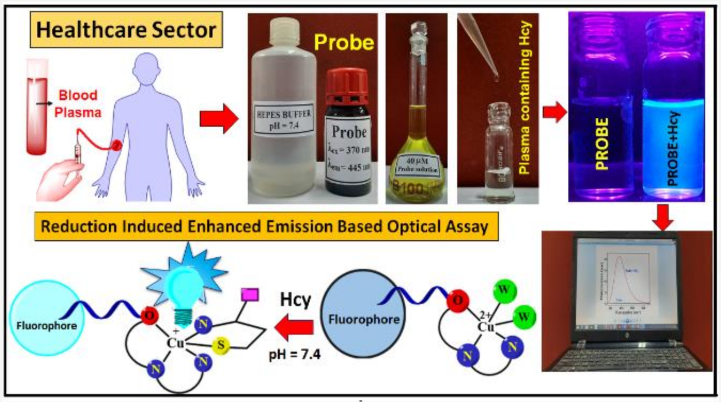
Hyperhomocysteinemia (HHcy, a clinical condition with elevated levels of homocysteine (Hcy) in human blood) is associated with various acute health disorders.[1] HHcy has been considered as one of the possible causes of developing cardiovascular diseases (CVDs), brain atrophy, cognitive impairment, renal dysfunction and Alzheimer's disease (AD).[2] Detection of these diseases at early stages and appropriate monitoring of therapeutics will certainly enable to improve the life standards of any patient. Despite recent progress in fighting with these fatal diseases, the best approach for achieving an early stage cost-effective diagnosis that will be operative in low-resource settings remained unsuccessful. In view of this, a major drive for developing point-of-care (POC) assay for measuring plasma Hcy could facilitate early detection of CVD and MCI as well as individualized therapy monitoring. Normal level of Hcy ranges between 5-15 μM, Hcy levels ≥15 μM, ≥30 μM and ≥100 μM indicates moderate, intermediate and severe conditions of HHcy, respectively.[2] Therefore, demand for plasma Hcy testing for determination of HHcy got increased momentum in recent times. However, global healthcare diagnostics market is yet to offer any solution for direct optical measurement of Hcy in human plasma. Herein, a series of water soluble optical probes has been developed, which displays turn-on response towards Hcy.[3] EPR and UV-vis studies has established reduction-induced-emission-enhancement of the sensor for its off-to-on behavior with Hcy. Furthermore, we demonstrate clinical testing of our probe in human plasma of cardiac patients and healthy volunteers. Validation using traditional HPLC and reliability against clinically approved commercial immunoassay kit confirms the diagnostic potential of the optical sensor. The presented optical sensor demonstrates the feasibility for the development of Hcy-selective diagnostic kit to be suitable for point-of-care uses.



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OL-16

Rh(III)-Catalyzed Dehydrogenative Annulation of 2-Arylquinoxalines with Allyl Alcohols: Synthesis of Benzo[*a*]phenazine-6-carboxylic Acids

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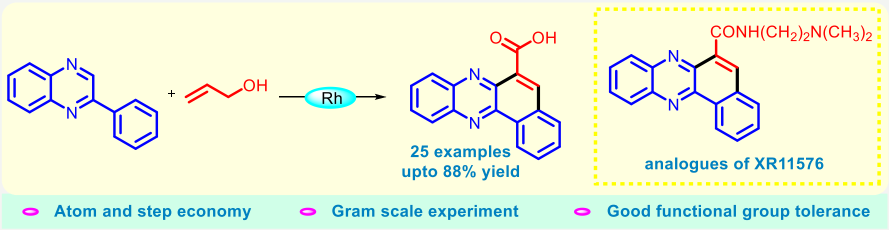
Transition metal-catalysed C-H activation/functionalization is one of the most attractive approach in organic synthesis for the construction of biologically active compounds with high atom- and step-economy.[1] A specific class of reactions as annulation reactions are widely used in the functionalization of easily available starting material into a highly valuable heterocyclic compound.[2] On the other hand, quinoxaline scaffold is an important class of *N*-heterocyclic compounds, and this skeleton has been showing different biological and pharmacological activities including anti-malaria, anti-viral, antibiotic, anti-bacterial, and anti-fungal activities.[3, 4] In the past few years allyl alcohols have been utilized as coupling partners in different metal-catalysed reactions.[5] In view of the importance of benzo[*a*]phenazine derivatives and our interest in transition metal-catalysed C-H activation reactions,[6, 7] we have developed an efficient synthesis of benzo[*a*]phenazine-6-carboxylic acid *via* rhodium (III)-catalysed dehydrogenative annulation of 2-arylquinoxalines with allyl alcohols **(Scheme 1)**. To the best of our understanding, this is the first report of the annulation reaction using allyl alcohol as a coupling partner. This methodology provides broad substrate scope concerning both the 2-arylquinoxalines and allyl alcohols, in moderate to good yield. Mechanistic investigation suggests that the activation of the C(sp^2)-H bond at the *ortho*-position of the phenyl ring is a reversible step whereas, cleavage of the C-H bond is a rate-limiting step. Additionally, the analog of **XR11576**, which is a dual inhibitor of the enzyme topoisomerase is also synthesized by the developed protocol.



Scheme 1: Rhodium (III)-catalysed dehydrogenative annulation of 2-arylquinoxalines.

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OL-17

Synthesis of Visible Light Triggered Pheophorbide-a Tryptamine Conjugate Photosensitizer for Photodynamic Therapy

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Photodynamic therapy (PDT) is an emerging non-invasive treatment modality that involves a photosensitizer, light and molecular oxygen to kill cancerous cells by producing reactive oxygen species(ROS).[1] Photosensitizer upon irradiation with laser light within therapeutic window[2] (max 600–800 nm) generates highly reactive singlet oxygen ($^1O_2$) which damages tumour cells by reacting with nearby biomolecules. Naturally occurring cyclic tetrapyrroles such as chlorins and bacteriochlorins resemble the typical features of ideal photosensitizers endowed with strong absorbance in long range (>650 nm), tumour tissue selectivity, preferential localization and low dark toxicity.[3] In efforts to enhance selectivity and accumulation towards cancer tissues, chlorin conjugates with tamoxifen[4], histamine[5], anti-cancer drugs[6], (2-pyridyl)ethylamine[7], and curcumin[8] have been studied. Biological effects of these conjugates are based on their nature and position in the macrocycle. Biogenic indole containing amines, such as tryptamine and 5-methoxytryptamine are considered as privileged scaffolds with high affinity towards multiple receptors and their multi-targeted hybrids are found to be potencially useful in cancer therapy.[9] Hormone melatonin is an indolamine involved in various physiological process as well as provide protection against wide spectrum of cancers like gastric, breast, prostate, oral, colon, liver and pancreatic. In our efforts to identify a potential photosensitizer,[10] we have prepared six methyl pheophorbide-a derivatives by linking tryptamine side chain at C-13^1, C-15^2 and C-17^3 positions of methyl pheophorbide-a. Prepared conjugates were characterized and evaluated for their photocytotoxicity against A549 cells and found to exhibit significant cytotoxicity. Molecular integration of pheophorbide-a (C-17^3) and tryptamine showed synergistic effects as the most conjugate was identified with enhanced photocytotoxicity when compared to methyl pheophorbide-a. The pheophorbide-a tryptamine conjugate (C-17^3) with strong absorption at 413 nm (Soret band), 663-671 nm (Q bands) along with comparable quantum yield (0.21) was smoothly taken up by A549 cells and exhibited intracellular localization predominantly to lysosome cells found in the cytoplasm. Detailed synthesis and photocytotoxicity results of the prepared pheophorbide-a tryptamine conjugates will be presented during the conference.

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OL-18

Deciphering a dissociative path to phosphoryl transfer mechanism catalysed by promiscuous Homoserine Kinase

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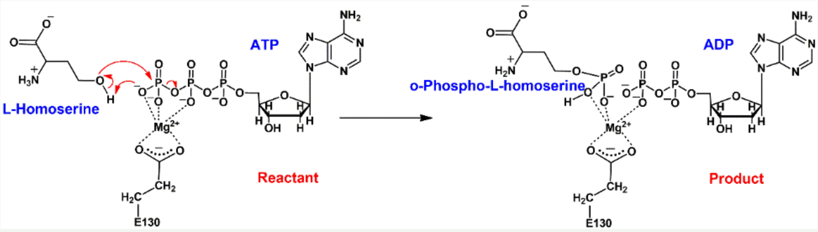
Abstract:

Phosphoryl transfer mechanism plays a central role in various metabolic pathways, protein synthesis, signaling, and energy transduction Kamerlin et al. [1]. Homoserine kinase catalyses ATP-dependent phosphorylation of L-homoserine to yield L-homoserine phosphate with a k_{cat}/K_M of 3.8×10^5 $M^{-1}s^{-1}$. It has a significant role in threonine biosynthesis in bacteria. Recently reported in Leishmaniasis disease, it is a strategy to inhibit the homoserine kinase to prompt pathogen mortality by deficiency of threonine, due to its unique activity towards the parasite and inactiveness in the human host Meshram et al. [2]. From previous studies, it is known that homoserine kinase also catalyzes a toxic antimetabolite L-4-hydroxythreonine with a robust k_{cat}/K_M of 4.8×10^3 $M^{-1}s^{-1}$ as a side reaction Kim et al. [3]. This suggests that promiscuous activities are not always inefficient.

Conventionally phosphoryl transfer reactions are classified into two pathways; a) concerted associative pathway, b) concerted dissociative pathway Kamerlin et al. [1]. According to previously proposed mechanism of homoserine kinase, it is initiated by the direct attack of the hydroxyl group of homoserine to γ-phosphate of ATP in the absence of base, following the associative pathway Krishna et al. [4].



In light of this prior knowledge, however, phosphoryl transfer by homoserine kinase has not been explored much. So, in this work, for the first time, we have complimented MD simulation with QM/MM calculations in the direction of investigating the mechanistic pathway adopted by homoserine kinase. We determined that homoserine kinase follows a dissociative pathway and the most probable base is His138.

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OL-19

Posterior silk glands of *Bombyx mori* show decreased levels of polyamines during degradation

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Abstract

Bombyx mori is an economically important lepidopteran and is a very good model organism for studying developmental biology. Autophagy is the cellular self-renewal process that helps in recycle of cytoplasmic components, and cell survivability. Several changes in the silk glands occur during larval–pupal transition which show signs of autophagy. Polyamines were shown to play an important role in autophagy in several organisms. Among the natural polyamines, spermidine enhanced autophagy in yeast, flies, and mice. The role played by polyamines in silk gland autophagy is not known. In the present work, the quantitative and qualitative changes in the silk gland polyamines of *Bombyx mori* during the late larval, prepupal, and pupal stages were checked. Results showed a correlation of silk gland degradation with a decrease in polyamine levels at the end of the prepupal stage. This is the first report to show the involvement of polyamines in the autophagy of silk glands

OL-20

Impact of heat stress on the development of embryo and its effect on the commercial traits of silkworm *Bombyx mori* L.

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ABSTRACT

The embryonic stage architects all post embryonic developments which also governed by genetic and environmental conditions. The effect of heat shock remains obscure in silkworm *Bombyx mori* L. APM1 and APHO1 silkworm selected to examine the impact of heat shock on the embryo and larvae. Different developmental stages of embryos were exposed to heat shock temperatures. After HS, eggs and larvae were reared under normal environmental conditions. Eggs of APM1 and APHO1 heat shocked at 35˚C exhibited increased hatching (91.66 & 69.33%), larval weight (1.72 & 3.33 g), ERR (72.39 & 81.93%), cocoon weight (1.01 &1.6 g), shell weight (0.12 & 0.29 g), shell ratio (13.11 & 20.52%) and pupal weight (0.87 &1.29g) compare to control. HS at 35˚C increased hatching compared to control. Increased total protein content observed in both strains after HS compared to control. Besides increased total protein content, expression of 205, 90 and 70 kDa heat shock proteins was noticed both in APM1 and APHO1 eggs HS at 35, 40 and 45°C compared to control. In addition, the glycogen content found more on day - 3 compared to day - 2 in the embryos of APM1 and APHO1 eventually declined as the embryonic development proceeds until hatching. Therefore, APM1 and APHO1 eggs had shown profound response to heat shock and exhibited thermotolerance.

Key words: *Bombyx mori.* Commercial traits, Heat shock, Thermo tolerance.

OL-21

UPLC is an effective tool for simultaneous analysis of Anxiolytic drugs

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Abstract:

Anxiolytics are a class of psychiatric medications that are typically used to control psychosis or treat mental illnesses including schizophrenia and bipolar disorder [1][2][3]. The assigned work comprises using the UPLC technology to simultaneously quantify and validation of a panel of widely used Anxiolytic drugs in the dosage form. The samples were separated using an Acquity UPLC@BEH shield RP C18 (100 mm X 2.1 mm id, 1.7 µm particle size) column with gradient elution using 0.1 % TFA and ACN and a PDA detector, 0.3ml/min flow rate, and 1µl Injection volume. The study was complete in 7 minutes with a 45°C column oven temperature. For different pharmaceutical dosage forms, time-consuming methods and separate mobile phases are typically utilized in quality control laboratories; nevertheless, the proposed technique saves time and money by eliminating the need to switch mobile phases. The presented method is mostly utilized in QC laboratories and forensic toxicology, where Anxiolytic drugs are mostly employed to track medicine delivery or to pinpoint the cause of intoxication during post-mortem and situations involving human performance.

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OL-22

Synthesis and characterization of Rare earth Doped Potassium Sodium Niobate for electronic application

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Key Word: - Synthesis of some rare earth doped piezoelectric crystals.

Rare earth metals well known for their rich structure and exhibiting extremely well electrical, magnetic, dielectric and optical properties[1]. The properties of piezoelectric materials are affected by composition, structure and lattice defect. KNN is an inorganic compound derived from combination of ABO_3 perovskite structure of $KNbO_3$ (NN) and Na NbO_3(NN) where A refers to K and Na ion while B refers to Nb ion, Bulk ceramics, thick and thin films[2] of lead free potassium sodium niobate have been prepared[3] . Doping [4]/substitution technique a dominant master plan to accomplish high performance piezoelectric materials. High temperature is needed for the preparation of the rare earth doped KNN. Due to the volatile nature of sodium and potassium, low density is achieved in the product the densification of the KNN by doping with rare earths would be done . Increment of the dielectric constant by reducing the dielectric loss and increasing the piezoelectric coefficient of KNN by rare earth doping technique is made. The impact of molar ratio of (k+Na)/Nb presence in liquid phase, chemical modification (doping) and different atmosphere (defects) during heat treatment process are discussed. The Crystal texture characterized by XRD ,phase structure studied by Raman spectrometer and Surface morphology, piezoelectric properties is investigated by SEM and Std. Piezometer.

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OL-23

Natural substance as a Tyrosine Kinase Inhibitor (TKI) and its efficacy in Thyroid Cancer

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The most prevalent endocrine malignancy with global impact is thyroid cancer. The first targeted therapy ever created for any cancer was radioactive Iodine ([^{131}I]-Iodine solution) treatment for papillary thyroid cancer. The uptake of RI using sodium/Iodine Symporter (NIS) and its integration into thyroglobulin residue, which increases the radioisotope's resistance time, is necessary for radioiodine therapy (RAI) for metastatic thyroid cancer to be effective. Unfortunately, thyroid cancer has the worst prognosis and exhibits little to no NIS expression because it cannot successfully absorb and trap iodine. It has been reported that small-molecule TKIs have been shown to restore radioiodine uptake in thyroid carcinoma. Keeping this in mind, we aim to screen anti-cancerous and MAPK inhibitory activity of three cheap, well-characterized natural products i.e. Apigenin, Berberine, and Epigallocatechin-3-gallate. The findings suggested that these natural products may be used as potent anti-cancerous drugs as they inhibit proliferation and induce apoptosis in human thyroid TPC-1 cells. The docking results showed that all three compounds adhere to Lipinski's rule of five, allowing for the creation of therapeutic medication. The substances are firmly lodged in the pockets of MAPK, ERK, and BRAF receptors, supporting the idea that they can inhibit the MAPK/ERK signaling cascade, which controls the proliferation of malignant cells. Further mechanistic studies are needed to validate the efficacy of Epigallocatechin-3-gallate, Apigenin, and Berberine for the therapeutic basis of drug development.

Keywords: Thyroid Cancer, RAI, NIS, MAPK, and TKI

Acknowledgment:
Author Juhi Rais is thankful to the CSIR, New Delhi for the Research Associate Fellowship award (CSIR-RA: 09/0590(11198)/2021-EMR-I).

OL-24

Fabrication of disposable and sensitive electrochemical biosensor based on (3-Aminopropyl)trimethoxysilane for new cancer biomarker detection, sperm protein 17

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Recently, cancer has emerged as one of the main causes of death throughout the globe. Nearly 10 million individuals worldwide lose their lives to cancer every year [1], as reported by the World Health Organization (WHO). By 2025, the world's population is projected to reach 8.3 billion, and annually, more than 20 million people are diagnosed with cancer [2-3]. Finding ways to identify cancer indicators in human fluids is a major area of study right now, since this may assist in the disease's early identification. Sperm protein 17 i.e., SP17 is a mammalian protein expressed in the spermatozoa and testis has been related to a variety of human malignancies [4]. In this study, we provide a novel approach for development of first label free, sensitive, and selective biosensor, in complex serum samples for SP17 determination, a novel cancer biomarker. The SP17 biosensor used in this study was the first of its kind to be fabricated on a disposable ITO sheet modified with (3-Aminopropyl)trimethoxysilane (APTMS). Multiple analytical and morphological methods were used to independently verify the immobilisation biological and chemical species onto the surface of electrode. Using electrochemical methods, researchers analysed the effects of incremental immunoelectrode changes. We used the DPV method to quantify the selectivity of the anti-SP17 and SP17 at doses ranging from 100 to 5000 pg mL ^{1}. The immunosensor's sensitivity was 0.013 mA mL pg^{-1} cm^{-2}, and its LOD as well as LOQ were only 70.07 as well as 233.57 pg mL^{-1}, respectively. Quantitative analysis of concentrations of SP17 in patient serum samples was used to evaluate the functionality of the manufactured immunosensor. The created immunosensor yielded data that was highly reproducible, repeatable, and selective in the presence of several different interferants, including cancer biomarkers. In addition, ELISA validation shows excellent agreement between the electrochemical findings and the observed ones. This has the potential to build a novel platform for the detection of additional cancer biomarkers and may be used in clinical diagnostics.

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OL-25

Wastewater treatment (photodegradation/fluoride removal) via 3D rod-like Fe-Al bimetallic metal-organic-framework prepared through solvothermal route

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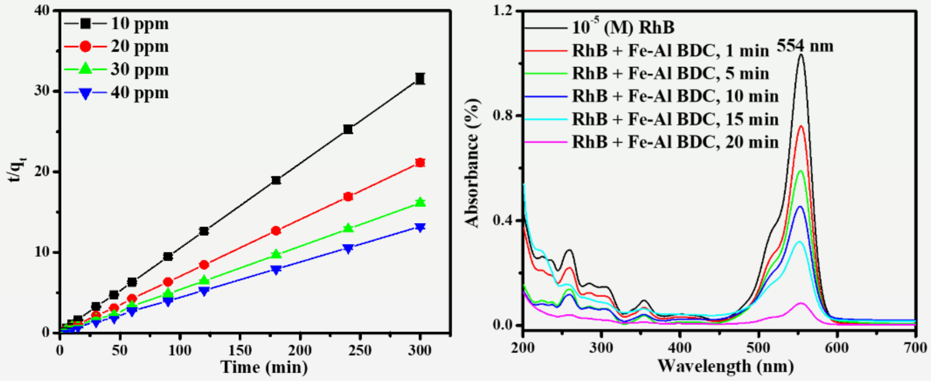
Abstract

A 3D rod-like, porous Fe-Al bimetallic metal-organic-framework (MOF) with 1,4-benzenedicaboxylic acid as an organic linker (abbreviated as Fe-Al BDC) was prepared using the solvothermal method. Fe-Al BDC with 120.255 m^2/g surface area was used for the photodegradation of carcinogenic water-soluble xanthene class of dye e.g., rhodamine B (RhB) ($10^{-5}/10^{-4}$ M) (pH range 2-11) under the Solar irradiation. The thermal and pH stabilities of Fe-Al BDC were checked by the thermogravimetric and ξ-potential studies. The 3D rod-like structure was confirmed by the FESEM study. Fe-Al BDC was also characterized by the PXRD, FTIR, Raman spectra, TEM, HRTEM, analyses. The photodegradation followed pseudo-1st-order kinetics and the mechanism was established using HPLC and LC-MS studies. The photodegradation mechanism was controlled by the in-situ generated $OH^{\bullet}$ radicals supported by ESR study. Fe-Al BDC was also able to chemisorb fluoride established using FTIR and XPS studies. The Fe-Al BDC MOF was reusable up to eight cycles.

Keywords: Photodegradation; Chemisorption; Kinetics; XPS study; HPLC studies; LC-MS studies



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OL-26

Sticky Hydrophobic Surface Patterning in Synergy with Biochemical Cue Augment Mesenchymal Stem Cells Proliferation, Differentiation,Epithelial Transition, and Curb Senescence

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The apposite *in vitro* maintenance of mesenchymal stem cells (MSCs) is an unmet need in regenerative medicine because of diminished proliferation due to excessive ROS generation expediting replicative senescence [1]. There are different biophysical stimuli-based ECM support to the MSCs for curbing this issue

[2] while of all the stimuli sticky hydrophobic rose petal surface patterns are significantly less explored. We report the fabrication of rose petal patterned silk fibroin porous scaffold embedded with 0.4% and 2% honey(PHSF0.4 and PHSF2 respectively) along with corresponding flat versions (FHSF0.4 and FHSF2) using a combination of soft lithography and freeze-drying. After fabrication, all the scaffolds were studied for surface morphology, topography, roughness, porosity, honey incorporation, and mechanical strength using SEM, AFM, liquid displacement method, FTIR, and NINT methods followed by examining *in vitro* swelling and degradation behavior. These studies and an antibacterial assay against MRSA proved PHSF2 to be superior to other variants with sustained honey-releasing potential. Hierarchical sticky hydrophobic topography provided by PHSF2 allowed MSCs sensors to grasp the features and eventually form cell sheets on the substrate surface which were further validated by NBT, fluorescence spectroscopy, and SABG assays by examining ROS generation and senescence respectively. Molecular gene dynamics of vimentin, fibronectin, p53, p21, SOX9, RUNX2, PPARϒ, CDH1, and CK-19 were studied to examine potential MSCs proliferation, trans-differentiation, and epithelial transition in which PHSF2 again stood out. Thus, PHSF2 surfaced as a stand-alone MSCs delivering regenerative healing tool with four-in-one technology for promoting proliferation, differentiation, epithelial transition, and inhibiting senescence.

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OL-27

A novel Ni(II)-thiocyanate complex with functionalized carbon nanotube as efficient catalytic activator for oxygen evolution reaction

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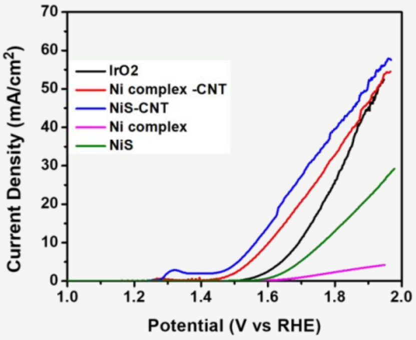
Oxygen evolution reaction (OER) is on the high demand for the crucial energy conversion and storage process[1].The sustainable development of cost-effective and high performance electrocatalyst for OER is the critical challenge. Recently, the earth abundant metal complexes and their derived materials have gained massive significance as electrocatalysts[2]. Among these, Ni(II) has immense importance due to its nature as earth-abundant, cost-effective, variable oxidation state and high electrical conductivity.In the present study, we report the novel Ni(II)-thionate complex (**1**) on functionalized carbon nanotube and NiS derived from single source precursor **1** as electrocatalyst for oxygen evolution reaction (OER). We designed and synthesized a novel Ni(II) complex $[(\mathbf{L1})_2Ni(NCS)_2]$ (L= 2-(pyridin-2-yl)benzothiazole) (**1**). The single crystal XRD data of complex **1** revealed the octahedral geometry around metal center. Complex **1** annealed at 350 °C for in inert atmosphere revealed NiS nanoparticles. Further, complex **1** sonicated with functionalized carbon nanotube and annealed at 350 °C for in inert atmosphere that revealed **1-CNT** composite. The OER electrocatalytic performance of the as prepared Ni complex (**1**), derived NiS, and **1-CNT** were evaluated in 1 M KOH. It was observed that the NiS showed appreciable increase in the electrocatalytic OER activity as compared to Ni complex. The incorporation of CNTs in the Ni complex (**1-CNT**) shows exceptional enhancement in the OER activity showing E_{onset} at 1.45 V vs RHE and 290 mV overpotential to reach current density 10 mA/cm^2, outperforming the state-of-the-art IrO$_2$ catalyst. The study provides an efficient strategy to design OER electrocatalyst using novel Ni(II)-thionate complex.



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OL-28

Honey ghee incorporated double stabilized alginate hydrogel to accomplish regenerative repair of full-thickness cutaneous wounds

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To overcome common complications associated with healing of full-thickness cutaneous wounds by providing holistic and systematic support, two natural products- Honey and Ghee, *Madhu Ghrita* (Udwadia, 2011), were mixed and embedded into an alginate hydrogel scaffold stabilized by dual cross-linking, and their synergistic healing efficacy was studied (Mukhopadhyay, 2020). These scaffolds were then thoroughlycharacterized in terms of physicochemical, and mechanical properties. Further, swelling and degradation studies exhibited these hydrogels' absorption capability and stability. The antimicrobial potential was studied in gram-positive *S. mutans* and gram-negative *E. coli* respectively. Cellular biocompatibility and viability were evaluated against 3T3 fibroblasts and regulations in the expression of markers for cellular recruitment, ECM formation, cell-cell communication, and scar tissue formation, respectively. Finally, the fabricated hydrogels were applied to full-thickness cutaneous wounds created in rats, and the subsequent wound contraction kinetics and real-time wound healing ability were explored using non-invasive stereozoom imaging and optical coherence tomography respectively. Histological staining helped to establish tissue components in normal and treated sections. Honey ghee embedded dual cross-linked hydrogels exhibit superior chemical stability, mechanical strength, surface roughness favoring cellular growth, cell-to-cell contact, deposition of ECM material, and decrease in expression of scar tissue. These showed remarkable antimicrobial properties against both Gram-positive and Gram-negative bacterial strains. Non-invasive imaging and histopathological studies revealed treated tissue properties closely resembling that of normal skin, indicating a regenerative repair pathway.

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OL-29

Flexible and freestanding Co (II) based metal organic framework/ carbon nanofiber hybrid mat for uric acid sensing

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Uric acid is a main product of the metabolic breakdown of purine nucleotide and the abnormal level UA in blood, results in several diseases like gout, hyperuricemia and pneumonia etc have become one of the major global extortions to human health. Therefore, the detection and monitoring the uric acid levels is significantly important for gout patient diagnosis. The rapid diagnosis capabilities, excellent repeatability, and good selectivity have contributed to the rapid growth of new biosensors in recent years. The present study focused on the novel flexible and freestanding uric acid sensor based on hierarchical cobalt (II) MOFs/ carbon nanofiber hybrid mat. In this approach, the carbon nanofiber (CNF) mat was taken as a substrate to grow cobalt metal-organic frameworks (Co-MOFs) via solvothermal approach. To explore the electrochemical application of the nanocomposite, the Co-MOFs/CNF modified glassy carbon electrode (GCE) was prepared and used as a non-enzymatic electrochemical sensor for uric acid. The hierarchical 3-D structure (sea-urchin like) of cobalt-based metal organic framework was defined by scanning electron microscopy; Fourier transformed Infrared spectroscopy and X–ray powder diffraction. The cyclic voltammetry and chronoamperometric study indicate that the uric acid sensor shows outstanding electrochemical response as well as stronger electro-catalytic activity. The novel uric caid sensor displayed a reasonable linear range 25-700 µM, low detection limit of 103.5 nM, and excellent sensitivity (5.78 µA μM^{-1} cm^{-2}) for uric acid detection. The detection outcomes of the real samples establish the Co-MOF/CNFs hybrid mat can be a favorable candidate for uric acid sensing applications. The as-fabricated biosensor also exhibited great accuracy, excellent selectivity and good reproducibility.

Keywords: Metal organic framework, Electro-oxidation, Sensitivity, Uric acid, Biosensor.

OL-30

A Glimpse on Effective Synthetic Strategy for Developing a Variety of Mitochondria Specific Ru(II)/Ir(III)/Re(I)-based Mixed Metallic Luminescent Complexes as Highly Efficient Cancer Therapeutic Agents

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Cancer is the most incurable pernicious disease till date after the cardiovascular disease with immeasurable rate of mortality. However, effective cancer therapy is still castles in the sky to the researchers being unable to develop appropriate anticancer drugs. In quest of an appropriate strategy to annihilate cancer, we have aspired to design a set of Ru(II)/Ir(III)/Re(I)-based mixed metallic complexes having the cancer cell imaging and damaging capability with higher degree of cytoselectivity. These mixed metallic complexes are fluorescent with high quantum yield displaying the capability of diagnosing the cancer cells and have shown remarkable cytotoxicity against a series of cancer cell lines (HeLa, Caco-2, MDA-MB468, MCF-7, HT-29) accompanied with excellent binding efficacy with biomolecules (HSA, DNA) being resistant to glutathione(GSH) rendering the normal healthy cells unaffected. In line with this, complexes are highly capable of targeting the organelles (nucleus, mitochondria) and can destroy the cancer cells causing mitochondrial dysfunction through reduction of mitochondrial membrane potential (MMP) as well as triggering the emergence of ROS in association with damaging DNA (**Figure 1**) (P. Paira *et al* and J. J. Wilson *et al*).[1, 2, 3] Optimistically, all the characteristics will attribute these complexes for being explored as brilliant cancer therapeutic agents in imminent future.

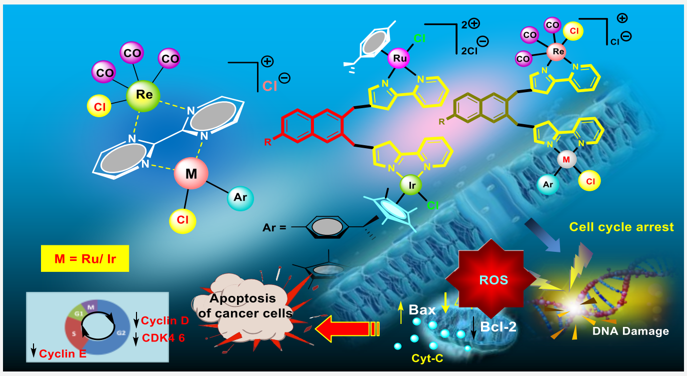

Figure 1. A Mechanistic Approach of the Synthesized Complexes in Destruction of Cancer Cells

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OL-31

A CLINICAL STUDY OF BACTERIAL PATHOGENS FROM HOSPITAL ACQUIRED INFECTIONS IN ANM MEDICAL COLLEGE AND HOSPITAL, GAYA

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Choice of Mode: - Oral Presentation
Name: - Pinky Gupta, DOB: 14.05.1995
Theme: - Clinical Trials on Nosocomial Infections along with Surgical Site Infections. AMR, HAI, Antibiotic Resistance and Susceptibility.

Hospital associated infections acquire while receiving health care. It appears 48 hours after Hospital admission or within 30 days after discharge (Horan et al. [1]). It is a major problem for patient's safety and has a high impact of poor medical condition as well as death. The most common Blood, Urinary Tract, Areas of Surgery, Wound infections, Skin infections. The microorganisms which cause these infections are *Escherichia coli*, *Klebsiella pneumonia*, *Pseudomonas aeruginosa*, *Citrobacter* spp., *Enterobacter* spp., *Proteus* spp., *Acinetobacter* spp., *Staphylococcus aureus*, *CONS*. The earlier study was based on use of standard specific antibiotic to test the pathogens. In this study, different antibiotics were used to test the sensitivity against these pathogens. The antibiotics were used for the study are Gentamycin, Ciprofloxacin, Amikacin, Ofloxacin, Nitrofurantoin, Norfloxacin, Penicillin, Nalidixic acid, Erythromycin, Amoxicillin, Chloramphenicol, Azithromycin, Cefixime, Levofloxacin, Moxifloxacin to test the pathogens. Out of 501 cultures, 398 positive cultures were taken, in which, 216 (54.27%) are urine samples, 46 (11.55%) are pus samples, 16 are swab samples, and 120 are surgical site infection samples. The Antimicrobial Susceptibility was done by Disk Diffusion Method (Kirby-Bauer Disk Diffusion Method). In this study, I have shown that *CONS* (95.2%) has the highest Antimicrobial Susceptibility to Chloramphenicol, than Ciprofloxacin and Gentamycin.

Keywords: Hospital Acquired Infections, Bacterial Pathogens, Antimicrobial Activity

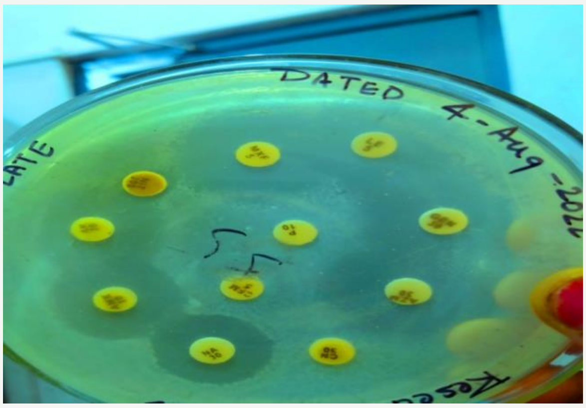

Figure :- The Antibiotics Nalidixic acid, Amoxicillin, Azithromycin, Moxifloxacin, Gentamycin, Levofloxacin, Amikacin, gives clear zone of Inhibition against *E.coli* in MHA Plate.

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OL-32

SCREENING AND PARTIAL PURIFICATION OF CRUDE BACTERIOCINS

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Bacteriocins are an assembly of polypeptides with antimicrobial properties, produced by the protein synthesis apparatus of bacteria and archaebacteria against predator cells (Juturu & Wu [1]). Along with their antibacterial nature, they also have antagonistic activity against viruses and fungi. As a bacterial immune weapon, these antimicrobial peptides kill or inhibit bacteria either from the same species or from different genera (Fahim et al. [2]). These bacterial peptides are used in the medicinal, agricultural, food processing, and livestock industries and are also acknowledged as a bio preservative that is an alternative to various chemical preservatives. In this study, soil samples were collected from the rice fields to isolate various bacterial strains. Twenty-four morphologically distinct colonies were selected and sub-cultured on Luria-Bertani agar plates. A screening technique is used to identify bacterial strains with antimicrobial activity. The restricted activity of the isolates was checked out against different disease-causing bacterial strains like *E. coli*, *S. aureus*, *K. pneumonia*, *P. aeruginosa*, *S. typhii*, and *V. cholerae* by the agar well diffusion method. Colonies with a zone of inhibition were selected to carry out partial purification of crude bacteriocin protein. The selected strains were precipitated with ammonium sulphate and dialysed using a dialysis membrane. Further on, crude dialysed bacteriocin-like inhibitory substances were extracted with butanol. Thus, it can be concluded that extracted crude bacteriocin exhibit different inhibitory activity against above mentioned disease-causing bacterial strains.

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OL-33

Influence of Gut Microbiome on Parkinson’s Disease due to the intake of Pesticides using Quorum Sensing Pathway

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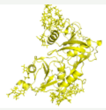
ABSTRACT

Gut microbes crucially influence several neurological disorders, including Parkinson’s disease (PD) in humans [1]. With a special emphasis on the Indian population, the effect of Fipronil sulfone (FS), a metabolite of Fipronil, on gut microbes *Enterococcus faecalis* and *Lactobacillus plantarum* has been studied through molecular docking and dynamic simulation studies. The damage incurred to the neurons due to the metabolism of FS increases the chances of PD, and this is compensated by to the Quorum-Sensing (QS) molecules released by the gut microbiome [2].

The interaction between FS and essential proteins required for the survival of the bacterium, Diaminopimelate epimerase (Q88V90) (DapF) from *Lactobacillus sp*. [3], and Tyrosine Decarboxylase (P0DTQ4) (TDC) from *Enterococcus sp*. [4] and Quorum Sensing molecule LuxS for each bacterial species were simulated. The values of molecular simulation analysis of TDC, DapF and each LuxS respectively were: RMSD = 4.9846 nm, 2.0648 nm, 4.43525 nm, 5.4524 nm and RMSF = 1.788071 nm, 1.237829 nm, 1.581939 nm and 1.51322 nm.
A concentration-based simulation was done for 100 ns at 92 mg/L, half the LD50 value for Fipronil sulphone.

Bacterial protein structure at 50 ns	 TDC from *Enterococcus sp.*	 DapF from *Lactobacillus sp.*
Bacterial protein structure at 100 ns	 TDC from *Enterococcus sp.*	 DapF from *Lactobacillus sp.*
MM-PBSA (kJ/mol)	-820.15	-764.25
RMSD (nm)	0.335866 nm	0.443469 nm
RMSF (nm)	0.133603 nm	0.166563 nm
SASA (nm^2)	156.1687 nm^2	295.278 nm^2

This work indicates a change in the conformation of the protein structure that could potentially inhibit the functioning of the bacteria, hereby reducing the amount of neurotransmitter produced and possibly influencing Parkinson’s Disease.

Key Words: Gut microbiome, Parkinson’s Disease, Quorum-Sensing Peptides, Pesticides

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OL-34

Development of 1,2-bis(hydroxymethyl)benzo[g]pyrrolo[2,1-*a*] phthalazine hybrids as potent anticancer agents to small cell lung cancer

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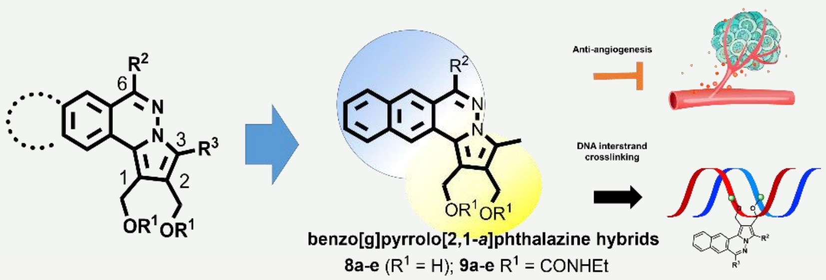
Designing hybrid molecules with dual functions is one approach to improve the therapeutic efficacy of combination treatment. We have previously conjugated phthalazine and bis-(hydroxymethyl)pyrrole pharmacophores to form hybrids bearing antiangiogenesis and DNA interstrand cross-linking activities. To improve the bioavailability, we adopted a benzology approach to design and synthesize a new series of 1,2-bis(hydroxymethyl)benzo- [g]pyrrolo[2,1-a]phthalazines. These new hybrids retained the dual functions and could be formulated into vehicles for intravenous and oral administration. Among them, we demonstrated that compound 19a with dimethylamine at the C6 position markedly suppressed the tumor growth of human small cell lung cancer cell line H526, squamous lung cancer cell line H520, and renal cancer cell line 786-O in nude mice, implying that compound 19a is a broad-spectrum anticancer agent. Our results implicated that the conjugation of antiangiogenic and DNA cross-linking is likely to be a helpful approach to improving the efficacy of combination therapy.[1]



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OL-35

Designing of a novel Curcumin Analog to inhibit MAPK 1 and MAPK 3: A Cheminformatics Approach

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Curcumin (diferuloylmethane), an orange-yellow component of turmeric or curry powder, is a natural polyphenol product isolated from the rhizome of the plant *Curcuma longa*. Curcumin has been used in medicinal preparations or as a food-colouring agent for centuries. In recent years, extensive *in vitro* and *in vivo* studies suggested curcumin has anticancer, antiviral, antiarthritic, anti-amyloid, antioxidant, and anti-inflammatory properties. The underlying mechanisms of these effects are diverse and appear to involve the regulation of various molecular targets, including transcription factors (such as nuclear factor-κB), growth factors (such as vascular endothelial cell growth factor), inflammatory cytokines (such as tumour necrosis factor, interleukin 1 and interleukin 6), protein kinases (such as mammalian target of rapamycin, mitogen-activated protein kinases, and Akt) and other enzymes (such as cyclooxygenase 2 and 5 lipoxygenase). Thus, due to its efficacy and regulation of multiple targets, as well as its safety for human use, curcumin has received considerable interest as a potential therapeutic agent for the prevention and/or treatment of various malignant diseases, arthritis, allergies, Alzheimer's disease, and other inflammatory illnesses. The potential of curcumin has also been examined in neoplastic, neurological, cardiovascular, pulmonary and metabolic disorders. This review summarizes various *in vitro* and *in vivo* pharmacological aspects of curcumin and the underlying action mechanisms. This research project aims to find a novel analog of curcumin that targets multiple pathways in the body as curcumin is found to have low bioavailability in vivo. Analog molecules are constructed with database search and the SmiLib combinatorial library approach. Docking studies of analogs referenced to curcumin and its derivatives revealed few analogs that could be gained as drugs to inhibit MAPK 1 and MAPK 3.

Keywords: *Curcuma longa,* Curcumin, Demethoxycurcumin, Bisdemethoxycurcumin, SmiLib

OL-36

Exploring the role of endophytic fungi in remediating industrially polluted soils using *Catharanthus roseus*

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Abstract

Catharanthus roseus is a plant that produces metabolites of high therapeutic value used for basic and applied research. However, *C. roseus* growing in industrially polluted soils have shown alterations in their physiological and metabolic activities. The endophytic fungi play a crucial role in providing host resistance against soil heavy metal stress. Therefore, studying the endophytic fungal colonization within metal stressed *C. roseus* might help us in better understanding of plant-soil-endophyte relations. In the present study, on *C. roseus*, the ITS region amplification and nanopore sequencing was applied to study the hypothesized alterations of host endophytic fungal communities within plants grown in industrially polluted soils. The study revealed that the roots acclimatized in industrially polluted soils exhibited elevated alpha diversity. These roots also expressed highest beta diversity with leaves of *C. roseus* grown in uncontaminated soils. The depiction of metagenomic data as Sankey plots and Krona charts indicates that endophytic fungi in *C. roseus* were host specific and exhibited noteworthy population changes under metal stress conditions. Several traits shared by the identified endophytes were deciphered based on plant responses that might help to strengthen the knowledge on plant metabolism in response to soil contamination. Also, permanent metagenomic repositories created can serve as an invaluable resource for future research.

OL-37

Synthesis, Characterization and Environmental applications of a graft copolymer of Guar gum

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Guar gum is a polysaccharide extracted from guar beans (*botanical name* **Cyamopsis tetragonoloba**) that is abundantly used in the field of research. It is a natural biopolymer that serves widely as a viscosifier, thickening agent. Owing to its numerous significant properties, it is used in cosmetics, pharmaceuticals, oil drilling industries, etc. The proposed research endeavors to synthesize a novel guar gum-based biopolymer through the grafting process via *microwave assisted* technique. The modified biopolymer was eco-friendly, non carcinogenic, non-acrylamide in nature. Ceric ammonium nitrate(CAN) was used as a free radical initiator to create free radical sites on the guar gum (polysaccharide) backbone [1]. The synthesized novel biopolymer was characterized by various physico-chemical characterization techniques namely Ultraviolet visible (UV-visible) Spectroscopy, Fourier transform infra red (FTIR) Spectroscopy, X-ray diffraction (XRD) study, Thermal gravimetric analysis(TGA), Scanning electron microscopy(SEM) and Intrinsic viscocity study. The modified biomaterial holds promise in diverse applications viz. as a flocculant for water and wastewater treatment, as matrix for controlled and targeted drug release, selective abstraction of metal ions, dye removal, antibacterial properties (bacteriostatic agent), wound healing, haemostatic agent and mineral ore benification.

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OL-38

EXPLORATION OF FOAM GRANULATION TECHNIQUE FOR PRODUCING FAST DISINTEGRATING TABLETS CONTAINING FLUPIRTINE MALEATE

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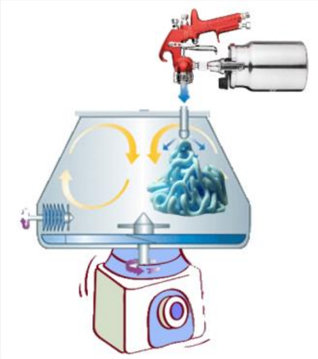
By employing a factorial design, the objective was to investigate a novel foam granulation technology in which foam serves as a binder for the formulation of a fast-disintegrating tablet (FDT) of flupirtine maleate for the treatment of pain management. FDT was developed using a cutting-edge foam granulation technique, which substituted foam for a liquid binder [1]. For the fabrication of granules, a foam granulator on a laboratory scale was devised [2]. A total of 2^3 factorial designs were used for the optimization, and different parameters were investigated. The marketed FDT and the optimised batch were contrasted. It was done to test the improved batch's short-term stability. Shorter disintegration time (DT) and wetting time were observed in prepared FDT using the foam granulation process, which demonstrated the combined effects of less binder (HPMC E5) and high porosity of granules. By integrating experimental design and the Design-Expert software, the variables were set to their optimum values. F9 (1.96% binder concentration, 296 RPM, 3.5 min granulator rotation duration) was discovered to be the best formulation batch. Without employing super disintegrants, this demonstrated DT of 25 seconds, Friability of 0.56 per cent, and wetting time of 11 seconds. It also revealed that a CDR of 93.87% in 10 minutes was optimal. According to stability research, accelerated conditions did not produce a discernible change. Using the foam granulation technology and optimal assessment criteria, FDT was successfully developed.



Schematic laboratory scale foam granulator

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OL-39

Synthesis and characterization of APTES modified ZnO loaded PVDF composites for energy storage application

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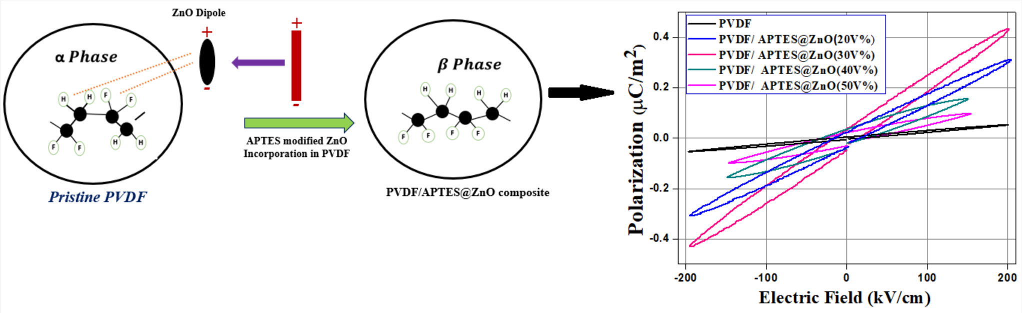
Dielectric nanocomposite plays a massive role in integrating a capacitor with high energy storage performance. Here, we synthesized environment friendly Polyvinylidene (PVDF) composites embedded with well dispersed surface modified zinc oxide nanorod (ZnO) through solution casting method. ZnO nanorod was obtained through wet chemical method reaction. Dried ZnO powder was hydroxylated with H_2O_2, followed by surface modification with APTES to acquire APTES@ZnO (APTES modified ZnO). Surface modification and high aspect ratio morphology of ZnO improved the breakdown voltage, polarization and overall energy storage performance of PVDF composite. The investigation of electrical properties of a series of synthesized PVDF/ APTES@ZnO (0, 20, 30, 40,50) V% composite films proclaimed loading of 30V% (zinc oxide @APTES) in PVDF act as optimized loading for enhanced energy storage performance. It showed an appreciable recoverable energy storage density about 36.7 mJ/cm^3 and energy storage efficiency of 91%. Relative comparison of the energy storage efficiency (ƞ) of PVDF/ APTES@ZnO (30) V% with recent published works verified its enhanced capacitive response [1,2]. The comparative study established PVDF/ APTES@ZnO (30V%) composite as a promising dielectric capacitor with application in energy storing portable device.



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OL-40

Repurposing of Anti Cancerous Drugs against Alzheimers disease for Targeting Tyrosine Kinase receptors

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ABSTRACT

Alzheimer's disease is a neurological issue that continuously decimates memory by influencing β-Amyloid and Tau-related proteins. Current research focusses on repurposing of anti-cancerous drug molecules for targeting Alzheimer's disease. Virtual Screening has been applied to generate library of small molecules based on prominent Anti-Cancerous drugs- vorinostat, tamibarotene, bexarotene, lenalidomide, thalidomide, dasatinib, masitinib, nilotinib, bosutinib and pexidartinib. These drugs have demonstrated to play significant therapeutic role in Alzheimer’s disease by improving restoration of synaptic activity, enhancing levels of IL-10, Blocking Fyn genes, eradicating senescent cells to decrease plaque formation and reducing Aβ and tau pathology. Chemical structures of these anti cancerous compounds were downloaded from Pubchem database followed by altering their pharmacophores by adding new functional groups or altering some heteroatoms in Chem sketch software. Around 151 Ligands were generated using this alteration strategy. Presence of proline-rich tyrosine kinases results in accelerated formation of neurofibril tangles and amyloid plaques. Tyrosine kinase inhibition has shown to improve conditions in Alzheimer's disease by reducing plaque formation and improving cell senescence. Structure of Tyrosine Kinase receptor was downloaded by RCSB database followed by docking of 151 ligands generated in chem sketch by using Autodock Vina wizard of PyRx software. Biovia discovery software was used for preparation of Tyrosine kinase receptor. Docking results have shown that conformers of Bexarotene, Lenalidomide and Nilotinib have highest binding affinity in the range of -9.2 to -11.4 Kcal/mol. Investigation of ADMET parameters have shown these conformers to be absolutely safe against Tyrosine Kinase receptors. Further molecular dynamics simulation studies are conducted to study the stability of these conformers.

KEYWORDS: *Alzheimers, Anti-cancerous drugs, Tyrosine Kinase receptors, Docking, Bexarotene, Lenalidomide, Nilotinib*

OL-41

Modeling studies of Hsp90 inhibitors with subtype selectivity

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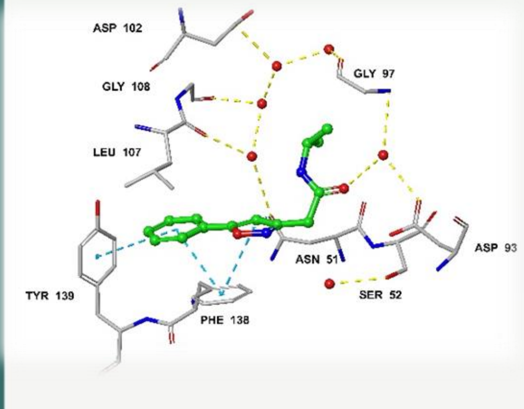
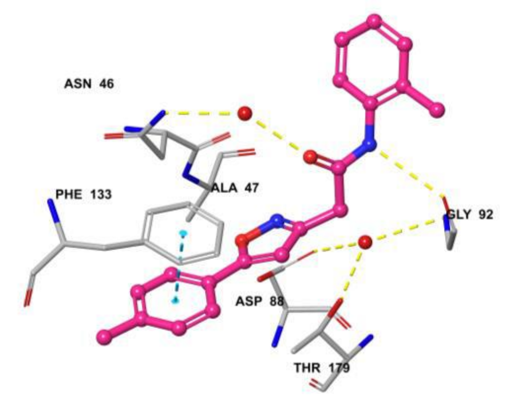
Heat shock protein 90 kDa (Hsp90) is a molecular chaperone whose functions include regulation of homeostatic conditions in the cells through the maturation of nascent polypeptide chains, refolding of denatured proteins, and disaggregation of the protein aggregates There are two cytoplasmic forms of HSP90, HSP90α, and HSP90β. The ATP binding cavity constitutes 29 amino acids in the four human paralogs. 70% of it is identical while the remaining 30% shows a high degree of similarity. This cavity is composed of central nucleotide-binding pockets encircled by three side pockets with conserved residues: Site 1, Site 2, and Site 3. These pockets form the basis of potential selectivity in Hsp90 isoforms as they show selective paralog binding by forming pairwise binding sites with the central cavity. An extensive network of water-mediated H-bonds is observed which play different roles in Hsp90α and Hsp90β. There is a difference only between two non-conserved residues in the ATP binding cavity: Ser52 and Ile91 in Hsp90α instead of Ala47 and Leu86 in Hsp90β. It has been extremely difficult to develop isoform-selective inhibitors of Hsp90a and Hsp90b because the two cytosolic isoforms have more than 95% identical binding site residues in the N-terminal ATP cavity. The only difference between these nucleotide-binding sites is the difference between the two amino acids. Hsp90 isoform-selective compounds can be utilized to diminish the toxicities of pan-inhibition and understand the contribution of particular isoforms from a pathological perspective. . The mechanism of selectivity is deciphered by a detailed thermodynamic study of the binding site analysis. . Known Hsp90α inhibitors are shown to manifest selectivity as well as binding affinity (reducing the entropic penalty) by inducing an opening of probe site 1 resulting from its hydrophobic occupation.





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[3] Authors acknowledge the High-End Computation Facility and Schrodinger Software support from BIT Mesra.

OL-42

Potential of marine fungi to biodegrade oil spillages in the most commonly contaminated sites of Visakhapatnam Port.

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Abstract

Oil spillage has become a major concern due to its huge impact on the marine ecosystem and mycoremediation is an effective strategy for clearing oil spills. The unique features that marine fungi possess are enhanced ability to tolerate crude oil and sustain in the oil- contaminated sites, elongated hyphae that spread to larger areas and provide more surface area for the degradation of crude oil, tolerance and adaptation to the fluctuations in pH and temperature make them better agents for bioremediation. The current study investigates the potential of marine fungi to degrade oil spills in the Visakhapatnam port, a major port involved in the transportation of oils. Samples from marine waters that are continuously exposed to oils are obtained from different oil berths and evaluated for their ability to degrade fossil fuels. *Aspergillus niger*, *A. fumigatus*, *A. flavus*, *Penicillium* and *Fusarium* species were isolated from the collected water samples and screened for their ability to degrade different types of oils (crude oil, petrol, diesel, and lubricant oil). The toxicity of the by-products that result from the bioremediation of oils is also assessed using a test organism. Thereby, this study helps in the determination of the potential of marine fungi that degrade various oils with higher capability and develop microbial consortia that can clean oil spills and establish a pristine marine ecosystem and environment.

OL-43

Use of Tropical Peptides for Cosmetic Medicine

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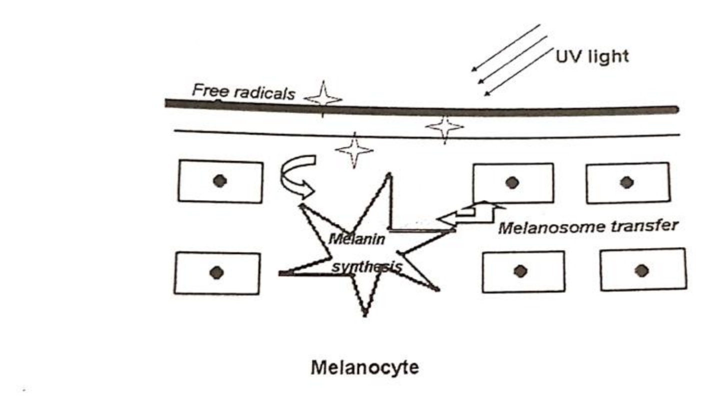
Peptides are known to have diverse biological roles, most prominently as signaling/regulatory molecules in a broad variety of physiological processes including defense, immunity, stress, growth, homeostasis and reproduction. These aspects have been used in the field of dermatology and cosmetology to produce short, stable and synthetic peptides for extracellular matrix synthesis, pigmentation, innate immunity and inflammation. The evolution of peptides over the century, which started with the discovery of penicillin has now extended to their usage as cosmeceuticals in recent years. Cosmeceutical peptides may act as signal modulators of the extracellular matrix component, as structural peptides, carrier peptides and neurotransmitter function modulators. Transdermal delivery of peptides can be made more effective by penetration enhancers, chemical modification or encapsulation of peptides. The advantages of using peptides as cosmeceuticals include their involvement in many physiological functions of the skin, their selectivity, their lack of immunogenicity and absence of pre-market regulatory requirements for their use. However, there are disadvantages: clinical evidence for efficacy is often weak, absorption may be poor due to low lipophilicity, high molecular weight and binding to other ingredients and prices can be quite high. Below figure shows a schematic representation of the effect of UV rays on skin leading to pigmentation.



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OL-44

Does perinatal development of locomotory muscles differ from postural muscles? Implication towards metabolic diseases and muscle defects

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The development of skeletal muscle during early ages is the projector of metabolic derailment during later life. While most of the studies are focused towards addressing locomotory disorders, very few have focused on addressing role of skeletal muscle development in metabolic abnormalities. Therefore, in our current study we have tried to investigate the distinct development of locomotory and postural skeletal muscles, and their implication towards metabolic diseases during adulthood. Goat as a precocial mammal, better depicts the developmental differences between locomotory and postural muscle and have more physiological similarity with human beings than mice. In our study postural muscles like trapezius and latissimus dorsi showed similar pattern of metabolic development as compared to gastrocnemius which predominantly performs locomotory functions. They showed significant difference in terms of mitochondrial oxidativeness and vascularization as observed in succinate dehydrogenase and alkaline phosphatase staining respectively. While gastrocnemius showed better distinction between oxidative and glycolytic fibers in terms mitochondrial density and vascularization; trapezius and latissimus dorsi contained more myofibers with intermediate mitochondrial density. They also differed in terms of expression of proteins associated with mitochondrial dynamics during development as well as adulthood. Both the fission and fusion associated proteins were elevated at term in all the three depots after which they are immediately downregulated in postural muscles. In contrast, their expression persisted till adulthood in gastrocnemius muscle. This difference in development suggests elaborating the metabolic development of postural muscles will implicate towards finding a suitable target to treat muscle associated metabolic diseases during adulthood.

OL-45

Tailoring Permeability of Acetazolamide Through Cocrystallization

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Acetazolamide (ACZ) is a carbonic anhydrase inhibitor primarily indicated for glaucoma and used as an ancillary therapy for epilepsy, diuresis, and high-altitude sickness, and oedema caused by congestive heart failure, as well as preventing drug-related side effects in the treatment of influenza [1,2]. ACZ, being a class IV member of biopharmaceutics classification system, possesses limiting solubility and permeability. In order to target the poor permeation profiles of such drugs, pharmaceutical cocrystals have emerged as novel tools in recent years [3,4]. Incorporation of a coformer inside the crystal lattice of a drug by means of weaker non-covalent interactions results in the development of cocrystal which exhibits modified crystal arrangement and molecular packing compared to the parent components. Since intrinsic properties of a molecule rely on its crystal structure, therefore rearranging the crystal packing of a drug is thought to manifest modulated permeability. In this regard, the ability of drug molecules to cross the biological membrane is a critical factor. Among the many cell-monolayer models currently available to mimic the human intestinal epithelium, the Caco-2 cell monolayer is most commonly employed because it is reliable and shows a strong correlation with the *in-vivo* absorption through the gastrointestinal epithelium. In the present study, the effect of cocrystallization of ACZ with p-aminobenzoic acid (PABA) on the CaCO-2 permeation profile of the parent drug has been shown methodologically (Figure 1).

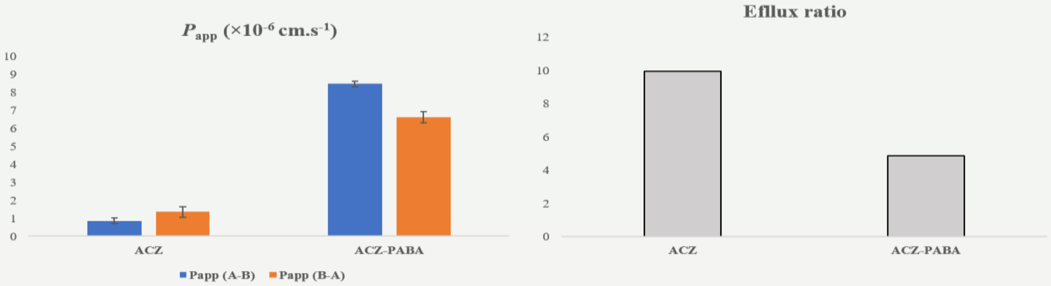

Figure 3. Comparative representation of modulation in permeability profiles of Acetazolamide (ACZ) and Acetazolamide-p-aminobenzoic acid cocrystal (ACZ-PABA) through CaCO-2 cell line.

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OL-46

Using free-ranging birds as model organism towards identification of targets in the skeletal muscle for countering metabolic diseases

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Avian cold adaptation is hallmarked by innovative strategies of both heat conservation and thermogenesis. While minimizing heat loss can reduce the thermogenic demands of body temperature maintenance, it cannot eliminate the requirement for thermogenesis. Shivering and non-shivering thermogenesis (NST) are the two synergistic mechanisms contributing to endothermy. We chose birds as the model for studying NST as they lack brown adipose tissue (BAT), the major organ of NST in mammals. In our studies, we have tried to critically analyze that skeletal muscle is the principal site of NST in birds via keeping seasonal cold adaptation to be the major challenge (i.e *Columba livia* for the experiment are taken in both summer and winter season from the local area). We have performed Real time PCR for almost all Ca2+ handling genes in skeletal muscle (Pectoralis, biceps, triceps and Ileo tibialis) and our results suggests that sarco(endo)plasmic reticulum Ca2+-ATPase (SERCA) and ryanodine receptor 1 (RyR1) are key in avian muscle NST, through their mediation of futile Ca2+ cycling and thermogenesis. Moreover, another novelty of our finding is the up regulation of sarcolipin (SLN) in winter muscles, which clearly shows that SERCA regulation by SLN facilitates muscle NST in birds. Further, from various histochemical staining assays, the up regulated Succinate dehydrogenase (SDH) and Alkaline Phosphatase (ALPL) activity in the winter acclimatized birds indicates the increase of mitochondrial oxidative capacity and capillary activity in the skeletal muscle fibers. Overall, our study highlights that birds are unlikely to be able to maintain their body temperature in cold climates by heat conservation and shivering, and therefore presumably recruit NST via SR-induced SERCA-based ATP utilization.

OL-47

Interaction of Sulfadiazine with Bioconjugates

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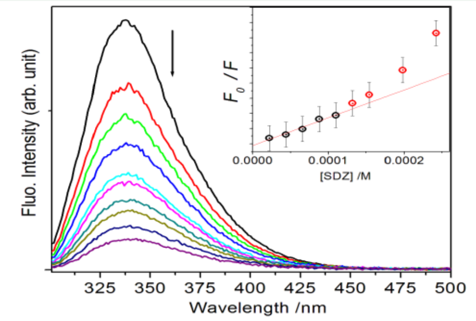
The modulated bioactivity of proteins immobilized on nanoparticle (NP) interfaces is having wide range of applications in designing better therapeutic, diagnostic and drug delivery tools [1]. Lysozyme (LYS) possesses a variety of important properties like antibacterial, anti-inflammatory, antiviral, immune modulatory and antitumor activity that enhances its application in pharmaceutical industries [2]. On the other hand sulfadiazine (SDZ) is a sulfonamide class having wide-spectrum antibiotic against both gram-negative and gram-positive bacteria. SDZ is commonly used drug to treat burn wounds. The interaction and binding behavior of LYS and SDZ was monitored by in-vitro fluorescence titration and molecular docking calculation under physiological condition. The quenching of LYS fluorescence on addition of the SDZ is due to the formation of protein-drug complex in the ground state.



Molecular docking calculation, Synchronous fluorescence results corresponding to Trp and Tyr residues as well as FTIR spectra in the amide-I region of LYS confirms minimal deformation in the LYS secondary structure on adsorption to spherical NP surface. Although the nature of LYS–drug interaction remains invariant, the extent of quenching interaction as well as the drug binding ability is strongly modulated in presence of NPs. Further, the antibacterial activity of LYS in presence of the investigated drugs shows upsurge with AuNP, in sharp contrast to decrease in AgNP.

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OL-48

Overexpressed Kinases (EGFR) as Therapeutic Tool in Targeting Oncogenesis

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Oncogenesis has emerged as a major threat with rapidly alarming incidences and mortality issues. Lung cancer among the top in terms of reported incidences worldwide is a multi-factorial, chronic diseases cohorted with simultaneous over-expression of multiple proteins and interconnected signaling pathways. EGFR is reported with many genetic as well as epigenetic modifications at molecular level leading to oncogenesis. Different kinase inhibtitors are reported in literature and approved by FDA to inhibit the overexpression with mutational modification as a frontline barrier. Majority of the approved drugs for the target are based on quinazoline scaffold. So, a vast library of synthetically feasible quinazolinone based derivatives was generated using structure based drug designing approach and the best hits retaining key interactions were figured out. This study can help in achieving better drug candidates in targeting mutationaly modified EGFR. Thus, structure based targeting of oncogenic proteins or deregulated pathways may result in achieving better drug candidates with better therapeutic outcomes.

KEYWORDS: Lung cancer, structure based, EGFR, Quinazolinones

OL-49

Pangenome analysis of ST147 *Klebsiella pneumoniae* reveals its genome evolution and functional diversity

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The rapid emergence of drug-resistant *Klebsiella pneumoniae* is being driven by the spread of fast-transmitting high-risk international clones such as ST147 but there are limited studies on their global prevalence and population dynamics. The current study aims at pangenomic characterization, evolution-based phylogenetic relationship and genomic diversity analysis of an Indian strain KP_ST147. AMR determinants were belonged to the antibiotics classes; β-lactamases, fosfomycins, peptide antibiotics, fluoroquinolones, outer-membrane porins, sulfonamides and aminoglycosides. 85.3 % of the genomes have KL64 capsular loci, while our strain belongs to KL10. Putative virulence classes are associated with type I/II-secretion, ent siderophores, yersiniabactin, type I/II-fimbriae, salmochelin, and CPS formation genes. The negative Darwinian selection rate indicates its higher rate of evolution. Our findings demonstrated a distinct lineage to acquire the *bla*$_{\text{OXA-232}}$ gene harboured in a ColKp3 plasmid. Integration of an insert in Tn6170 transposon element found to be interesting in this study. Overexpression of RND efflux genes and their regulators in response to colistin exposure results in led to a colistin resistance phenotype. The most commonly found BGCs were NRPS, redox-cofactor, polyketide synthase, Ripp-like, and thiopeptide, providing an avenue for exploring the therapeutic prospects of secondary metabolites produced by this clone. The timeline of emergence and understanding of the evolution of this clone determined in this study may aid in the identification of newly emerging lineages of *K. pneumoniae* and provide knowledge on the spreading of this high-risk clone across the globe.

OL-50

Bisphosphonates beyond Osteoporosis: Emergence as an anti-cancer agent and future potential upon nanoencapsulation

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Bisphosphonates (BPs) are agents that can prevent bone loss by direct action on osteoclasts. Amongst BPs, Zoledronate (Zol), a third generation aminobisphosphonate binds to mineralized bone with highest affinity and remains in the skeleton for a prolonged time thereby carrying the potency to create imbalance in bone niche. Zol has direct antitumor ability preventing RasGTPases modification and stimulating apoptosis, similar to that in osteoclasts. Despite its advances in maintaining balance in skeletal related events and direct anticancer property, Zol is also known to cause some cytotoxicity to normal healthy preosteoblast cells, hampering mineralization and differentiation which is also observed in the present study(Petcu et al. [1]). Therefore, to use Zol as a potential sole anticancer agent against osteosarcoma, poly(lactic-co-glycolic acid) (PLGA) is employed in the present study to nanoencapsulate the drug and deposit it in the tumor cells with less toxicity to preosteoblast within safer dose range. Results revealed that NPs in the nanometer range having smooth and spherical morphology demonstrated good encapsulation efficiency with sustained release of the encapsulated Zol. The in vitro cellular studies reflected the higher uptake of NPs more towards the cancer cells and thus *retained* cytotoxicity. Cell-death inducing ability of the nanoformulation is observed with the ability to *rescue* the normal preosteoblast cells from the damage native drug was imposing. Thus, in this study it is shown that a slow dug release nanosystem can open up novel venture as a safe delivery for Zol with retained and rescuing effect.

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OL-51

Polymerization Kinetics and Swelling-Contraction of Acrylate based Hydrogels

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The application of acrylate-based hydrogels has gained much research attention. The uses of these hydrogels are varied. Industrial applications include environmental engineering, agriculture, tissue engineering, biomedical, construction, oilfield and electrical products, personal care products, and wastewater treatment. In this study, the swelling, contraction behavior, and polymerization kinetics were followed by varying concentrations of monomer and the initiator. The temperature effect was also studied. Hydrogels were obtained by polymerization in an aqueous solution in the presence of initiators and crosslinkers. When acrylate was neutralized with NaOH by taking them in equimolar proportion in H2O and the resulting mixture was subjected to polymerization in the aqueous solution of (NH4)2S2O4 in presence of a crosslinker at ambient temperature for 24hr, the whole polymerization mixture was transformed to a solid glossy mass which was taken out, washed properly to remove soluble materials and dried. The hydrogel was placed in water till water absorbance equilibrium was reached. The degree of swelling contraction was found to be 100 to 1000 of its weight. The purpose of this investigation was to report the synthesis of an intelligent pH-sensitive acrylate-based hydrogel by polymerizing the co-monomers- acrylic acid, acrylamide, and sodium acrylate (NaAC). Through these studies, we found that the hydrogels show a sharp change in water absorbency and gain pH sensitivity, they are stable and able to undergo swelling-deswelling cycles suggesting their reversible characters. The hydrogels obtained through these processes are superabsorbent and have numerous applications in the areas mentioned above.

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OL-52

Near-IR Plasmonic and Anisotropic Silver Nanocrystals: Zero rpm Synthesis and the Effect of Sequence of Reagent Addition

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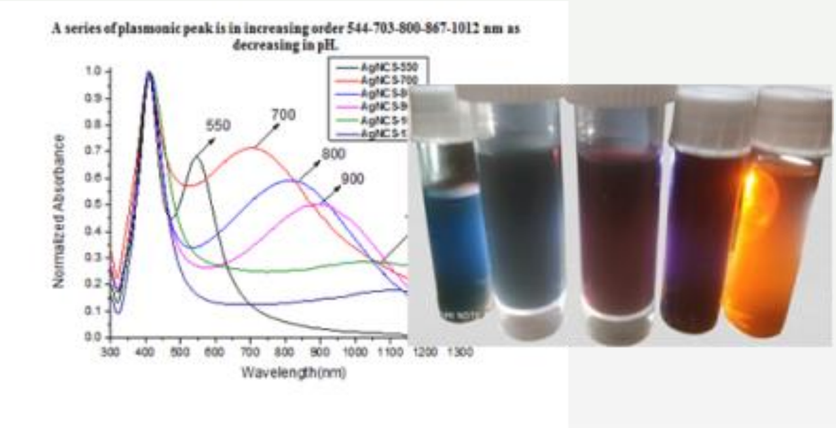
Anisotropic plasmonic nanomaterials of gold and silver have attracted the attention of scientists due to interesting optical phenomenon called surface plasmon resonance (SPR). The asymmetric shapes overcome the limitation of spherical nanoparticles in which SPR peak cannot be tuned to the near-IR spectral region [1]. For in-vivo biomedical applications, it is desirable to have nanoparticles with SPR peak in the near infrared (NIR) spectral region (650-1200 nm) which represents a biologically transparent window.

In this work, the effect of stirring speed and the sequence of addition of hydrazine hydrate has been thoroughly investigated. When the reaction mixture was not shaken or stirred, i.e, at zero rpm, plasmon peak was tuned to the near IR region and the FWHM was also less as compared to other stirring speeds. At 5^0C and at pH 5, the maximum redshifted peak was obtained at 880 nm. As the stirring speed is gradually increased in the order, 0®200®400®600 rpm, the plasmon peak moved to shorter wavelengths, 880®834®820®719 nm. Zero rpm was selected as the optimum condition to synthesize spectrally narrow silver nanoparticles with redshifted plasmon peaks. This also makes the process greener and cleaner as it makes the use of magnetic stirrer totally redundant. TEM analysis revealed that nanoparticles have a pentagonal pyramidal shape , with edge-length ranging from 18 to 30 nm. Such NIR plasmonic nanocrystals are weel-suited for biomedical applications.



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OL-53

Functional 3-D Smart Materials: Properties, absorption investigation, and usage

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In today's world, there are numerous functions of polymer hydrogels (PHGs) in various fields of modern technology. PHGs are defined according to their main properties and raw materials. PHGs are materials which exhibit both viscous and elastic network structures and properties. They are 3-D cross-linked hydrophilic polymers that are insoluble but absorb, swell and hold large amounts of water. The water absorbency of PHGs was found to be more than 1000 times their mass. The hydrophilic functional group such as hydroxylic (-OH), carboxylic(-COOH), amidic(-CONH-), primary amidic(-CONH2) and sulphonic(-SO3H) attached to the polymeric backbone gives the ability to uptake water in hydrogels. Findings show that small quantities of divalent or trivalent ions drastically decrease water uptakes of gels[4]. However, absorbency remains unaffected by urea because of its non-dissociating behavior and having a similar group as that of monomers[4]. These materials exhibit both solid and liquid-like properties. These properties are affected by concentration and nature of monomer, environmental conditions, and cross-linker used. The cross-linking of these polymers is a result of covalent, hydrogen bonding, Van der Waals forces, or physical entanglements. These responsive smart materials have pervaded daily life in different forms due to vast worldwide usage in industrial applications such as agriculture, textile, pharmaceutical, biomedical, biotechnology, wastewater treatment, and many other areas.

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OL-54

Synthesis and Study of a Novel Graft Copolymer With Mosaic Grafting And Assessment Of Its Suitability Towards Sugarcane Juice Clarification

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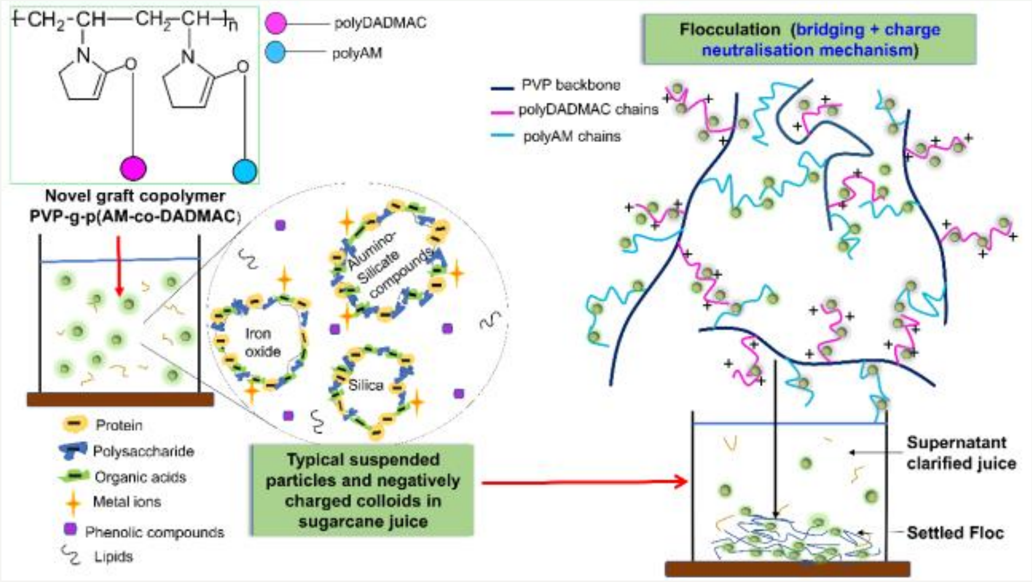
The study entailed the green microwave-assisted synthesis, characterization of novel graft copolymer poly (acrylamide-co-diallyldimethylammonium chloride) grafted polyvinylpyrrolidone (PVP-g-p(AM-co-DADMAC)) and ascertainment of its suitability as a sugarcane juice clarifier. The mosaic grafting of the two monomers harnesses dual property onto the parent polymeric backbone which was hypothesized to give effect to synergistic bridging and charge neutralization mechanism of flocculation. The flocculation efficacy and optimum dosage of different grades of material were corroborated by average floc size determination, zeta-potential measurement, and observed lowering of turbidity and optical density of the supernatant juice post flocculation.

Clarification remains an arduous but critical step in the industrial processing of sugarcane juice for obtaining high-quality products and by-products. However, commonly used techniques like liming and sulphitation are heavily chemical-based, posing both environmental and food safety threats. Whereas, newer membrane-based techniques require feedstock pre-treatment by clarification essentially to prevent membrane fouling. The novel polymer with biodegradable components facilitates relatively simple clarification via flocculation, opening avenues for future studies to test the flocculant in tandem with the prevalent clarification processes for greater sustainability. Additionally, the degree of brix (ºbx) of the juice changed negligibly for the best grade of flocculant at an optimum dosage indicating no loss of sucrose content.



OL-55

Solvent Effects on Regioselectivity: Sodium Fluoride Catalysed Synthesis of Mono- and Di-Substituted Benzimidazoles

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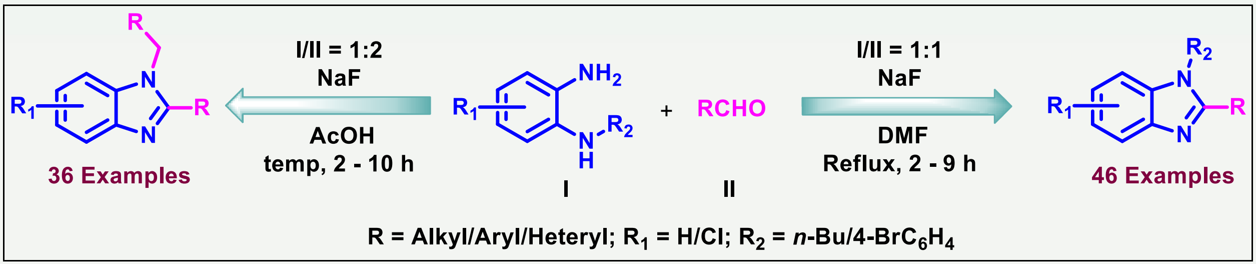
The regioselective formation of 2-substituted and 1,2-disubstituted benzimidazole derivatives have been achieved from the reaction of *o*-phenylenediamine derivatives with different aldehydes in presence of sodium fluoride (NaF) in two different polar solvents. This method is simple, easy, safe, economical, and applicable to a wide range of aldehydes. The method aid to form 2-substituted benzimidazole in dimethylformamide and 1,2-disubstituted benzimidazole in acetic acid using NaF as catalyst in excellent yield. The electron density of aldehyde and *o*-phenylenediamine exhibit significant influence on the selectivity of the formation of benzimidazole compound in acetic acid. Therefore, in acetic acid, with *N*,*N*-dialkyl- and nitro substituted benzaldehydes, 2-substituted benzimidazole derivatives were formed instead of their corresponding 1,2-disubstituted benzimidazoles.



Key words: Benzimidazole, mechanistic studies, *o*-phenylenediamine, regioselectivity, sodium fluoride.

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OL-56

Design and Development of effective drugs against Histone deacetylases in Alzheimer's disease using Computational Biology tools

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Current Research focuses on designing and development of effective drugs against Histone deacetylases (HDACs) in Alzheimer's disease using computational biology tools. Here, the repurposing of anti-cancer drug molecules targeting Histone deacetylases, a macromolecule has to be performed for the design and development process. Histone deacetylases have arisen as alluring focuses in anticancer medication improvement. The 3D crystal structure of HDAC of the hydrolase transferase class has utilized PDB ID 2GH6 and obtained through X-Ray Diffraction. In Alzheimer's disease, anticancer drugs such as vorinostat, tamibarotene, bexarotene, lenalidomide, thalidomide, dasatinib, masitinib, nilotinib, bosutinib, and pexidartinib play a rational therapeutic role by rebuilding synaptic pliancy, developing long-term potentiation of memory, and reducing Aβ and tau pathology. A virtual screening has performed on these drugs by downloading their chemical structures from PubChem and altering their pharmacophores in Chem sketch by adding new functional groups or changing some heteroatoms. Because of this alteration strategy, 652 ligands have been designed. Conducting the docking of 652 ligands to the HDAC through auto dock vena in PyRx gives the most elevated restricting partiality i.e. the binding affinity. Selection of the binding affinity in the range of -9Kcal/mol to -10.7 Kcal/mol gives the prominent results for the bio radar analysis using SWISS ADME tool. Compounds generated by pharmacophore alteration gives after virtual molecular docking is of Bexrotene followed by Tamibarotene and Dasatinib. Further bio radar analysis has been conducted using SWISSADME that provides the bio-ethnicity of the compounds showing their pharmacokinetics effects.

Keywords: Histone deacetylases; Computational modelling; Virtual Screening; Alzheimer’s Disease; Anticancer drugs

OL-57

Designing of nano drug delivery system based on polyoxometalates and MCM-48 for poorly soluble drug, Glipizide

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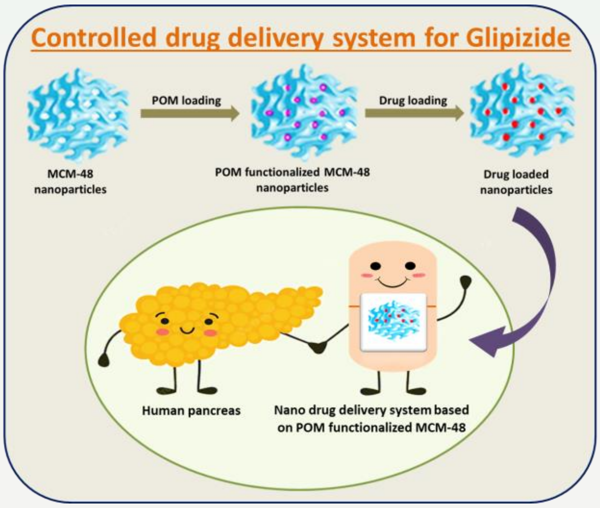
Diabetes mellitus (DMT2) is a heterogeneous disease associated with many health disorders including fluctuations in blood glucose concentration which can cause major side effects. To overcome this concern, a controlled drug delivery system (DDS) can be designed which can help in maintaining a constant drug concentration in blood. Amongst various types of DDS, mesoporous silica nanoparticles (MSNs) have been explored due to their unique properties like high surface area, ordered porosity, and adsorption capacity. It is known that functionalizing the surface of MSNs increases the drug-surface interactions which effects the release mechanism and mainly organic moieties have been used for the same. Hence, it was thought to use an inorganic moiety, especially Polyoxometalates (POMs), which already have been explored in medicinal chemistry [1].



In this work, 12-tungstosilicic acid (TSA) functionalized MCM-48 nanoparticles (nMCM-48) was synthesized for controlled release of Glipizide (GLP) and characterized by various techniques. In-vitro release study was carried out and compared with release profile of marketed formulation (Glynase). The comparison study indicates that TSA acts better as a functionalizing agent rather than as a capping agent and when compared with the marketed formulation, GLP/TSA/nMCM-48 shows more controlled release.

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OL-58

Poly pyridyl based Cobalt complexes as electrocatalysts for water oxidation

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To mimic the process of photosynthesis and access the ability to oxidize water to molecular oxygen is one of the most awaited dream of human and hence we try to take a step towards it .The present work reports the effect of electron donating substituents on terpyridine cobalt complexes as water oxidation catalysts $[Co(L_1)_2]$,$[Co(L_2)_2)]$,$[Co(L_3)_2]$.where L1= (4'-(3,4,5-trimethoxyphenyl)-2,2':6',2"-terpyridine),L2= (4'-(3,4-dimethoxyphenyl)-2,2':6',2"-terpyridine) and L3 = (4'-phenyl-2,2':6',2"-terpyridine). The metal complexes were observed as ML_2 on Single crystal XRD and Mass spectroscopy. FTIR, NMR and UV spectroscopy of the ligands and metal complexes were studies to unveil their nature, structural integrity and core characteristics. The ultimate goal is to produce a photo-catalyst but studies and production of electro, chemical, electrochemical and photo-electrochemical catalysts is also important. Here the complexes have shown promising results as electrocatalyst at higher pH while assessing their abilities as water oxidation catalyst on potentiostat.
Keywords- Water oxidation, Earth abundant metals, electrochemical water oxidation.

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OL-59

Monomeric Ru^{II} complexes with anionic ligand: Electrocatalysts for water splitting reaction

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Three highly active monomeric ruthenium complexes with anionic ligands as electrocatalysts for water oxidation: [Ru^{II}(L)(L^1)(DMSO)][ClO$_4$](**1**), [Ru^{II}(L)(L^2)(DMSO)] [PF$_6$](**2**) and [Ru^{II}(L)(L^3)(DMSO)][PF$_6$](**3**) [L = pyrazine carboxylate, L$_1$ = 2,6-bis(1H-benzo[d]imidazol-2-yl)pyridine, L$_2$ = 4,5-dmbimpy = 2,6-bis(5,6-dimethyl-1H-benzo[d]imidazol-2-yl)pyridine, L$_3$ = 4-Fbimpy = 2,6-bis(5-fluoro-1H-benzo[d]imidazol-2-yl)pyridine, dmso = dimethyl sulfoxide] are reported here. All the complexes are isolated and characterized by Single crystal XRD, NMR, ESI-MS, elemental analysis, UV-Vis, and EPR spectroscopy. Redox properties of the complexes and their electrocatalytic activity are studied by linear sweep voltammetry(LSV), cyclic voltammetry(CV), and bulk electrolysis. A systematic variation on the ligand scaffold has been found to display a profound effect on the rate of electrocatalytic oxygen evolution. Systematically studied the O-O bond formation by WNA mechanism by density function theory(DFT) and LSV study on all ruthenium complexes. At pH = 1, maximum turnover frequency (TOF$_{max}$) has been experimentally obtained as 110.41 s^{-1}, 2567.89 s^{-1}, and 2.05 s^{-1} for complex 1, 2, and 3 respectively from the foot of wave analysis (FOWA).

OL-60

Green Synthesis, Antimicrobial Activity and Corrosion Inhibition of Divalent Transition Metal Complexes of A Bidentate Amide Ligand

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The stable, non-electrolytic and coloured monomeric solid complexes of the amide ligand derived from N-acetylisatin with Co(II), Ni(II) and Cu(II) ions were synthesized under microwave irradiation in solvent-free condition with excellent yields. This method of synthesis of ligand as well as metal complexes is environmentally benign having simple work-up procedure, short reaction times and non-hazardous to environment. The divalent metal complexes were characterized with their stereo-chemical structures and geometries (tetrahedral & square planar) suggested were depending upon data of elemental microanalyses, IR, UV-Visible, 1H, 13C NMR spectra, mass spectral analyses, magnetic susceptibility and molar conductance measurements. Ligand field transitions were determined from observed absorption band positions in their electronic spectra and the band energies and Racah parameters were calculated by applying observed data on Tanana Saugano diagram of the investigated metal complexes.

The antimicrobial activity of the free ligand and its divalent transition metal complexes clearly indicates that the ligand has less potency towards tested micro-organisms than the investigated metal complexes. The complexes also inhibit the growth of bacteria and fungi to a greater extent as the concentration was increased. The antimicrobial activity is in the order of Co> Cu>Ni> Ligand.

The investigated ligand and its divalent metal complexes were used as nano-coating and inhibitors in acidic medium of stainless steel and found that the investigated metal complexes were weaker corrosion inhibitors than the ligand.

OL-61

Eco-Friendly Synthesis and Antimicrobial Activity of A Schiff Base Ligand & it's Divalent Transition Metal Complexes

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A facile, efficient and environmentally benign method using microwave irradiation has been applied for the synthesis of an unsymmetrical tetradentate bi-anionic Schiff base and its mononuclear square planar Co(II), Ni(II) and Cu(II) complexes in ethanolic-aqueous green solvent. A comparative analysis of the synthesized Schiff base and its Co(II), Ni(II) and Cu(II) complexes via conventional reaction and environmentally benign method have been described. All the eco-friendly synthesized compounds were characterized by elemental analysis, conductivity and magnetic moment measurements and IR, UV-Visible & ^{1}H NMR spectroscopic methods. The biological evaluation as anti-bacterial and human pathogenic anti-fungal activities of investigating compounds revealed that the M (II) complexes are found to be more active than the free ligand towards the tested microbes under the identical experimental conditions and the antimicrobial activity trend is in the order of: Cu-complex > Co-complex > Ni-complex > Ligand

Key words: Schiff base; transition metals; anti-microbial activity; microwave-assisted reaction; square-planar geometry

OL-62

Synthesis, Characterization, Cytotoxicity, and In Vitro Antibacterial Activity of Novel N'(di-2-pyridylmethylene) morpholine-4-thiocarbohydrazide Complex of Manganese

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Thiosemicarbazones and their derivatives exhibit a wide variety of biological and therapeutic applications. Moreover, its several metal complexes and their derivatives mark the dawn of a new era of specific treatment for various microbial infections, cancer, various neurological diseases, etc. Here, we have synthesized a manganese complex with N'(di-2-pyridylmethylene) morpholine-4-thiocarbohydrazide ligand and characterized using different techniques like IR, UV- Vis spectroscopy, Mass spectrometry, etc. Thermal stability was analyzed by thermogravimetric analysis, magnetic studies were carried out using a vibrating sample magnetometer at room temperature. From the biological studies, we have found that the metal complex possessed an outstanding resistivity against gram-positive Staphyloccocus aureus ATCC 25923 (S.aureus)] and gram-negative bacteria [Escherichia coli ATCC 25922(E. coli)] with MIC values 6.580µg/mL and 29.205µg/mL respectively. The in vitro antitumor activity of the complex was determined against L929 Fibroblast cells. These tests revealed that it has considerable cytotoxicity with IC50 135.45094µg/mL. Hence, the synthesized novel metal complex can be considered as a notable agent with superior antibacterial activity along with the potential antitumor activity.

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OL-63

Zero-rpm synthesis of Hollow Silver Nanocubes with high monodispersity and Near-IR Plasmon Tunability

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Folic acid plays a unique role as a capping agent in nanocrystals, directing their form and structure ability [1][2]. Folate-capped Ag_2O nanospheres were changed into hollow silver nanocubes with a cube-like nanocrystal and a spherical void-like space [3]. The hollow plasmonic nanocrystals are less massive than similar-sized solid particles, resulting in a weight advantage [3]. Hollow plasmonic nanocubes were synthesized by a unique synthesis technique in which no shaking or stirring is involved, hence called ‘zero-rpm synthesis. The HAgNCs were exhibited plasmon tunability from the visible-to-NIR region, 500 ® 850 nm, simply by altering the molar ratios. The zero-rpm synthesis yielded HAgNC have less fwhm signifying high monodispersity. The zeta-potential of HAgNC-500 and HAgNC-800 was found to be -62.6mV and -36.5mV, respectively. Thus, folate-capping imparts a high amount of surface charge and robust stabilization of nanocubes was achieved. Further, HAgNC-500 was relatively more stable than HAgNC-800. FTIR and Raman Spectroscopy confirm surface capping by folic acid. Enhanced SERS signal for folate was also observed under irradiation by 532nm laser, making it an excellent candidate in photocatalysis hydrogen evolution[4] and degradation of pollutants[3].

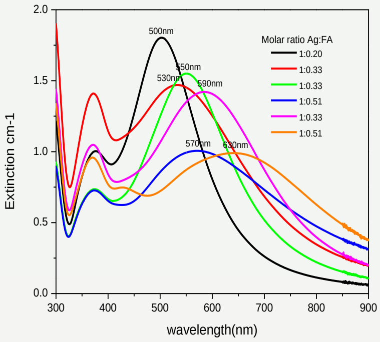

Figure: Effect of molar ratio Ag+:folic Acid on plasmonic properties of HAgNCs.

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OL-64

One-pot synthesis of pyrazole fused polyclic heterocycles

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Abstract Awaited

OL-65

Spermidine supplementation helps performance of sex-limited breeds of *Bombyx mori* (Lepidoptera: Bombycidae)

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Abstract

Sericulture has immense economic significance. The separation of male and female silkworm moths for egg production in commercial grainages is a laborious task. Sex-limited breeds of cocoon color are advantageous in the selection process. The major constraint in sex-limited breeds is low fecundity. The number of eggs laid by the sex-limited female moths is very low in comparison to non sex-limited breeds. Spermidine was shown to improve egg production of silkworm, *Bombyx mori*.L. In the present study, cocoon color sex-limited breeds were selected and fed with spermidine to improve fecundity and nutritional efficiency of the breeds. The 5th instar silkworm larvae of selected breeds were subjected to standard rearing conditions with and without spermidine supplementation up to spinning. Three replications were maintained for each breed. Results showed that spermidine supplemented sex-limited breeds showed better performance in fecundity, and nutritional indices when compared to control sex-limited breeds. The treated breeds also showed better economic performance. Of the three sex-limited breeds tested, one of the breed showed best result for taking it to field level trials.

OL-66

Chalcone Complexes as Anticancer Agents

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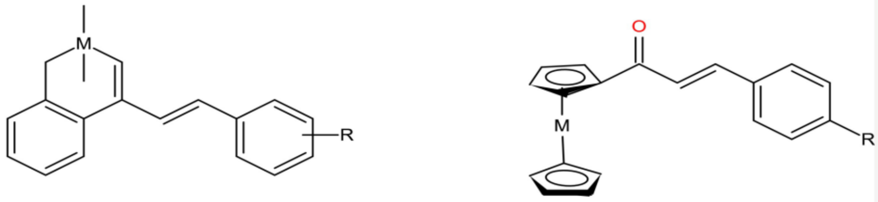
Cancer is a group of diseases characterized by the uncontrolled growth and spread of abnormal cells. There is at present, much optimism about the possibility of finding selective anticancer drugs that will eliminate the cytotoxic side effects associated with conventional cancer chemotherapy. Many chalcone and its derivatives target ‘cancer-specific’, which will allow the targeting of cancer cells while normal cells are spared. Several chalcones were synthesized and their *in-vitro* cytotoxicity against various human cell lines, including human breast adenocarcinoma cell line, MCF- human lung adenocarcinoma cell line A549, human prostate cancer cell line PC3, human adenocarcinoma cell line HT-29 and human normal liver cell line WRL-68 was evaluated. Most of the compounds being active cytotoxic agents, four of them with minimal IC50 values were chosen and studied in detail with MCF-7 cells.

Metal complexes of chalcone have played key role in the development of chemotherapy. The synthesis, characterization and applications of metal complexes containing chalcone and its derivatives as ligands, and the particular coordination chemistry indicates pharmaceutical potential in some areas such as anticancer activity and selective cytotoxicity, antioxidant and antibacterial effects. The anticancer activities of the chalcones and their Pd(II) complexes have been evaluated.
Ruthenocenyl chalcones is reported having *in-vitro* anti-proliferative activities. Chalcone complexes displayed remarkable inhibitor cytotoxic activity against NCI lung cancer cell line with 45 % inhibition whereas 91% inhibition against MDA-MB-4355 breast cancer cell line. The pyridyl chalcone derivatives and their complexes were also reported against the human colorectal cancer cell lines HT-29, HCT-116 p53+/+, HCT-116 p53_/_ and ARPE-19 . We have also worked on metal complexes of chalcone having bioactive motifs. The prototypes of our synthesized molecule are shown below.



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OL-67

Expression profile of differentially expressed genes associated with Oral Submucous Fibrosis

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Abstract

Oral submucous fibrosis (OSMF), is a premalignant ailment of the mouth which results in advanced juxtaepithelial fibrosis of the spineless tissues inside the mouth, ensuing the damage caused in the tissue which reduces the mobility, noticeable inflexibility leading to an ultimate incapability to open the mouth. In this study, microarray dataset was used for the entire genome analysis of the oral submucous fibrosis, which was later compared with the normal and tumorous samples from Gene Expression Omnibus (GEO) database; a repository of NCBI. Weighted Gene Co-expression network analysis helped in determining the differential gene expression using the Bioconductor package. A total 47323 differentially expressed genes were acquired. Each genes was then forecasted with human protein atlas which aided in determining **the expression profiles of genes which are associated with oral submucous fibrosis both on the mRNA and protein level.** The core upregulated and downregulated genes in the present study would help us in understanding the exact characteristics of these genes which play a major role in the progression of oral submucous Fibrosis.

Keywords- Differentially Expressed Genes, Oral submucous Fibrosis, Microarray dataset and Human Protein Atlas

POSTER

P-1

Rational design of nucleic acid aptamers against snake venom protein: An approach for snakebite management

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Abstract

Management of snakebite faces a major challenge in terms of diagnostic as well as treatment. Inefficacy and associated risks of current antivenom has raised the need for safer therapy as well as accurate diagnostic of envenomation. Aptamers are one such alternative which is being pursued for therapeutic interventions as well as for design of diagnostic kits due to its high specificity. Hence, the present study focussed on designing and validating nucleic acid aptamers against snake venom $PLA_{2,}$ a hydrolytic enzyme present in all venomous snakes. The aptamers were designed by adding nucleic acid chain on the surface of Daboxin P, a major PLA_2 enzyme of *Daboia russelii* venom using molecular docking. The designed aptamers were synthesized and studied for their inhibitory property. It was observed that the synthetic aptamers could inhibit the catalytic as well as the tested biochemical activities of Daboxin P. The IC_{50} of the aptamers against $sPLA_2$ activity of Daboxin P was found to be in the range of 0.52 µM to 0.77 µM. Moreover, the aptamers inhibited the anticoagulant activity of Daboxin P when tested on goat blood platelet poor plasma. In addition to the *in-silico* studies, binding of the aptamers to Daboxin P was confirmed by electrophoretic mobility shift assay. Thus, the present study demonstrates that designed aptamers can be a potential therapeutic molecule to inhibit the biochemical activities of Daboxin P which can be explored for management of snakebite patients.

Keywords: Aptamers, Daboxin P, PLA_2

P-2

A study on *Bungarus fasciatus* venoms of India and their immuno-crossreactivity with Indian polyvalent antivenoms.

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ABSTRACT

Bungarus fasciatus (Schneider, 1801) is a venomous medically important elapid snake abundant in Eastern and North-Eastern India along with the whole of Indo-Chinese region, Indonesian archipelago and Malay peninsula [1]. The wide distribution of the species indicates the possibility of variation in venom composition due to different geographical conditions which may impact the clinical management of snakebite [2]. The present study compares the crude venom of *Bungarus fasciatus* from three different locations of India *i.e* Assam, Mizoram and West Bengal to understand the variation in venom compositiom. The venom proteome profiles were compared using sodium dodecyl sulfate-polyacrylamide gel electrophoresis (1D-SDS) and reverse phase high performance liquid chromatography (RP-HPLC). There was significant variation in the elution pattern of RP-HPLC profiles under the same chromatographic conditions. Moreover *in vitro* enzymatic assays such as PLA_2 activity, proteolytic activity and anticoagulation activities exhibited differences. Furthermore, immuno-crossreactivity of the venoms with different commercially available Indian Polyvalent antivenoms such as Premium Serums Polyvalent antivenom and Bharat Serums Polyvalent antivenom were evaluated and the results showed significant differences in their neutralizing capabilities. Studies on venom variation due to geographical locations may provide insights for various pathological conditions arising out of snakebite envenomation and may help identify unique proteins which may have role in possible therapeutic interventions in various disease management.

KEYWORDS: Bungarus fasciatus, Indian polyvalent antivenom, immuno-crossreactivity.

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P-3

Cytotoxicity of monocellate cobra *Naja kaouthia* venom (North-east India origin): Exploration of Anti-cancer potential

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Cancer is one of the leading causes of morbidity and mortality worldwide. Development of naturally derived small molecules as sensitizing agents target gene products that regulate the apoptotic pathways and allow therapeutics to be effective for treatment of cancer. In the past three decades, natural products from plants or venom from animals played major roles in novel drug design and development. Snake venom is a highly complex mixture of organic and inorganic compounds that include peptides, enzymes, low molecular mass proteins that have specific chemical and biological activities [1]. A lot of components have been identified from different snake venoms as therapeutic agents. A group of polypeptides (60–70 amino acid residues) called cytotoxins or cardiotoxins present in elapid family of snakes have a wide variety of pharmaceutical applications and show cytotoxicity against cancer cells [2]. The aim of the present study is to evaluate the cytotoxic effect of protein/s purified from Indian monocellate Cobra (*Naja kaouthia*) venom against human breast cancer (MCF-7 and MDA-MB-231) and lung cancer cell lines (A549). The reverse phase HPLC fractions of crude *Naja kaouthia* venom were found to exhibit cell cytotoxicity (MTT assay), inhibit cell migration (wound healing assay) as well as apoptotic (AO/EtBr) activity. These results suggest that the venom might contain bioactive molecule with a potential to develop new anticancer drug for effective management of cancer.

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P-4

Small molecule mediated regulation of genes of the incretin signaling pathway: An epigenetic paradigm to ameliorate type 2 Diabetes and Obesity.

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Abstract:

Glucagon-Like Peptide 1 Receptor (GLP-1R) after activation associate with heterotrimeric G proteins at the plasma membrane to initiate second messenger signaling following which the receptor-ligand complex undergoes desensitization, internalization and is either recycled back to the plasma membrane or degraded in lysosomes. Contrary to this canonical pathway, our laboratory has discovered a novel molecular mechanism in which a Class B GPCR, GLP-1R, supports sustained cyclic AMP generation following activation and internalization at endosomes. GLP-1R agonism is known to provide glycemic benefits as well as lowers body weight gain. Our studies show that MS-275, a small molecule inhibitor of Class 1 Histone Deacetylase, enhances signaling response of GLP-1R to achieve better metabolic regulation. In pancreatic beta cells, MS-275 enhances GLP-1R-mediated sustained cyclic AMP generation resulting in increased Glucose stimulated insulin secretion and improved glucose tolerance in diet induced obese mouse model. MS-275 treatment enhances energy dissipation through enhanced β-oxidation; chronic administration of MS-275 and Liraglutide increases energy expenditure of white adipose tissue causing depot specific reduction of adiposity associated with decrease in body weight gain in diet induced obese mice. The data taken together highlight the therapeutic ability of Class 1 Histone Deacetylase Inhibitor MS-275 in enhancing GLP-1R response to regulate type 2 diabetes and obesity.

P-5

RyjB is an acid stress inducible small RNA regulated by PhoP in *Escherichia coli*.

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Small RNAs (sRNAs) in bacteria are primarily induced in response to changing environmental cues and modulate their target gene expression at the post-transcriptional level (1). Many sRNA-mediated regulations have been reported to achieve through the base pairing to their target RNAs. These sRNAs participate in the regulatory mechanisms of virtually all physiological circuits in bacteria. These regulatory sRNAs are encoded in cis and trans relative to their mRNA targets (2-4). One such small RNA found in Escherichia coli is RyjB, an 80 nucleotide long small RNA, the function of which is yet to be understood. In the current study, we have systematically investigated the regulation of RyjB expression in a growth phase-dependent manner and identified that RyjB expression is regulated neither by stationary phase-specific σ-factor nor by RNA chaperon Hfq and thus, its stability at the post-transcriptional level does not require the assistance of Hfq. Interestingly, RyjB was detected as a novel acid stress-induced sRNA. A DNA binding protein PhoP, a component of PhoP/Q regulon, was found to regulate ryjB expression, as the elimination of phoP allele in the chromosome exhibited no induction of RyjB expression under acid stress (5). RyjB has potentially been shown to act as a regulator of the expression of the sgcA gene, with which RyjB shares a 4-nt overlap. The current study increases our knowledge substantially regarding the regulation of ryjB expression in E. coli cells.

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P-6

I-M-150847, A NOVEL GLP-1R GIPR DUAL AGONIST AMELIORATES TYPE-2 DIABETES & OBESITY

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ABSTRACT

Multi-agonism of incretin receptors showed potential impact on glycemic regulation in pre-clinical as well as in clinical studies [1]. The non-canonical activation of receptors by different agonists leads to the differential second messenger generation, impacts the downstream outcome [2]. Our lab has shown the activation of different spatiotemporal cAMP pool upon receptor activation by different ligands and investigated to dissect the functional aspect of different cAMP pool in T2DM regulation [3, 4]. Our study reports a stepwise discovery of a novel GLP-1R/GIP-R dual agonist by replacing the tryptophan cage of exendin-4 with the C-terminal sequence of Oxyntomodulin with non-canonical activation of cAMP generation with great potential in pathological character regulation. I-M-150847 activates both GLP-1R and GIP-R in a balanced manner which leads to plasma membrane exclusive cAMP generation with I-M-150847 unlike other GLP-1R agonist Liraglutide. In-vitro administration shows increased glucose stimulated insulin secretion in a dose dependent manner and glucose vesicle exocytosis on the plasma membrane vicinity in cultured pancreatic β cells. The in-vitro ability is translated in hyperglycemia regulation in HFD fed diabetic obese mice. The subcutaneous treatment of I-M-150847 shows decrease in the fasting blood glucose to baseline. The IPGTT also reveals the improvement in glucose excursion upon chronic administration. I-M-150847 administration also shows significant decrease in body weight gain through regulating the acute and chronic food intake with decreased adiposity. The findings together highlight the novel designing approach of a dual agonist with potential ability to regulate hyperglycemia, obesity and food intake.

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P-7

Formulation of Anti-tuberculosis Drug Loaded StarchPropionate Microparticles for Controllable Drug Delivery

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ABSTRACT

The goal of this study was to use an emulsification solvent evaporation approach to formulate anti-tuberculosis drug (isoniazid, rifampicin, and pyrazinamide) loaded starch propionate microparticles (ATD-SPMPs). Fourier transform infrared spectrometry revealed that starch propionate (SP) exhibited new bands at 1749cm^{-1} and 1236cm^{-1}, whereas SPMPs had identical peaks. The A-type pattern of native starch was entirely changed into the V-type pattern of SP by X-ray diffraction, while SPMPs showed a similar type pattern with SP having reduced crystallinity. Propionylation improved the thermal stability of native starch by reducing the number of hydroxyl groups in the modified starch molecule. SPMPs have superior thermal stability than SPMPs due to their semi-crystalline structure. In the optimized formulation, the highest percentage encapsulation efficiency of isoniazid, rifampicin, and pyrazinamide was determined to be 37.6%, 45.2%, and 43.1%, respectively. Scanning electron microscopy revealed that propionylation partially disturbed the granule morphology of native starches, and the imperfections and porosity structures of SP granules were completely changed into the uniform-sized spherical shape of SPMPs. The geometric particle sizes of the blank SPMPs, isoniazid, rifampicin, and pyrazinamide loaded SPMPs were 1.243

± 0.3 µm, 1.65 ± 0.2 µm, 2.73 ± 0.7 µm, and 2.69 ± 0.5 µm, respectively. The dialysis bag method was used to study drug release from ATD-SPMPs and in-vitro drug release data was also analyzed using several kinetic models. The in-vitro drug release investigation revealed that drug release from SPMPs was controlled in comparison to pure ATD using the Korsmeyer-Peppas model, indicating drug release by anomalous diffusion, i.e., non-Fickian diffusion. Overall, the formulated ATD-SPMPs may be regarded as a potential anti-tuberculosis micro-drug, offers a path forward for tuberculosis clinics.

P-8

Asymmetric synthesis of propargylamine by using chiral glycoconjugate copper (II) complex

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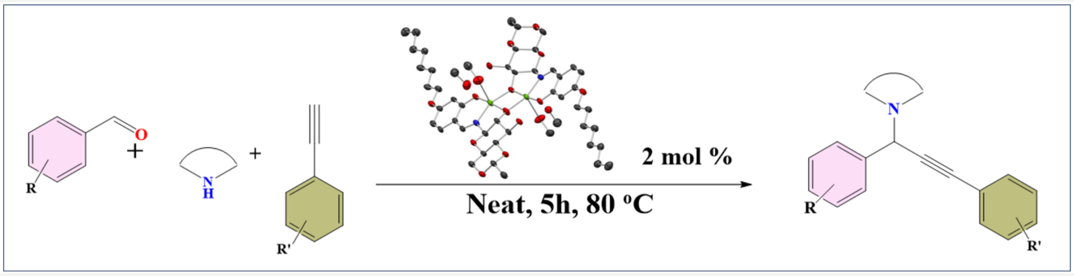
Abstract: The coexistence of carbohydrate and metal ions in living organisms have already been established, which facilitates several biological processes such as cell-cell recognition, bio-catalysis, etc. Inspired by these facts, we are exploring the catalytic activities of glycoconjugate transition metal complexes, which might enable asymmetric synthesis due to the chiral nature of the complex. Among various metal complexes, currently, we are investigating the catalytic applications of Cu(II) and Mo(VI) complexes in oxidation as well as coupling reactions. Along this line, currently we are working on Cu(II) complex catalyzed chiral synthesis of propargylamines. This class of compounds has wide applications, from synthetic precursors to pharmacological and pharmaceutical uses in the form of natural products and organic substrate for the treatment of neurodegenerative diseases, etc.[1]. Several reports are available on the copper-catalyzed synthesis of propargylamines, including few asymmetric ones, however, they require hazardous solvents, longer reaction time and high catalyst loading[1, 2]. We have developed a one-pot catalytic synthetic protocol for the chiral propargylamines under solvent-free conditions using aromatic aldehydes, phenylacetylenes, and secondary amines. Various propargylamine derivatives have been synthesized including new ones in good to excellent yield (75-95 %) and up to 99.9% enantiomeric excess. The molecular structure of the catalyst, and two of the synthesized new derivatives have been established by single-crystal X-ray diffraction studies. The thermal stability of ligand and metal complex has been explored by thermogravimetric analysis (TGA) and the catalyst has been recycled five times without any appreciable loss in the catalytic activity.



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P-9

Application of Ring-Rearrangement Metathesis in Organic Synthesis

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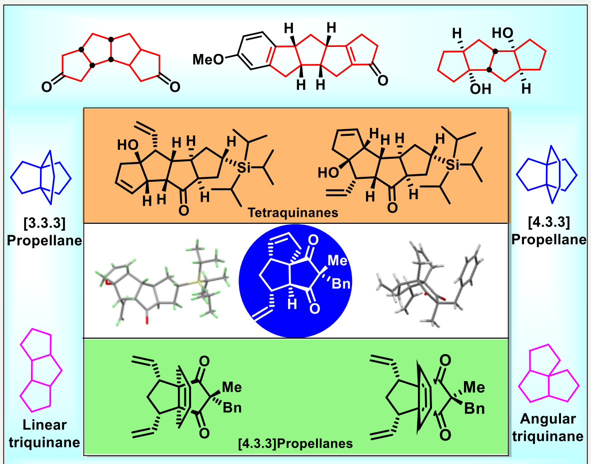

 # Complex polyquinanes are synthesized using RRM as key step
 # 5-8 contiguous chiral centres are present
 # Stereochemistry is well defined using single crystal X-ray data.

Abstract: Triquinanes, tetraquinanes and propellanes belongs broadly to polyquinanes which consists of cyclopentane fused rings. Polyquinanes have several applications in medicinal chemistry and natural product synthesis and their importance is increasing with time. Creation of such complex systems having contiguous stereocenters and dense functionality in economical way is always a challenging task for chemists. Usually the synthesis of such molecules involves a large number of steps which is not only associated with high cost but also results in low yields. In this context, we have developed new strategy to make angularly and linearly fused polyquinanes which are present as core units in certain natural products such as silphinene, (+)-3-oxosilphinene, hirsutane, capnellane, modhephene, bukittinggine etc. Our strategy involves the combination of operationally simple reactions like Diels–Alder reaction (DA), alkylation, Grignard addition and ring-rearrangement metathesis (RRM). Utilization of such reactions leads to reduction of the total number of steps and hence good yields. The structures and relative stereochemistry of targeted molecules are well defined by various characterization techniques and further supported by single crystal X-ray diffraction studies. The present strategy is useful to design various "drug-like molecules" and expand the chemical space of cyclopentanoids that are useful in medicinal chemistry.

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P-10

NCSe Palladium Pincer Complexes for Sterically Favoured Regioselective C-H Activation Reaction

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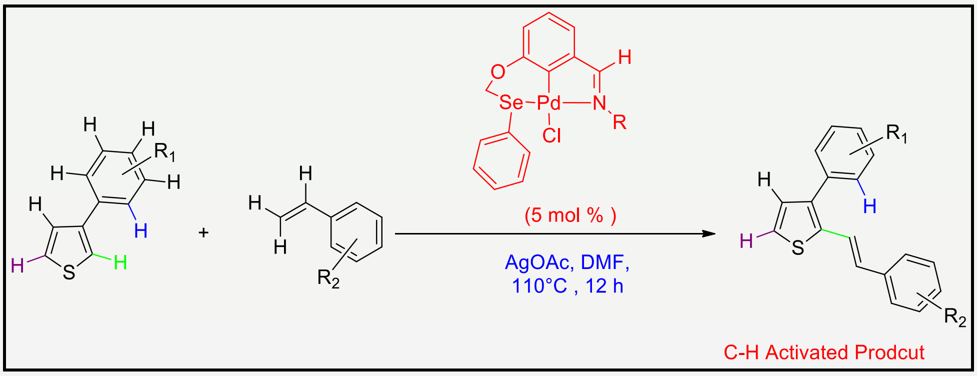
Organochalcogens-based Pd pincer complexes are efficiently employed for various organic transformations including C-H activation, C-X (X= C, O, N, S, Se) bond formation reactions, dehydrogenative coupling reaction, CO_2 conversion, *O*-arylation of phenol, transfer hydrogenation of aldehydes and ketones, aldehyde–alkyne– amine, coupling, hydration of nitriles, conversion of aldehydes to amides, cross-dehydrogenative coupling (CDC), photodegradation of substrates (formic acid, methylene blue), reduction of nitrophenols, electrolysis (hydrogen evolution reaction and oxygen reduction reactions) due to their thermal stability, air insensitivity and high reactivity.[1] Here we have designed NCSe pincer type ligands by the reaction of 3-((phenylselanyl)methoxy)benzaldehyde with t-butylamine and 1-admentylamine respectively. The palladium pincer complexes were synthesized by the reaction of ligands with $PdCl_2(ACN)_2$. The catalytic efficiency of the catalyst was tested for C-H activation from 3-phenylthiophne with styrene derivatives in the presence of suitable oxidants and solvents. Previous reports depicted that either the C5 position of thiophene moiety (less sterically favoured) or the *ortho* position of the phenyl ring of 3-phenyl thiophene was activated through transition metal catalysts. Here we have activated the highly sterically hindered C2 position of thiophene ring. The C-H activated products can be isolated in >70% yield with 5 mol% catalyst loading *via* cross dehydrogenative coupling reaction.[2] The catalyst showed very high tolerance for different functional groups.



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P-11

Synthesis of α-Amino α-Aryl Esters by Electrochemical Oxidative CouplingBetween Benzylic C(sp^3)-H and N-H of Secondary Amines.

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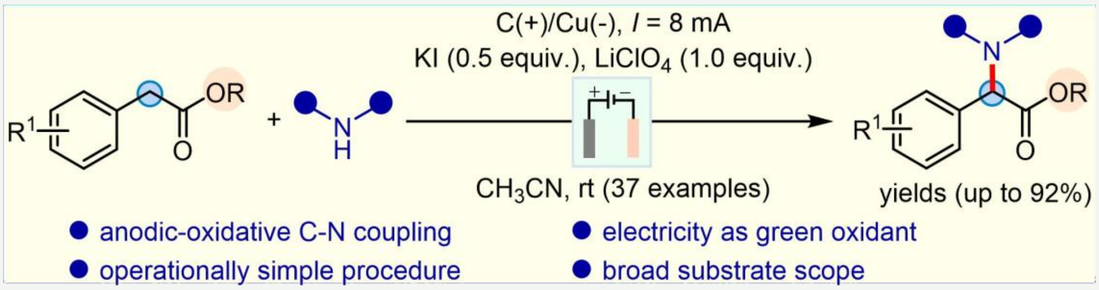
ABSTRACT: The α-amination of carbonyl compounds remains a central attraction in synthetic and medicinal chemistry as a straightforward route to versatile building units widely present in natural products and pharmaceuticals [1].On the other hand, electrochemical organic transformations have recently gained much attention as sustainable protocols under mild conditions [2].The electrochemical oxidative C-H functionalization for C-C, C-O, and C-N bond formation has been achieved using metal-catalysis or metal-free conditions. Despite these efforts, the direct electrochemical amination of the C(sp^3)-H bond remains elusive [3].Recently, we reported an intermolecular electrochemical coupling between the benzylic C(sp^3)-H bond with various secondary amines [4].A series of acyclic/cyclic secondary amines and α-aryl acetates were tested to furnish the corresponding α-amino-esters with high yields (up to 92%) under mild conditions (Scheme 1). Details of the work will be presented in the poster.



Scheme 1. Electrochemical amination of the α-aryl acetates

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P-12

Metal-Free, Site-Selective Oxidative C3-Alkenylation of Indoles and Imidazo[1,2-*a*]pyridines

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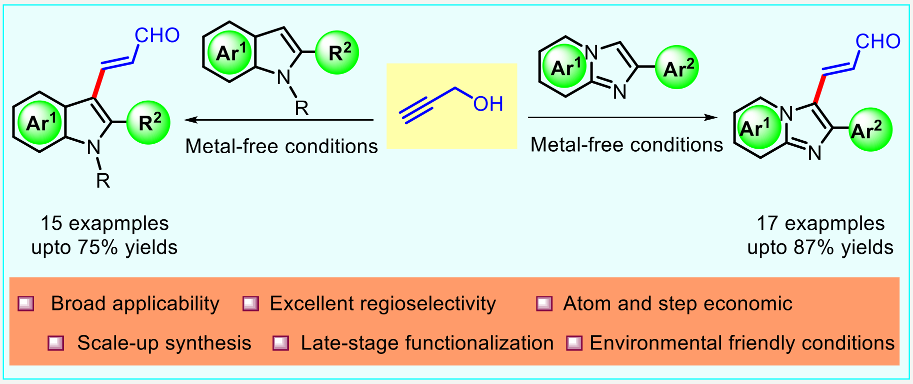
Fused heterocyclic compounds are of immense importance due to their eminence importance in pharmaceuticals, material chemistry, and organometallics.[1] They are found to be prominent building blocks of many natural products and drugs.[2] Among various heterocyclic scaffolds, indole and imidazo[1,2-*a*]pyridine have grabbed special attention of chemists due to their widespread importance as anti-cancer, anti-microbial, anti-fungal, anti-inflammatory and anti-pyretic agents.[3] From the past half century, continued efforts have been made for the simpler and effective synthesis and functionalization of these fused π-extended heterocycles.[4] With our interest in the direct functionalization of such heterocyclic motifs, an effort has been made to develop an efficient method for a sustainable oxidative C3-alkenylation of indoles and imidazo[1,2-*a*]pyridines with propargyl alcohol. Developed protocol features high functional group tolerance resulting in moderate to good yield, broad substrate scope, site- selectivity, and metal-free reaction conditions. The generated method can be further applied for formal synthesis and late-stage modifications of related drug molecules. Details of the reaction conditions, mechanism and substrate scope will be presented.



Scheme 1. Oxidative C3-alkenylation of indoles and imidazo[1,2-*a*]pyridines with propargyl alcohol

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P-13

Preparation of Chalcones by Catalytic Carbonylative Heck Coupling using Heterogeneous Nano-Pd/g-C_3N_4 Composite

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Generally, α,β-unsaturated ketones are called Chalcones which have wide applications in pharmaceutical chemistry [1]. Carbonylative Heck coupling occurs via catalytic insertion of olefins into acyl palladium complexes and the acyl palladium complexes in turn can be prepared either by CO insertion in Pd-Aryl species or by the oxidative addition of benzoyl precursors [2]. Recently palladium catalysed Carbonylative Heck coupling was done by using $[(Cinnamyl)PdCl]_2$/dppp [3]. The main problem with these is, they are homogeneous in nature. So, separation of catalyst from reaction is difficult, low yields and low selectivity towards Carbonylative products. Hence, to overcome these problems we have prepared a novel nano-catalyst. Pd-nanoparticles can be used as heterogeneous catalyst due to the availability of active surface area, high surface to volume ratio, unique position in 5th period and 10th group in periodic table, etc.

Here we have prepared chalcones by carrying out Carbonylative Heck reaction of aryl halide and aryl alkenes in presence of heterogeneous nano-Pd catalyst which implements the concepts of the green chemistry approach. Here we have used highly active, air- and moisture-stable Pd-nanoparticles supported on g-C_3N_4 matrix to obtain a composite, as a reusable catalyst for Carbonylative Heck reaction under conventional thermal heating. The optimized catalytic reaction was studied in details followed by study of recyclability and stability of the catalyst proved that this method is an economic and eco-friendly process. The major highlights of this approach are high product yields (90-95%), short reaction time, wide substrate scope and easy catalyst-product separation and high catalyst stability.

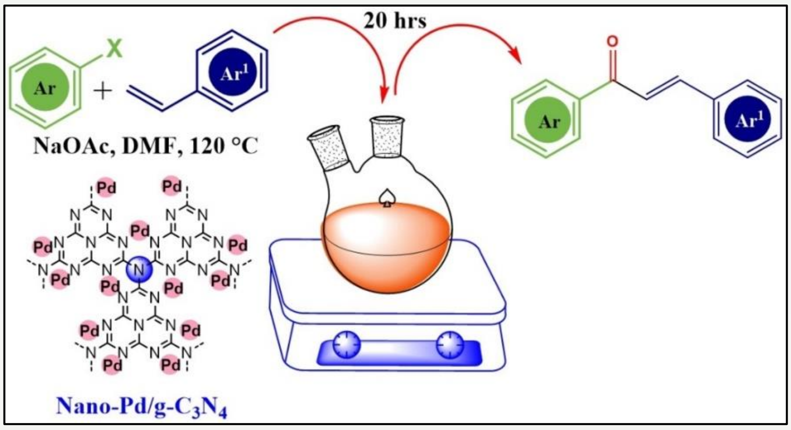

Fig: Carbonylative Heck Coupling reaction using Heterogeneous Nano-Pd/g-C_3N_4 Composite

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P-14

Pyridinium-based Fluorescent Chemosensor for Detection of TNP and Cr(VI)

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Owing to the escalating threat of criminal activities and pollution aroused by 2,4,6-trinitrophenol (TNP), the development of a proficient sensor for the detection of explosives is highly demanded [1]. TNP is a potent nitro explosive that is even more powerful than TNT [2]. The expanding use in numerous industries, including steel production, paint manufacturing, and leather tanning, $CrO_4^{2}/Cr_2O_7^{2}$ has emerged as environmental non-biodegradable contaminants [3]. Hexavalent chromium is a human carcinogen, therefore its detection and removal in wastewater discharge and drinking water distribution are essential. Excess intake of these anions leads to DNA damage and disruption of the protein and enzyme system of the human body [4]. Therefore, the effective monitoring and detection of trace amounts of TNP and chromate anions are very crucial for public safety, homeland security, and preventing damage to life [5]. Pyridinium-based moieties have gained attention due to their hydrophilic nature and photostability [6]. Herein, a water-soluble pyridinium-tagged fluorescent probe has been designed and synthesized for the dual detection of hexavalent chromate anions ($CrO_4^{2-}/Cr_2O_7^{2-}$) and 2,4,6-trinitrophenol (TNP). The probe displayed strong neon yellow fluorescence that is quenched on the addition of TNP and chromate anion. This probe can be a promising candidate applicable in environment protection, water treatment, and safety inspection.

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P-15

Pyrazinium-based Fluorescent Chemosensor for Selective Detection of TNP

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There has been a significant increase in research on the detection of nitro explosives concerning national security and environmental protection [1]. 2,4,6-trinitrophenol also known as Picric acid (PA), has been classified as a potent nitro explosive substance [2]. Although RDX and 2,4,6-trinitrotoluene (TNT) are the most often used explosives, owing to their poor safety coefficient and rapid detonation velocity, TNP is more potent than TNT [3]. The excellent water solubility of PA and its widespread use in the manufacture of rocket fuel as well as in the pharmaceutical, dye, and fireworks industries and forensic investigations [4], it can easily contaminate water and soil, leading to health hazards viz., sycosis, cancer, anaemia, severe eye, and skin irritation, and potential destruction of the liver, kidney, and respiratory organs [5]. Ion-tagged compounds are a fascinating class of organic materials because they have unique, tuneable features that come from a balanced ratio of cations and anions [6]. Because of their photostable properties, pyrazines are widely used in sensors, semiconductors, and luminous materials. Additionally, the pyrazine nucleus provides room for one of the N atoms to be quaternized, increasing its hydrophilicity and providing the ability to sense in aqueous media [7]. Herein, we report the highly selective detection of PA at nanomolar levels using pyrazinium-based chemosensor. Detection of PA is also demonstrated in simulated water and soil samples assessing the its sensing efficacy.

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P-16

Novel Spiro/non-Spiro Pyranopyrazoles: Eco-Friendly Synthesis, In vitro Anticancer Activity, DNA Binding, and In silico Docking Studies

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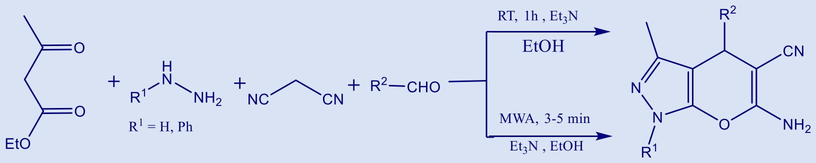
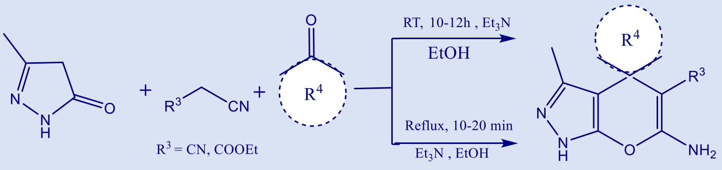
Abstract: Pyrazole derivatives have much importance in synthetic organic chemistry and pharmaceutical science. Moreover, the utilization of the 4H-pyran ring was found useful in medicinal and synthetic chemistry. Thus, Pyranopyrazole, nitrogen and oxygen ring fused heterocycles play a vital role in a biologically active compound and show antibacterial, anticancer, and anti-inflammatory properties. Pyranopyrazole derivatives were firstly synthesized by H. Otto in 1974 by reacting malononitrile with 4-arylidene-3-methyl-2-pyrazoline-5-one (*Otto et al.*[1]). In 2010, *Hamad et al.* [2] synthesized pyranopyrazole which exists in 2H-form as confirmed by the NOE experiment. Herein, using a multicomponent reaction strategy, our group synthesized two series of pyranopyrazole (spiro and non-spiro) by mixing ethyl acetoacetate, hydrazine hydrate or phenylhydrazine, aldehydes or ketone, and malononitrile or ethylcyanoacetate in presence of triethylamine (*P.shukla et al.*[3]) Our group synthesized this substituted pyranopyrazole via the conventional method and also microwave-assisted method. Building up on our work, we propose to synthesize the pyridine/pyrimidine fused pyrazoles. The synthesized series of spiro and non-spiro pyranopyrazoles were found to possess anticancer activity as evinced by the studies on Hep-3b cells and mainly the non-spiro derivatives inhibited the growth of cancer cells in a dosage-dependent manner. DNA binding interaction of these molecules was observed especially non-spiro ones using UV-visible absorbance spectroscopic study and the docking studies corroborated well with the experiment results. The scheme of the reaction is given below:



Scheme 1 : Synthesis of Non-spiro Pyranopyrazole via Conventional method and Microwave assisted method



Scheme 2 : Synthesis of Spiro Pyranopyrazole via Conventional method (i)RT (ii)Reflux

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P-17

Design, Synthesis and Catalytic Activity of *N*-Heterocyclic Carbene-Based Unsymmetrical Palladium(II) CNN Pincer Complex

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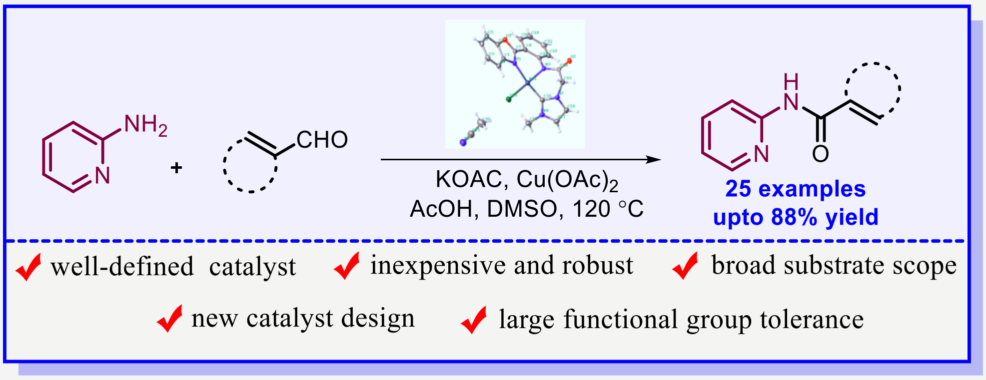
The transition metal-catalyzed C–H bond functionalization strategy represents a paradigm shift for the construction of C–C and C–heteroatom bond in organic synthesis.[1, 2] Direct functionalization of C–H bond provides an atom- or step-economical, cost-effective, and environmentally friendly synthesis of important building blocks, natural products and medicinally relevant molecules.[3, 4] However, the typical catalysts employed in these transformations suffer with thermal stability and selectivity issues. Pincer ligands show tight coordination ability with metal because of tridentate coordination, resulting in their high thermal stability, which has led to widespread exploration of pincer complexes in several cross-coupling reactions.[5-8] Keeping this in mind, we have developed a new *N*-heterocyclic carbene-based CNN pincer complex of palladium. A C_{NHC}NN-Pd(II) based pincer complex was synthesized and characterized using NMR (^{1}H and ^{13}C) spectra and single crystal X-ray crystallography as well as oxidation state and chemical composition by XPS. Further, the catalytic efficiency of C_{NHC}NN-Pd(II) pincer complex was investigated for carbonylation of 2-aminopyridine with aldehydes. Various functional groups both on the 2-aminopyridine ring as well as on aldehydes were tolerated and a wide range of amidation products were obtained in moderate to good (37-88%) yields (Scheme 1). Details of the developed protocol will be presented in the poster.



Scheme 1: Pd(II)-catalyzed cross-dehydrogenative coupling of 2-aminopyridine and aldehydes

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P-18

1-D Zn(II) Coordination polymer with positional effect of pyridyl groups for the selective degradationof anionic dyes.

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Abstract: Zn(II) based three coordination polymers were synthesized using **L1** = 1,2-bis(pyridin-3-ylmethylene)hydrazine, **L2** = 1,2-bis(1-(pyridin-3-yl)ethylidene)hydrazine and **L3** = 1,2-bis(1-(pyridin-4-yl)ethylidene)hydrazine ligands. Ligands **L1, L2** differ from **L3** in terms of position of nitrogen on pyridyl group, while **L1** and **L2** differs in the context of hydrogen or methyl group on imine carbon. Due to these minor structural variations in the ligands have affected on Zn(II) coordination polymers $\{[Zn(\mathbf{L1})](I)2\}n$ (**CP1**), $\{[Zn(\mathbf{L2})](I)2\}n$ (**CP2**) and $\{[Zn(\mathbf{L3})](I)2\}n$ (**CP3**). Single crystal XRD was used for the determination of the molecular strucutre of these three coordination polymers. Using Hirshfield analysis on **CP1**, **CP2** and **CP3** intermolecular interactions were determined in the crystal lattice that were in agreement with the hydrogen bonding present in the single crystal XRD analysis. All the coordination polymers were used for the selective dye adsorption study. Out three coordination polymers only **CP3** was selective towards dyes, Methyl orange(MO) and sodium salt of Methyl Red(MR). CP3 didn't show any adsorption for the cationic dyes such as Methylene ble(MB), Malachite green(MG), Rhodamine-B. These studies showed the importance of chemical nature of different ligands in the coordination polymer on the adsorption properties. These 1D chain coordination polymers in the absence of pores were able to adsorb the dye due to the presence of electronic effects relsulted from **L3** with the coordination centre**Zn(II).**

P-19

Rhodium-Catalyzed Annulation of Vinylated Tyrosines with Internal Alkynes to Access Oxepine-Mounted Unnatural Tyrosines and its Peptide Late Stage Functionalization

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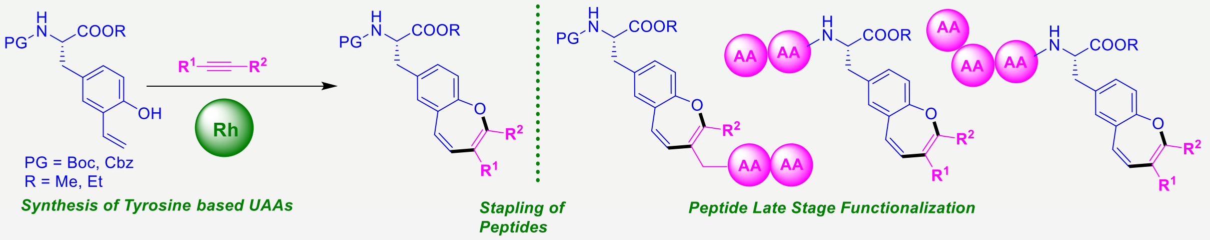
Abstract: Proteins perform differentiated functions such as metabolic reactions catalysis, DNA replication, stimuli response and transportation of molecules in living organisms.[1] Though, genetic code expansion of natural amino acids results in the synthesis of most proteins, yet, co-translationally amalgamation of a few unnatural amino acids (UAAs) into proteins offers unprecedented capability for site-specific protein manipulation in living systems.[2]

The application of the described Rh-catalyzed strategy towards late stage functionalization on tyrosine-containing dipeptides and tripeptide with internal alkynes with the aid of a benzo[*b*]oxepine framework offers an excellent addition to the toolbox of methods known for designing complex UAAs. Rh(III)-catalyzed [5+2] annulation of *N*-protected vinyl tyrosines with symmetrical and unsymmetrical internal alkynes which furnish a series of oxepine-mounted tyrosine based unnatural amino acids.

In sharp contrast, benzo[*b*]oxepine is a privileged heterocyclic scaffold that constitute an integral part of several natural products (*e.g.* Heliannuol C , Pterulone), [3] and found immense application in the discovery of bioactive drug candidates.[4] We envisioned that merging structural diversities of tyrosine with oxepine in a tailored manner would foster interesting modified tyrosine-based biomolecules with potential applications in drug delivery and protein engineering studies. Anticipating the applications of designer tyrosine-based UAAs, and embracing the rich possibility of amalgamation between vinyl tyrosines and internal alkynes, Further, late stage functionalization of the developed strategy was also achieved on tyrosine containing dipeptide and tripeptide.



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P-20

Synthesis of Quinoxalinetacrines Analogues as Cholinesterase Inhibitors for Potential use Against Alzheimer's Disease

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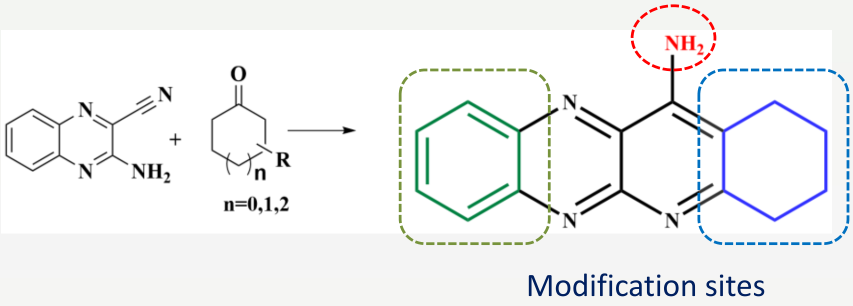
Abstract: Alzheimer's Disease (AD) is a progressive multifarious neurodegenerative disorder and the most common cause of dementia in late adult life. Etiology of AD is very complex and exact cause is not known yet. A key strategy for the development of novel anti-Alzheimer's disease (AD) is to develop multi-target inhibition drugs. One major strategy for the development of new therapeutics relates to the enhancement of cholinergic systems through anticholinesterase inhibitors such as inhibition of acetylcholinesterase (AChE) and butyryl cholinesterase (BuChE) activities. Tacrine (1,2,3,4-tetrahydro-9- aminoacridine; THA) was found to be a potent inhibitor for AChE and BChE in 1953, and administered to thousands of patients for the treatment of Alzheimer's disease (AD). The clinical use of tacrine, as a reversible AChEI and Butyrylcholinesterase (BuChE) inhibitor, was discontinued due to the short half-life, adverse side effects at high dosage and high hepatotoxicity. However, tacrine has been selected as the ideal active fragment because of its simple structure, low molecular weight, clear activity, ability to cross BBB easily and its superiority in structural modifications.In current search for non-hepatotoxic tacrines for AD therapy, quinoxalinetacrine (1,2,3,4-tetrahydroquinolino[2,3-b]quinoxalin-12-amine) is less toxic than tacrine at high concentration and less potent as acetylcholinesterase (AChE) inhibitor, but shows highly selective butyrylcholinesterase (BuChE) inhibition. Various studies have suggested that BuChE inhibition is a potential strategy for the treatment of advanced AD.[1] Based on reported IC_{50} value of Quinoxalinetacrines and selectivity towards BuChE[2], we plan Quinoxalinetacrines array of qunoxaline tacrine analogs with change in ketone and linker on amino leading to high selective and potent for BuChI.The scheme for the synthesis of desired compounds is as given below:-



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P-21

Two-pot synthesis of 1,6-disubstituted 5-aza-indoles from succinaldehydeand *N*-aryl propargylic-imines

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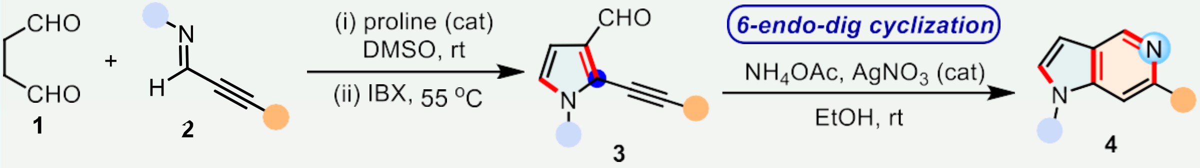
Abstract: 5-aza-indoles have been synthesized from aqueous succinaldehyde and *N*-aryl propargylic-imines in a two-pot protocol. This two-step synthesis initially involves the metal-free [3+2] annulation of aqueous succinaldehyde and *N*-aryl propargylic-imines to access 2-alkynyl-pyrrole-3-aldehydes followed by silver- catalyzed 6-endo-*dig*-cyclization to obtain substituted 5-aza-indoles in the second pot. We have synthesized 20 examples of 2-alkynyl-pyrrole-3-aldehydes (**3**) with good yields and finally 10 examples of substituted 5-aza- indoles (**4**) and along with the gram-scale access of synthesis 5-aza-indole.



Scheme 1. Synthesis of 1,6-disubstituted 5-aza-indoles

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P-22

Synthesis, structural elucidation, chelation competency, DFT and molecular docking of indole based thiosemicarbazone ligand with Co(II), Ni(II), Cu(II) and Fe(III) metal ions

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Indole moiety is known for many biological and catalytic active compounds in the area heterocyclic chemistry [1,2]. Therefore, the Schiff bases obtained by the condensation of 1H-indole-3-carboxaldehyde with amines and their metal complexes have received considerable attention in medicinal chemistry [3-5]. Hence, novel indole based ligand (*E*)-2-((1-benzyl-1*H*-indol-3-yl)methylene)hydrazine-1-carbothioamide (BIMHC) have been designed and synthesized by following the condensation reaction at optimum conditions. A series of 3d metal complexes *i.e.* Ni(II) (C1), Cu(II) (C2), Co(II) (C3) and Fe(III) (C4) have been prepared by the reaction of BIHMC ligand with suitable metal precursors in 1:2 metal- ligand ratio. Chemical structure of ligand and its all complexes has been elucidated by using various analytical and spectroscopic techniques. The solid state structure of BIMHC has been determined by using single crystal X-ray diffraction data. The spectroscopic study suggested the chelation of ligand as tridentate for C1, C2, C3 and bidentate for C4. The molar conductance values for complexes (C1), (C2), (C3) have been found in the range of 2.79-4.38 and for (C4) 62.5 Sm^2mol^{-1} and these values suggested non ionic and ionic behavior of complexes, respectively. Magnetic moment, IR, UV-visible and EPR studies results indicate that all complexes have six coordinated octahedral geometry. Further molecular docking study of BIMHC and complexes has been also performed against the 2DN1 (crystal structure of human hemoglobin in the oxyform) for evaluating the binding energies of protein-compounds (synthesized) interaction.

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P-23

PHENOL NITRATION AND CHLORINATION AT A TRIPODAL COPPER(II) SITE VIA PROTON-COUPLED-ELECTRON-TRANSFER (PCET)

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Oxidatively modified tyrosine (Tyr) such as nitro-tyrosine (Tyr-NO_2) and chloro-tyrosine (Tyr-Cl) serve as biomarkers for various age-related cardiovascular, neurodegenerative and inflammatory diseases.[1,2] In this perspective, oxygenase-type modifications of such phenolic substrates by different reactive copper-oxygen intermediates such as dicopper(II)-peroxo and dicopper(III)-(bis-μ-oxo) have gained enormous interest over several decades.[3] However, examples of phenol oxidation under anaerobic and ambient conditions remain underexplored in comparison. Notably, utilizing a nitrito-copper(II) cryptate, our previous study outlines phenol oxidation coupled to the reduction of NO_2^- to NO through proton-coupled-electron-transfer (PCET).[4] Intriguingly, phenol reactivity of the nitrito-copper(II) cryptate with a protonated outer-coordination-sphere has been illustrated to provide an unusual anaerobic route for phenol nitration.[4,5] Aiming to disclose the underlying mechanism towards anaerobic oxidation of phenol, the present work illustrates the synthesis and spectroscopic characterization of copper(II)-chloride and copper(II)-nitrite complexes supported by a newly designed *N*-nitrosated ligand ($\mathbf{L^{3NO}}$).[6] Unlike the copper(II) complexes of parent tripodal amine ligand ($\mathbf{L^{3H}}$), the copper(II) complexes of $\mathbf{L^{3NO}}$ facilitate the anaerobic oxidations of various phenolic substrates resulting in nitrophenol and chlorophenol derivatives. Detailed kinetic investigations including kinetic isotope effect (KIE) and Eyring analyses reveal a proton-coupled-electron-transfer (PCET) as the rate determining step for phenol chlorination mediated by copper(II)-Cl complex of $\mathbf{L^{3NO}}$. Finally, reactions of isolated 2,4,6-tri-*tert*-butylphenoxyl radical with copper(II)-X (X = Cl and NO_2) lead to chlorophenol and nitrophenol, respectively, thereby suggesting a radical-recombination step succeeding the initial rate-limiting PCET step. Thus, this work outlines the mechanism of phenol nitration and chlorination mediated at copper(II) sites under anaerobic conditions.

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P-24

PIFA-Promoted Oxidative Cyclodehydrogenative Strategy to Forge Pyrrolo[1,2-a]quinoxalino-Fused porphyrins with Enhanced Near-Infrared Q-bands

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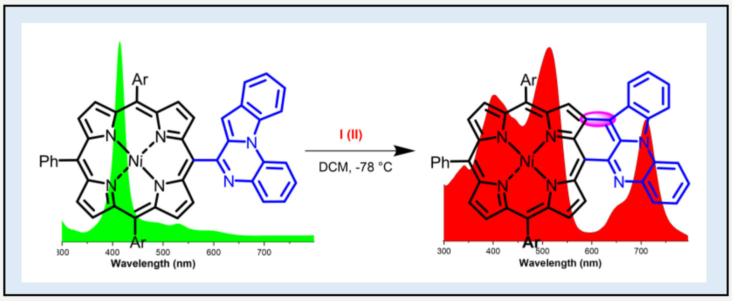
Heteroaromatic π-conjugated metalloporphyrins with unique optical and electronic properties[1] are widely used as photo-chemotherapeutic agents in PDT and photo-electron storage and transfer systems in light harvesting devices.[2] The fusion of an aromatic segment directly to the porphyrin macrocycle is one of the promising methods to expand electronic conjugated systems.[3] Recently, heteroaromatic-fused porphyrins could be more effective[4] with the co-planarization of the lone pair of peripheral heteroatoms[5] with the conjugated porphyrin macrocycle.[6] In continuation of our efforts to identify effective photosensitizers[7] herein, we have developed a facile protocol for the synthesis of *meso-β*-pyrrolo- and indolo[1,2-a]quinoxalino-fused porphyrins by PIFA-promoted intramolecular oxidative cyclization of easily accessible *meso*-pyrrolo- and indolo[1,2-a]quinoxalino-appended porphyrins. The *meso*-pyrrolo- and indolo[1,2-a]quinoxalino-appended porphyrins were prepared from *meso*-formyl porphyrins. The absorption spectra of *meso-β*-pyrrolo- and indolo[1,2-a]quinoxalino-fused porphyrins displayed bathochromic shifted (100-150 nm) broadened Soret and Q bands in addition to intense bands in emission spectra near IR region as well shows reduced energy band gap. Synthesis, characterization and photophysical studies of pyrrolo and indolo[1,2-a]quinoxalino-appended/fused porphyrins will be discussed in the conference presentation.



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P-25

Bioactive compound of cinnamon alleviates chemotherapy-induced cachexia

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Abstract

Chemotherapeutic agent, a staple approach, which besides imparting anti-cancer efficacy also contributes to a wide range of complications including cachexia (loss in muscle mass and strength) due to alteration in protein metabolism and myogenesis (process of muscle formation).Till date, there is no approved therapy/drug/treatment available against cancer cachexia. In the present study, we explored the anti-cachectic effect of cinnamaldehyde (CNA), a bioactive compound of cinnamon, on cisplatin-induced myotube atrophy and myogenesis in skeletal muscle specific cells i.e. C2C12. Myotubes were treated with cisplatin in the presence or absence of CNA. Data shows that myotube treatment with cisplatin (50 □M) contributes to reduction in the mean myotube diameter and enhances the degradation of muscle specific proteins i.e. creatine kinase while CNA supplementation counteracts cisplatin-induced myotube atrophy and protects the myotube diameter by suppressing the calpain-dependentmuscle proteolytic system. Likewise in myogenesis, CNA (50□M) administration prevents the negative effect of cisplatin (50□M) in myogenesis and helps in the formation of healthy myotubes compared to cislatin-treated cells. Collectively, our preliminary data suggests that CNA may represent a possible potential compound against cisplatin-induced cachexia.

Keywords: Chemotheraputic agent, C2C12 myotubes, atrophy, myogenesis

P-26

Stress mediated C2C12 myotube atrophy: Protective role of CNA analogues

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Abstract

Skeletal muscle loss is a consequence of many pathophysiological and physiological conditions including cancer, COPD, HIV, aging etc and is often associated with increased human morbidity, mortality and poor quality of life. Oxidative stress is one of the key mediators of muscle loss, therefore, supplementation of antioxidant with multi-targeted approach may provide a new therapeutic outlook. The present study reveals the structure activity relationship of synthesized analogues of cinnamaldehyde (CNA) in respect to observed effects and their efficacy as antioxidant agent and protecting agent against H_2O_2-mediated myotubes atrophy in cultured C2C12 cells. Various approaches were used including anti-oxidative & biochemical assay, immunofluorescence, and bright-field microscopy etc in the study. Our data demonstrate that the anti-atrophic effect of CNA analogues in H_2O_2 induced cultured myotubes was different than their *in vitro* anti-oxidative potential. From various analogues, CNA, BzCNA (2-Benzyloxycinnamaldehyde) and MeCNA(2-methoxycinnamaldehyde) showed pronounced protective effect in H_2O_2 induced atrophied myotubes. Overall data depicts the anti-atrophic effect of CNA analogues (BzCNA and MeCNA) on C2C12 myotubes suggesting their therapeutic use in atrophy conditions associated with oxidative-stress.

Keywords: C2C12 cells, myotubes, Cinnamaldehyde analogues, oxidative stress

P-27

S-allyl cysteine ameliorates skeletal muscle loss by preventing alteration in protein metabolism: An *invitro* to *invivo* translation study

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Abstract

Skeletal muscle loss is a common altered protein metabolic phenomenon that occurs under diverse conditions including starvation, aging & chronic diseases (heart failure, diabetes etc), which is characterized by decreased myoproteins and reduced muscle strength. Up to 1/3rd of all cancer patients die from direct consequences of muscle loss (cachexia), not from cancer. Moreover anti-cancer chemotherapy also induces cachexia. Beyond a reduced survival rate, muscle loss is also related to poor functional status and health-related quality of life. Over more than two decades, new insights into the etiology of muscle loss (atrophy) have been established in the literature even than the treatment of atrophy remains an unresolved challenge and no drug is recommended by the FDA (USA) till today. *Invitro*&*Invivo* studies from our lab demonstrate the active potential of SAC, a bioactive compound of garlic (*Allium sativum*), against atrophy. Cell culture data illustrates that SAC supplementation significantly impedes H_2O_2-induced protein loss by suppressing protein-catabolic systems and endogenous level of inflammatory molecules (TWEAK, IL-6). Likewise in denervation-induced skeletal muscle atrophy, SAC pre-administration reduces the negative effects (i.e. decreased cross-sectional area, up-regulation of proteolytic systems, and degradation of total/specific protein) of denervation on muscle mass. Overall findings show that protective effect of SAC against atrophy is well translable from *Invitro* to *Invivo* level.

Keywords: C2C12 myotubes, Mice, Denervation, Muscle loss

P-28

"Design, Synthesis and characterization of furan bearing dihydro-1,3,4-oxadiazole hybrids as potential antimicrobial and antitubercular agents"

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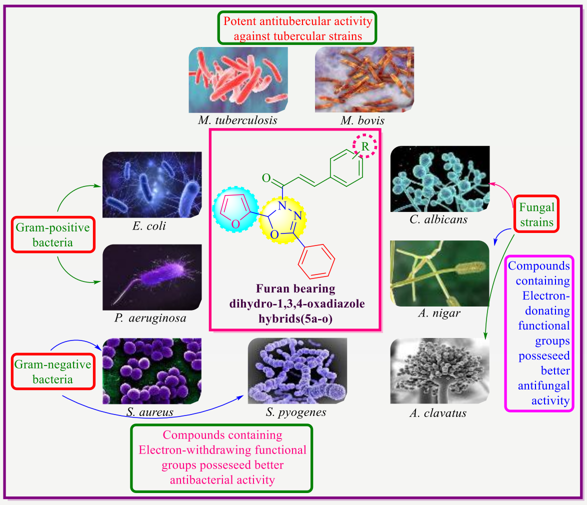
***Choice of mode:** poster*

1,3,4-Oxadiazoles are very good bioisosteres of amides and esters, contributes in enhancing biological profile of hybrid molecules by participating in hydrogen bonding interactions with the biological receptors [1, 2]. In In continuation to this, we have designed and synthesized a novel series of fifteen furan bearing dihydro-1,3,4-oxadiazole hybrids as potential antimicrobial and Antitubercular agents. A unique series of 1-(2-(furan-2-yl)-5-phenyl-1,3,4-oxadiazol-3(2*H*)-yl)-3-phenylprop-2-en-1-ones (**5a-o**) were synthesized utilizing conventional and microwave assisted synthesis. Structures of all the newly synthesized compounds were confirmed using various analytical techniques. These compounds were evaluated for their *in vitro* antimicrobial activity against various bacterial and fungal strains using serial broth dilution method. From the results, compounds with electron withdrawing groups found to possess excellent antibacterial activity while compounds containing electron donating groups found to possess excellent antifungal activity. The synthesized compounds were further screened for antitubercular activity using a Nitrate reductase assay and an XTT Reduction Menadione assay against *Mycobacterium tuberculosis* $H_{37}Ra$ (ATCC 25177) and *M. bovis* BCG (ATCC 35734) strains and rifampicin as positive control. The synthesized compounds were found to possess promising antitubercular efficacy.



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P-29

Charge contribution to SARS-CoV-2 spike protein-ACE2 interaction

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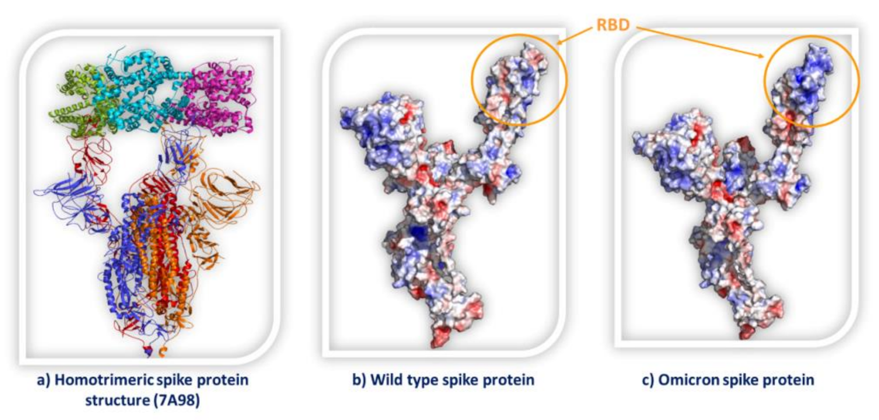
Spike protein is one of the structural proteins of the deadly virus SARS-CoV 2 that has caused the recent worldwide pandemic COVID-19. The spike protein is constantly changing its structural and functional features by mutating important binding residues in the Receptor Binding Domain (RBD) [1][1]. Till now, several variants of this virus are already introduced with varying mutations leading to an increase in infectivity rate, increase in overall charge of spike protein, and binding affinity of the spike protein [2-3]. Here, we have performed a computational study to compare the change in charge, binding affinity, and stability of protein structures of different variants (alpha, beta, gamma, delta, omicron) described as variants of concern by the World Health Organisation (WHO). Electrostatic interactions of naturally evolved mutant residues of the spike protein have increased due to the negatively charged binding surface of the human ACE2 receptor. Most of the mutations in spike protein RBD have increased charge (**Figure 1**) and interactions that may enhance the spike's affinity towards ACE2. The conformational changes due to mutations in each variant might have changed its energy and stability, thus analyzing the energy landscape of each variant will help us understand the energy of contributions of mutated residues in stabilizing spike protein.



a) Homotrimeric spike protein structure (7A98)

b) Wild type spike protein

c) Omicron spike protein

Figure 1: (a) Trimeric structure of spike protein (dark blue, orange, red) bound to ACE2 receptor (green, light blue, pink) is shown using protein data bank ID 7A98[4]. The electrostatic potential surface of **(b)** wild-type spike protein and **(c)** spike protein with omicron mutations, highlighting circled RBD region where blue, red, and white colour indicates positive, negative, and fairly neutral potential.

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P-30

Ni(II) Incorporated Porphyrin-Based Conjugated Porous Polymer Derived from 2,6-Diformyl-4-Methylphenol as a Catalyst for Urea Oxidation Reaction

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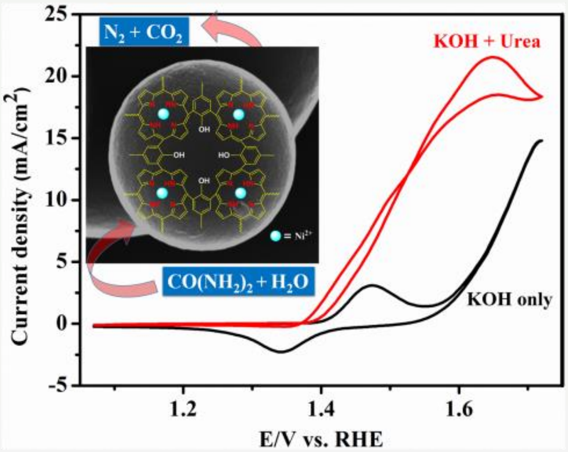
Urea oxidation reaction (UOR) is an excellent alternative to sluggish oxygen evolution reaction (OER) as an anode reaction for hydrogen generation via electrochemical water splitting. [1][2] Here, a porphyrin-based conjugated porous polymer (CPP) has been developed through the polycondensation reaction of 2,6-diformyl-4-methylphenol and pyrrole (DMP-POR).

The nickel(II) complex of this conjugated polymer Ni-DMP-POR shows efficient UOR in an alkaline medium. The as-synthesized materials were characterized by solid-state ^{13}C CP-MAS, thermogravimetric analysis (TGA), Fourier transform infrared (FT-IR) spectroscopy, X-ray photoelectron spectroscopy (XPS), powder X-ray diffraction (PXRD), scanning electron microscopy (SEM) and transmission electron microscopy (TEM). The porous property of the materials was characterized by N_2 adsorption/desorption isotherms at 77 K. Both DMP-POR and Ni-DMP-POR showed excellent thermal stability. The Ni-DMP-POR exhibits very good UOR in 1 M KOH and 0.33 M urea with an overpotential of 200 mV at 10 mA cm^{-2} and Tafel slope of 73 mV dec^{-1}. The catalyst also shows excellent chronoamperometric and chronopotentiometric stability, suggesting its future scope in sustainable hydrogen production from waste water resources.



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P-31

Ruthenium-Catalyzed (Spiro)Annulation of *N*-Aryl-2,3-dihydrophthalazine-1,4-diones with Quinones to Access Pentacyclic Spiro-Indazolones and Fused-Cinnolines

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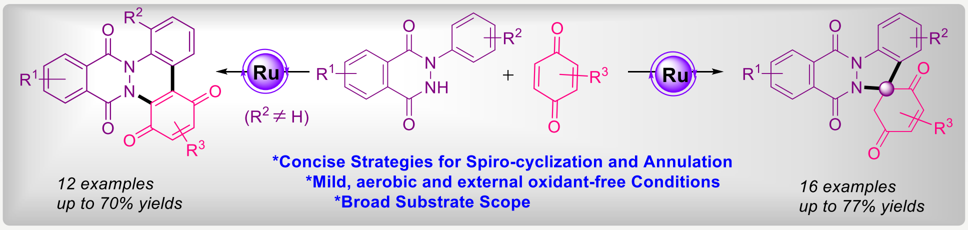
The expedition for the construction of complex heterocyclic architectures has become uncomplicated with the synthetic shortcuts pioneered by chelation-guided directive C-H functionalization under transition-metal catalysis in the last one decade [1]. In this realm, a plethora of strong and weak directing groups (DGs), including *N*-heterocycles (*e.g.* pyridine, pyrimidine, triazole, pyrazole, oxazoline, 8-aminoquinoline, picolinamide) and functionalities (*e.g.* aldehyde, ketone, carboxylic acid, thioether, amide, sulfonamide) have showcased remarkable reactivities with varied coupling partners for the site-selective C(sp^2)-H bond functionalization and/or subsequent oxidative annulations [2]. In recent years, the spotlight on heterocyclic moieties possessing inherent chelation-aided directive capabilities to endow unprecedented molecular frameworks by annulative cyclization remains desirable.

Phthalazine is one such diazaheterocyclic moiety of paramount importance that has displayed interesting pharmacological profile, and its derivatives have exhibited anti-inflammatory, antitumor, antihypertensive, antimicrobial and anticonvulsant activities. Using the above highlighted DG-aided functionalization notion, powerful methods have been developed in recent times for the annulation of *N*-phenyl-2,3-dihydrophthalazine-diones with varied coupling partners, including isocyanates, nitroolefins, propargyl alcohols, alkynes, allenes, sulfoxonium ylides and α-diazo compounds *via* transition-metal catalysis [3].

In striking contrast, 1,4-benzoquinone (BQ) has exemplified selective C1 or C2 synthon reactivity as a coupling partner with a few (hetero)arenes under Rh or Ir catalysis. Determined by our ongoing interest in the transition-metal catalyzed annulations, we herein describe two Ru-catalyzed divergent strategies for (spiro)annulation of differently substituted *N*-aryl-2,3-dihyrophthalazine-diones with benzoquinones to afford spiro{cyclohexane-indazolo[1,2-*b*]phthalazines} and benzo[c]phthalazino[2,3-*a*]cinnolines in high yields [4].



*Concise Strategies for Spiro-cyclization and Annulation
*Mild, aerobic and external oxidant-free Conditions
*Broad Substrate Scope

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P-32

Generation of Dimethyl Sulfoxide Coordinated Thermally Stable Halogen Cation Pools for C- H Halogenation

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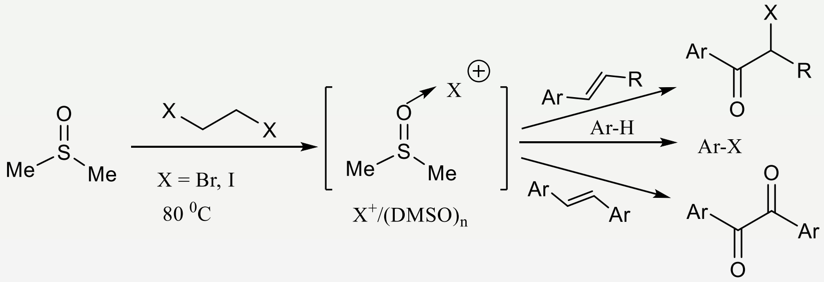
Zoretic et al.[1] reported that the dimethyl sulfoxide, a common aprotic polar solvent, has been regarded as a *magic* solvent in the halogenation process, specifically for the bromination of electron-rich arenes, using HBr. Majetich et al.[2] have proposed that the *in situ* generation of bromodimethylsulfonium bromide from the reaction of DMSO and HBr, which is the effective reagent to enable brominated products. Consequently, Yoshida et al.[3] employed a sophisticated method involving the low temperature anodic oxidation of halide ion (X^+ =Br^+ , I^+) for effective production of halonium ion which could be stabilised by the coordination of DMSO to form a pool of cations (DMSO-X^+) for effective transformation. This method was to generate halogen cation pools from the reaction of 1,2-dihaloethanes (hal= Br, I) and dimethyl sulfoxide (DMSO) for C- H halogenation of arenes and heteroarenes. The initial reaction of DMSO and 1,2- dihaloethane generates the sulfur ylide, which undergoes pyrolytic elimination of ethylene by affording halonium ions. These ions were accumulated and stabilized by DMSO through coordination by forming halogen cation pools for the halogenation reaction. This protocol was selective for electrophilic monohalogenation of arenes at room temperature; however, polyhalogenated products were formed by raising the reaction temperature. Late-stage halogenation of heteroarenes and some commonly marketed drugs signifies the synthetic utility of this protocol in pharmaceutical chemistry. Unlike the classical methods, the in-situ generated electrophilic bromonium ion was further exploited for the direct synthesis of α-diketones from the alkenes under base-free conditions.

Scheme



References:

P-33

Functional assessment of underutilized moth bean protein hydrolysate obtained using static simulation of gastrointestinal digestion

Nancy Goyal, Sachin N. Hajare*, and S. Gautam

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Moth bean (*Vigna aconitifolia*) is a drought tolerant underutilized pulse that was primarily grown as forage in earlier days. Recently, it is gaining importance owing to the presence of various bioactive compounds of pharmacological relevance [1, 2]. However, functional assessment of moth bean proteins after proteolysis is not been reported. The current work was intended to further investigate the functionality of moth bean seed proteins after proteolysis by mimicking gastrointestinal digestion conditions. Functional assessment of this protein hydrolysate was carried out via *in vitro* antioxidant assays, and cell survival assays as well as elucidation of antimutagenic potential. The hydrolysate displayed high 2,2′-azinobis (3-ethylbenzothiazoline-6-sulfonic acid), ($ABTS^+$) radical scavenging activity (1419.6 μg TE/100 mg), Ferric reducing/antioxidant power (FRAP) of 164.9 ±1.5μg AAE/100 mg and ferrous ion chelation capacity with IC_{50} value of 140 ± 4 μg of hydrolysate. It also showed a significant increase (~20%) in the survival of TK-6 cells treated with 0.3 mM H_2O_2. Along with this, hydrolysate also possessed strong antimutagenic potential as assessed using TK-6 cell assay system. The hydrolysate displayed significant reduction in mutagenicity (45%) against EMS (0.5mM). In addition to this, moth bean protein hydrolysate possessed a significant angiotensin converting enzyme (ACE) inhibitory activity with an IC_{50} value of 6.9 ± 0.9 mg/ml. Findings thus provide credible evidences ascertaining broad spectrum functional properties of moth bean thus opening an attractive avenue of using the hydrolysate as a functional food ingredient.

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P-34

Betulinic acid inhibits SYK phosphorylation in platelets to lessen platelet adhesion and activation

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Abstract:

Betulinic acid is a pentacyclic triterpenoid, and is found in various plant species [1]. Betulinic acid is produced by betulin oxidation and is widely distributed in nature. Betulinic acid has been shown to exhibit several biological activities such as antiviral, anticancer, immunomodulatory, anti-inflammatory, antimicrobial, anti-diabetic, anti-parasitic, and anti-HIV properties etc. [1]. Further Betulinic acid has been found to exhibit antithrombotic effects in many studies. Betulinic acid and Betulin has been shown to exhibit inhibitory effects against Thrombin Receptor Activator Peptide (TRAP), Adenosine Diphosphate (ADP), and Arachidonic acid (AA) induced platelet activation and aggregation in a dose-dependent manner [2]. However, signalling pathways inhibited by Betulinic acid in platelets is yet to be explored. Therefore, we proposed to investigate the effect of betulinic acid on collagen induced platelet adhesion and activation. Platelets were isolated from mice. Platelets were labeled with CD41 PE-Cy7 and Phospho-SYK PE at 37° C for 1 hour followed by 20 minutes of incubation either with betulinic acid (500µM) or Cytochalasin D (1µg/ml) for 20 followed by addition of collagen (25µg/ml) and was analyzed by flow to determine the platelet activation. Further, washes platelets were labeled with Phalloidin-FITC and CD41 PE-Cy7, then treated with either betulinic acid (500µM) or Cytochalasin D (1µg/ml) followed by 30 minutes of incubation on collagen coated-cover slip for platelet adhesion studies by confocal microscopy. Betulinic acid inhibited the collagen-induced platelet activation by inhibiting protein tyrosine kinase SYK-phosphorylation at 500µM. Further, it inhibited the platelet adhesion on collagen-coated surface in imaging studies at the same concentration. The Betulinic acid inhibited the collagen-mediated platelet activation and reduced the total platelet population from 82.1% to 49.8%, respectively. These studies indicate that the Betulinic acid exhibits anti-platelet activity by inhibiting SYK phosphorylation.

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P-35

HPLC and UPLC method comparison followed by Validation and Forced Degeneration study of Xarelto tablet

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This work offers a Comparative method development of Xarelto tablet with the help of two Sophisticated Instruments, HPLC (Waters-2489) and UPLC (Waters Acquity UPLC$^{TH)}$[1]. The existing work represents the Validation comparison between HPLC and UPLC methods, it also shows the forced degeneration study by Acidic, Alkali, Hydrolysis, Photolysis and Thermal degradation. The observation and consequences obtained from each validation research lie well inside the getting criteria of ICH guidelines Q2(R1)[2].

	Experimental conditions	**HPLC Method(Waters 2489)**	**UPLC Method(Waters Acquity UPLCTH)**
1	Mobile Phase	0.1% OPA: ACN (60: 40 v/v)	**0.1 % OPA: ACN (55:45 v/v)**
2	Column	Phenomenax C8 100A (250mm X 4.6mm X 5µm)	**Acquity UPLC (R) BEH C8 (100mm X 2.1 mm X 1.7 µm)**
3	Flow rate	1 ml/min	**0.25 ml/min**
4	Column oven temperature	30˚C	**30˚C**
5	UV detection	280 nm	**280 nm**
6	Run time	15 minutes	**5 minutes**
7	Injection volume	20 µl	**2 µl**
8	Stock solution (standard and test)	500 ppm	**500 ppm**
9	Sample solution (standard and test)	50 ppm	**25 ppm**
10	**Diluent**	**Water:ACN (50:50 v/v)**	**Water:ACN (50:50 v/v)**

Keywords: HPLC, UPLC, Validation, Method Development, Forced Degeneration Study

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P-36

Cycloaddition of Oxidopyrylium Ion and Cyclization Reaction of Oxocarbenium Ion Involved in Natural Product Synthesis

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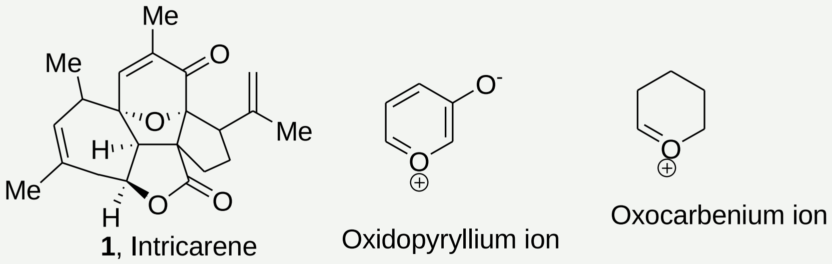
Abstract:

Enantioselectivity and molecular complexity from simple molecule is become challenge to build up completely bioactive natural product. Multicomponent reaction, cascade reaction, and cycloaddition reaction use to achieve synthesis of complex molecular structures. Due to stereoselectivity in [5+2] cycloaddition of oxidopyrylium species cycloaddition method uses in synthesis of the natural products. Dipolar cycloaddition of oxidopyrylium ion from literature will be presented. Utilization of oxidopyrylium cycloaddition towards, natural products will be reviewed. Oxocarbenium ion cyclization in synthesis of natural products will be cited. Problem citation of oxidopyrylium ion cycloaddition and oxocarbenium ion cyclization on the basis of literature will be presented and possible solution on problem will be concluded.

Key words: Cascade reactions, Cycloaddition, Dipolar, Oxocarbenium ion, Oxidopyrylium ion

.

Graphical Abstract



1, Intricarene

Oxidopyryllium ion

Oxocarbenium ion

Fig.1

References :

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P-37

Enantioselective imine reduction of dihydro-β-carbolines and dihydroisoquinolines by chiral bifunctional pyrrolidinyl-carboxamide and thiosquaramide catalysts

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Abstract: Enantioselective imine reduction of dihydro-β-carboline (DHBC) and dihydroisoquinolines (DHIQs) is a reliable and powerful technique to construct important bioactive tetrahydro-β-carbolines (THBCs)[1] and tetrahydroisoquinolines (THIQs)[2]. Here, we have developed an efficient enantioselective imine reduction protocol by employing two different types of chiral bifunctional organocatalysts such as pyrrolidinyl-carboxamides (**1**) and thiosquaramides (**2**)[3] to produce chiral THBCs (**5a-f**) and THIQs (**6a-d**). However, both the catalysts **1b** and **2a** found to be efficient at the catalytic load of 10 mol% for the enantioselective imine reduction of DHBCs and DHIQs to afford corresponding chiral THBCs and THIQs with an excellent enantioselectivities (up to ee 98% and 96% respectively).

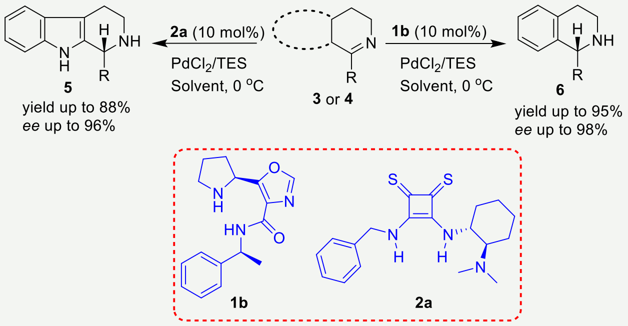

Figure 1: Enantioselective imine reduction of dihydro-β-carboline (DHBC) and dihydroisoquinolines (DHIQs).

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P-38

Molecular tiltation and supramolecular interactions induced uniaxial NTE and biaxial PTE in bis-imidazole based co-crystals

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Variable temperature single crystal X-ray diffraction(VT-SCXRD) study reveals the unusual thermal expansion behaviour of two new co-crystals prepared by solvent drop grinding using flexible ligand [1,4-bis[(2-methylimidazol-1-yl)methyl]benzene] (**BIMB**) and aromatic carboxylic acids viz. terephthalic acid (**TA**) and 4,4'-biphenyl dicarboxylic acid (**BPDCA**). Tiltation of the carboxylic acid molecules along certain crystallographic axis induces uniaxial negative thermal expansion (NTE). Supramolecular interactions such as,O−H···N, C−H···O C−H···π, π···π and van der Waals interactions play important role for biaxial positive thermal expansion(PTE) in both the co-crystals.

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P-39

Characterization of an Aminopeptidase (BfAp) from the Outer Membrane Vesicles (OMVs) of *Bacteroides fragilis* for hydrolysis of Soy protein allergens

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Abstract: Soy-protein although serves as dietary protein, it is also listed as one among “9 major food allergen” [1]. Its Glycinin and β-conglycinin proteins are resistant to complete digestion by gut enzymes [2,3] and known to act as immunogen as well as substrate for predominant proteolytic bacterial phyla of gut, Bacteroidetes [4]. *Bacteroides fragilis* constitute > 50% of total Bacteroidetes and produce OMVs containing a consortium of proteins with hydrolytic potential for various complex-polysaccharides and proteins [5]. In view of this, *B. fragilis* and *B. ovatus* were allowed to grow in media with Soy-protein as nitrogen source. Soy protein supported the growth of *B. fragilis*, but not that of *B. ovatus*. Thus, proteome analysis of OMVs of *B. fragilis* was carried out to identify soy-protein processing enzymes. Among different proteins, a putative Zn-metallopeptidase (BfAp) was expressed exclusive in soy-protein OMVs. Structurally, the protein shared highest homology (29% identity) with AminopeptidaseS of *S. griseus*. BfAp showed aminopeptidase activity against Leu, Ala, Arg & Lys with optimum activity at pH 8.5 and at 55ºC. It showed 20-fold activation in presence of 250 µM Co^{+2}. The enzyme also showed activity against peptide substrates with 5-15 residues long with Leu, Arg and Met at N-terminus. In vitro gastric digestion of Soy-proteins produces peptides with same amino acids at N-terminus whose immunogenicity can be modified by disturbing the primary sequence by hydrolysis [6]. Hence, BfAp can be considered as potential enzyme to alter the immunogenicity of soy proteins.

Key Words: Soy-protein, Bacteroidetes, Outer membrane vesicles (OMVs), proteomic analysis, AminopeptidaseBF

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P-40

Manufacture of Nano Carbon Materials incorporated with Palladium, Gold, and Gold–Palladium for Cyclohexane Oxidation: A Review

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Abstract:

Transition metal doped porous carbon materials have become a promising aspirant in energy storage, solid catalysis, and material chemistry. Palladium, gold, and gold-palladium anchored carbon composites (**CPC-25/170**, **CGC-25/170**, and **CGPC-25/170**) with two different sized carbon cages (~ 25 and 170 nm) were constructed using nano-silica ball (NSB) as the template and a pyrolysis fuel oil (PFO) based pitch residue as the carbon source. The Pd, Au, and Au-Pd doped carbon nanoreactors were characterized by various Physico-chemical analysis methods. The developed materials were used as heterogeneous catalysts for the oxidation of cyclohexane to cyclohexanol and cyclohexanone using H_2O_2 at room temperature (25 °C) and atmospheric pressure. The most active catalyst **CGC-170** showed combined cyclohexanol and cyclohexanone yield of 7.7 % after 4 h reaction time. The conversion of 2.4 %, 0.05% and 0.32 % was achieved using **CGC-25**, **CGPC-25** and **CGPC-170** catalysts, respectively. Recyclability of the catalysts maintains no observable performance loss during catalytic oxidation reaction.

Keywords: Carbon cage; Carbon nanoreactors; Cyclohexane; Metal doped; Oxidation.

Reference:

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P-41

Manufacture of Nano Carbon Materials incorporated with Palladium, Gold, and Gold–Palladium for Cyclohexane Oxidation: A Review

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Abstract:

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[2] V J Mayani, S V Mayani, S W Kim, Bulletin of Korean Chemical Society, 35, 2014, 1312-1316.
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P-42

Calixarene Based Fluorescent Chemosensors Containing Ru(II)/Re(I)-Bipyridyl Unit: Synthesis and Ion Recgnition Study: A Review

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Abstract

A series of metallo-receptors containing Ru(II)/Re(I)-bipyridine moiety as signaling unit and modified calix[4]arene as ionophore have been synthesized and characterized. These molecules exhibit metal to ligand charge transfer (MLCT) absorption band at 456 nm and ^{3}MLCT luminescence band at 614 nm. Ion-binding property of these molecules has been studied using a large number of metal ions and anions with the help of luminescence spectral change, which revealed that all of the receptors bind Hg^{2+} and Pb^{2+} strongly, as evident from the enhancement in emission intensity with red shift of λ_{max}. The Re(I) based calixarene chermosensor has strong affinity towards Cu^{+2} ion. This is observed in naked eye colour change. This Re(I) based molecule behaves as a dual sensor, it exhibited highly selective turn-on fluorescent sensing for Hg^{2+} and naked eye colourimetric detection of Cu^{2+} over a wide range of metal ions. The ion-competition study revealed no significant interference from any other metal ion used in this study. Among anions, $H_2PO_4^-$ and F^- exhibited substantial quenching in emission intensity, suggesting their strong interaction with the receptors. To evaluate the binding constants (*Ks*), luminescence titration of the receptor molecules with the strongly interacting ions have been performed and the *Ks* values have been calculated from the titration data.

Keywords: Chemosensors, Ru(II)/Re(I)-bipyridine unit, MLCT absorption band, calixarene

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P-43

Pharmacophore mapping and virtual screening for designing potent telomerase inhibitors as anti-cancer agents

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Telomerase is a ribonucleoprotein (RNP) responsible for the maintenance of chromosomal integrity by stabilizing telomere length [1]. This enzyme is considered one of the most common factors in almost all cancer cells and is mainly responsible for regulating telomere length [2]. Malignant cells are more susceptible to anti-telomerase inhibitors [3]. As normal cells, which lack telomerase activity, are unaffected by anti-telomerase cancer therapy utilizing telomerase inhibitors, it is implied that this medication has a high selectivity for cancer cells, making it less toxic and having a lower chance of adverse effects. Inhibition of telomerase by different Telomeres, also known as telomere terminal transferase, nowadays are the focused targets in treating cancer. heterocyclic scaffolds provides a path that leads to a new target for the development of cancer therapy. For the development of novel entities, several potent compounds that were reported in numerous articles and the molecules in various stages of clinical trials were used to design a pharmacophore model. A five-point pharmacophore model (AHRRR_1) was developed with a survival score of 4.5283, using 19 compounds with IC_{50} values ranging from 0.1 to 50.0 µM bearing one hydrogen bond acceptors (A), one hydrophobic site (H), and three aromatic rings (R) using Phase module of Schrodinger software. Based on the features generated by the pharmacophore model, substructure searching and virtual screening were done using high throughput (HTVS module of Schrodinger). The top hits were found to have similar characteristics to the developed pharmacophore model. Based on their fit values and anticipated activities (pIC50) greater than 5.1, the top 15 hits were determined. Results from the current study were first used to gain an understanding of the structural feature that promotes bioactivity, and then, during the screening process, the generated hits and/or their bio-isosteric replacement might serve as novel possible telomerase inhibitors prior to their synthesis and biological screening.

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Available at: https://doi.org/10.1158/0008-5472.CAN-05-1215.

P-44

Pharmacophore based Virtual Screening for designing PI3K/AKT/mTOR inhibitor for the treatment of Triple negative breast Cancer

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Cancer is the number one cause of death worldwide, over 10 million people died in 2020. This figure includes 685,000 deaths from breast cancer in women. The most common cancer in the world by the end of 2020 will be breast cancer, which accounts for 10-20% of all cases. Triple-negative breast cancer (TNBC) is particularly common in this group. Despite the fact that advances have been made in the treatment of hormone receptor-positive and human epidermal growth factor receptor 2-positive breast cancer, proven treatments for TNBC remain elusive.[1] All subtypes of breast cancer were affected by PI3K/AKT/mTOR pathway mutations, which were among the most common genetic abnormalities. The PAM pathway controls several cellular and physiological pathways in breast cancer, including the development of malignant cells.[2] There are four distinct isoforms (α, β, δ, γ) of PI3K, which are heterodimers made up of the regulatory (p85) and catalytic (p110) subunits. The same route is initiated by simulating receptor tyrosine kinases, which then activates PI3K and eventually phosphorylates AKT and the mTOR complex (mTORC1/mTORC2). A PI3K/AKT/mTOR inhibitor should therefore be incorporated as a promising pharmacological drug. Our research work has used Phase module of Schrodinger software to generate five-point pharmacophore models[3] for PI3K and mTOR individually utilizing 18 small molecules from clinical trials and literature reviews. To find a hit, a 3D query was utilized to search against a 3D database using the statistically significant pharmacophore hypotheses of ADDRR_1 (survival score 4.111) and DDHRR_1 (survival score 4.5355) for PI3K and mTOR, respectively. The Hit were screened virtually in high throughput (HTVS module of Schrodinger). The pharmacophore hypothesis as well as hit identification finally point us in the direction of a potential bioisosteric replacements to obtain the principal scaffold.

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P-45

Palladium-Catalyzed Suzuki Coupling and NIS-Mediated Dehydrogenative Cylco-etherification: A Concise Approach to 6,6-Disubstituted 6*H*-benzo[*c*]chromenes and Total Synthesis of Didehydroconicol

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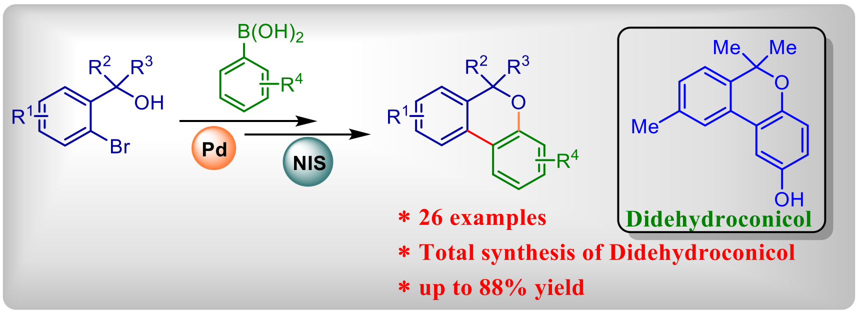
Abstract: Benzo[*c*]chromones are valuable tricyclic systems of natural and biological significance. Herein, we report a concise approach of 6,6-disubstituted 6*H*-benzo[*c*]chromenes in a two-step sequence starting from ortho-bromo benzylic alcohols and arylboronic acids, using intermolecular palladium-catalyzed C−C and intramolecular *N*-Iodosuccinimide (NIS) mediated key C−O bonds construction. Besides, the current method explored broad substrate scope under robust conditions. Notably, the practicality of the present approach is further extended for the total synthesis of Didehydroconicol.



* 26 examples
* Total synthesis of Didehydroconicol
* up to 88% yield

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P-46

Synthesis and Spectroscopic Characterization of Pyrimidine-fused Porphyrin Analogues

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Porphyrins are strongly conjugated aromatic heterocycles that are a crucial component of naturally occurring pigments like chlorophylls and bacteriochlorophylls, which are recognised for storing sun energy and facilitating photosynthesis in both plants and bacteria. Porphyrins have also showed a wide range of uses in many fields, including photodynamic therapy for the treatment of cancerous tumours, supramolecular chemistry, optoelectronic devices, and catalysis [1–5]. *meso*-Tetraarylporphyrins have been successfully used as raw materials for the peripheral functionalization to construct a wide range of complex porphyrinoids [6, 7]. Based on earlier research, it has been determined that the electronic characteristics of these molecules can be tailored by functionalizing their *β*-pyrrolic and *meso*-positions. To this end, we have developed a new synthetic strategy to integrate a pyrimidine ring on porphyrin periphery. In this way, a novel series of pyrimidine fused porphyrins were effectively produced with good yields. The synthetic details and structural characterization of newly created porphyrinoids will be presented.

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P-47

Pyranose sugar-based macrocycles with peptidic scaffolds as potential host for carboxylate anion recognition

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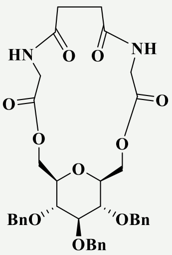
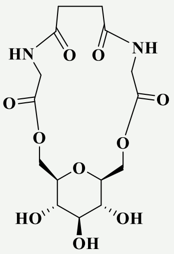
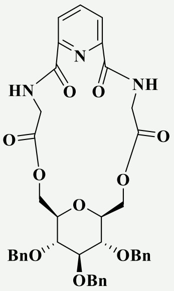
Macrocycles are important class of compounds having applications in drug development, bioinorganic chemistry and in material sciences. Recently sugar-based macrocycles have gained wide recognition because of easy accessibility, low cost, multifunctionality and inherent chiral nature. In the area of supramolecular chemistry anion complexation, specially carboxylate anion complexation is currently receiving much attention due to their biochemical properties, such as enzyme-substrate interactions, carboxylate anion in carboxypeptidase A, carboxylate anion in biological activity of vancomycin family of antibiotics etc. We have synthesized three macrocyclic compounds using 2,6-anhydro-glucoheptitol, glycine and dicarboxylic acid linkers, *viz.* succinic acid and pyridine dicarboxylic acid. The anion inclusion capabilities of synthesized macrocyclic compounds were evaluated using boc-GlyCOO$^-$ anion *via* ^{1}H NMR titration studies in $CDCl_3$. The macrocyclic compounds **I** and **III** have shown strong binding affinity towards carboxylate anion present in TBA salt of *N*-boc-glycine. The detailed synthetic pathway and binding studies will be discussed during the poster presentation.



Macrocycle I



Macrocycle II



Macrocycle III

Key References:

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P-48

Development of Thiourea based derivatives as potent inhibitors of Hepatitis B Virus

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Hepatitis B Virus is a hepatotropic virus that may cause acute and chronic liver infection in humans. Currently, 3.5 percent of the total world population is chronically infected with HBV that are managed using a combination of antiviral and immune modulatory therapies. A candidate molecule 1-(3-(1H-imidazol-1-yl)propyl)-3-(2,4-difluorophenyl)thiourea (coded as IR-415) exhibiting excellent antiviral efficacy in cell culture model was identified after a high-throughput screening of the Maybridge library. We undertook the synthesis of twenty derivatives of IR-415 and evaluated them for their in vitro activity against hepatitis B virus. It was observed that on changing the linker carbon between the phenyl thoiurea and imidazole ring of the parent compound from three carbon propyl to four carbon n-butyl there was a significant improvement in anti-hepatitis B viral activity. The human hepatoma HepG2 cells transfected with HBV genomic DNA or HBV-permanent cells (HepG2.2.15) were treated with different concentrations of synthesized 20 IR-415 derivatives. Inhibition in the expression of viral proteins (HBsAg, HBeAg, HBx etc.) was observed significantly in two antiviral candidate drug out of 20 derivatives compared to IR415. The in vitro results corresponded with the in-silico studies performed on these two selected thiourea derivatives with HBx protein.

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P-49

Modified starch based selective flocculant for the beneficiation of low-quality iron ore: experimental and theoretical studies

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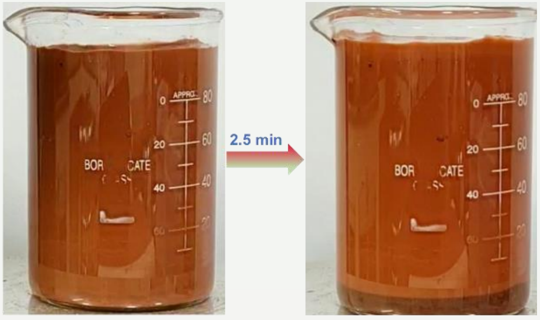
A selective flocculant, St-Meth-Co-PAM has been synthesized by functionalization of starch (St). Starch methacrylate (St-Meth) has been first developed by methacrylation of the starch with methacrylic anhydride (MAh) followed by formation of a 3D network like structure which has been achieved by free radical polymerization among St-Meth molecules and then grafting simultaneously with polyacrylamide chain on the St-Meth network backbone [1]. The developed selective flocculant has been characterized by several characterization techniques. The selective flocculation efficacy of the synthesized selective flocculant has been studied and compared with the industrial selective flocculant starch [2]. It has been established from the selective flocculation study that the material exhibit very good selective flocculation efficiency by means of settling velocity and iron recovery. Also, from the theoretical analysis, it can be said that the material form coordination with the hematite particles selectively [3]. That's why the material St-Meth-Co-PAM can be affordably used for industrial purpose as displayed very high settling speed and high iron recovery rather than the conventional selective flocculant starch.



Iron ore suspension
Before Selective Flocculation

After Selective Flocculation

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P-50

Thermally Activated Delayed Fluorescence and Room-Temperature Phosphorescence in Asymmetric Phenoxazine-Quinoline (D2−A) Conjugates and Dual Electroluminescence

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Advanced Photofunctional Materials Research Laboratory, Department of Chemistry, School of Natural Sciences, Shiv Nadar Institution of Eminence deemed to be University, Delhi NCR, Uttar Pradesh, India 201314
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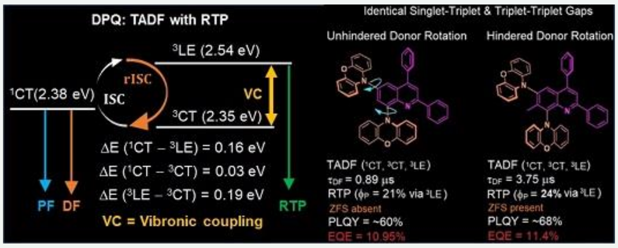

Abstract: Thermally activated delayed fluorescent (TADF) materials combining high photoluminescence quantum efficiency and short delayed emission lifetime are highly desirable in organic light-emitting diodes (OLEDs)[1] and sensors.[2] It is also well known that harvesting triplet state (i.e, phosphorescence at ambient conditions, RTP) from an organic molecular system is a difficult task due to inefficient spin-orbit coupling (SOC)[3] and localized nature of the triplet states, which can be quenched easily by molecular vibrations and oxygen under ambient conditions. Herein, we report two phenoxazines-quinoline conjugates (**DPQ**, **DPQM**), in which two phenoxazine donors are covalently attached to the 6,8-positions of the 2,4-diphenylquinoline and/or 7-methyl-2,4-diphenylquinoline acceptors. Detailed spectroscopic investigations and quantum chemistry calculations ensured that both conjugates show TADF *via* rISC from the charge transfer triplet (^{3}CT) to singlet (^{1}CT) states mediated by vibronic coupling (VC) among ^{1}CT, local triplet (^{3}LE) and ^{3}CT states due to close energy gaps. Further, RTP with quantum yields (ϕ_P) of ca. 21−24% was also observed due to radiative decay of ^{3}LE states caused by small triplet-triplet gaps and VC effect. Phosphorescence measurements of **DPQM** at low temperatures (T = 77, 10 K) ensure a distinct zero-field splitting (ZFS)[4] of T_1^{CT} state into sub-states. Both compounds showed dual-electroluminescence with external quantum efficiencies of ca. 11−12% due to the efficient triplet harvesting *via* TADF and RTP channels. In this lecture, I will address how a simple asymmetric D2-A systems can generate high efficiency TADF and RTP which may find potential applications in OLEDs[5].

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P-51

Polymeric Micelle Derived from Modified Alginate and N-Boc-Glycine via RAFT Polymerization for pH Triggered Release of Hydrophobic Drug

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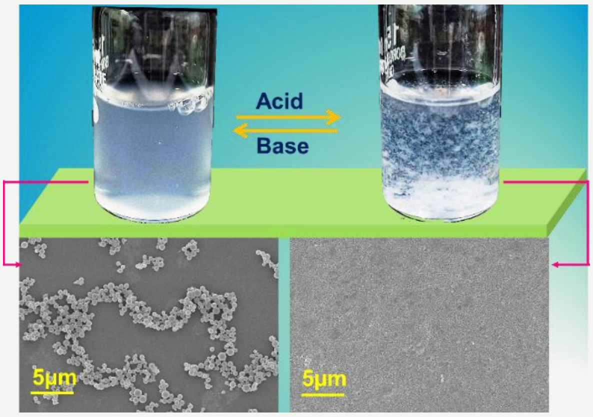
Reversible pH responsive biopolymeric micelles have been prepared by the self-assembly of amphiphilic Alg-g-p(Gly-HEMA) copolymer. Herein, a hydrophobic monomer N-Boc glycine-hydroxy methyl methacrylate (Gly-HEMA) has been synthesized by chemical modification of N-Boc glycine. This monomer has further been grafted through RAFT polymerization on the backbone of raft reagent modified alginic acid to obtain a new amphiphilic copolymer with attached hydrophobic segment. The controlled polymerization is assessed using Advanced Polymer Chromatographic (APC) analysis with a narrow distribution. The critical micelle concentration (CMC) of the developed copolymer has been determined by surface tension, photoluminescence spectroscopic (PL) and dynamic light scattering (DLS) analyses. The size and shape of the developed micelle has been investigated by FESEM and HRTEM analyses, which reveal that the size of the copolymeric micelle is ~ 200 nm with spherical in shape. Alg-g-p(Gly-HEMA) has demonstrated pH-responsive reversible micellization behaviour. The process of micellization to phase separation and vice versa can be controlled just by altering the pH. The formed micelle is able to uptake and release a model hydrophobic drug in controlled manner.



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P-52

A Comprehensive Review on Various Synthetic Strategies and Structure Activity Relationship (SAR) Study for the Discovery of *Plasmodium falciparum* DihydroorotateDehydrogenase (*Pf*DHODH) Inhibitors as Antimalarial Agents

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Abstract:
One of the deadliest infectious diseases, malaria, still has a significant impact on global morbidity and death. *Plasmodium falciparum* dihydroorotate dehydrogenase (*Pf*DHODH) catalyses the fourth step in *de novo* pyrimidine nucleotides biosynthesis, a critical mechanismfor Plasmodium parasites survival. *Pf*DHODH has been clinically validated as an innovative and extremely promising target for the development of novel targeted antimalarial drugs. *Pf*DHODH inhibitors has the potential to significantly slow down parasite growth at the blood and liver stages by blocking the *de novo* pyrimidine biosynthesis. Several *Pf*DHODH inhibitors based on various scaffolds have been explored over the past two decades. These include triazolopyrimidines, dihydrothiophenones, benzimidazole-thiophene-2-carboxamides, pyrrole-based derivatives, isoxazolopyrimidines, hydroxyazole-based compounds, and others.Many scientists from numerous research organisations across the globe have synthesised *Pf*DHODH inhibitors with various substitutions on different heterocyclic ring systems and scaffolds. For the first time, this review provides an overview of all the synthetic approaches used for the synthesis, alternative synthetic routes, and novel strategies involving various catalysts and chemical reagents that have been used to synthesise *Pf*DHODH inhibitors as antimalarial agents. We have also summarised SAR study of all these *Pf*DHODH inhibitors. In an attempt to assist readers, scientists and researchers involved in creating new compounds as *Pf*DHODH inhibitors as antimalarials, this review provides accessibility of all synthetic techniques and SAR study of last two decades of work.

Keywords: Plasmodium falciparum, Dihydroorotate dehydrogenase, Malaria, Scaffolds.

References:

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P-53

Prussian Blue Insoluble – A Life Saving Innovation

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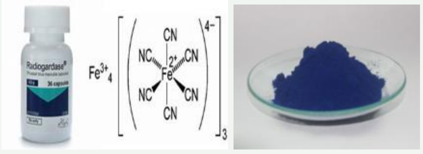
Introduction: Prussian Blue was first prepared in 1704 and used as an inorganic pigment. A work in the 1960s investigated the use of PB as an antidote for thallium poisoning and a decorporation agent for radio cesium. From the 1970s PB was recommended as an antidote in thallium 59 intoxication and it is now routinely used for this purpose.
There are two forms of Prussian blue, **ferric (III) hexacyanoferrate (II)** (Insoluble PB) and **potassium ferric (III) hexacyanoferrate (II)** (colloidal PB). PBI is used to treat patients with internal contamination of **radioactive cesium, radioactive thallium and non-radioactive thallium,** to increase their rates of elimination.

$$4\ FeCl3 + 3\ K_4\,[Fe\,(CN)_6] \rightarrow Fe_4\,[Fe\,(CN)_6]_3 + 12\ KCl$$



Properties: PBI is Dark blue in color, insoluble ion exchange resin. PB breaks the entero-hepatic cycle by binding cesium in the gut so that the bound cesium is not reabsorbed and gets eliminated with PB in feces. The average effective half-life of Cs-137 gets reduced by 3 factors with PB therapy. Dosage of Prussian blue: one gram orally 3x daily for 3 weeks reduces T_b to about 1/3 normal value.

Importance: India has been declared as a **Nuclear State**, there are **22 nuclear reactors** placed at **7 nuclear power plants**. India's vulnerability to nuclear accidents like Fukushima Nuclear accident in Japan is very high. Also a possible nuclear detonation cannot be denied. Many rdionuclides are produced during a nuclear fission reaction, and Cs-137 is most significant among all.**Cs-137 mimics potassium ion** and it gets incorporated in the cells/tissues very easily. Hence, there is an unmet need of the drug in India.**Till date, only PBI has been reported as an antidote of Cs-137**. USFDA has approved Radiogardase-Cs capsule comprising Prussian blue insoluble. In view of this, DRDO developed PB formulations-PruDecorpTM and PruDecorp-MG.

References: List of drugs approved by CDSCO, USFDA – Guidance for Industry – Prussian Blue Drug Products, Research Papers related to use of PB during Goinaia incident of Cs-137 contamination in 46 subjects.

P-54

Design and synthesis of porous carbon materials for energy production and storage applications

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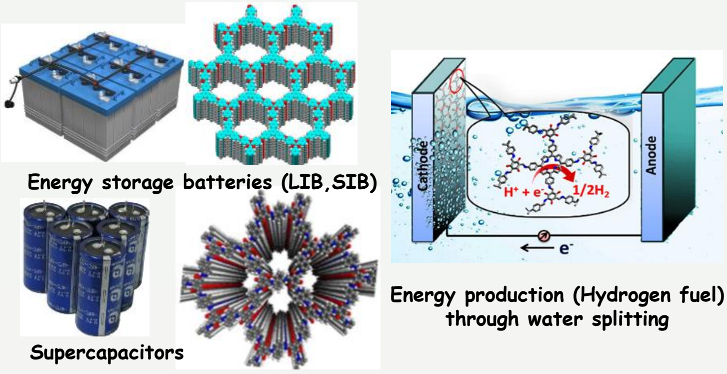
Since the last two decades, we have been constantly threatened by global warming and natural resource scarcity. This situation forced us to move from non-renewable to green renewable energy. Cost-effective renewable energy production and storage technologies have recently received a great deal of attraction from several industries for day-to-day applications. Plentiful, economically viable, reproducible, and easily processed materials are now commercially crucial for energy production and storage. Technological implementation of the optoelectronics[1-4] field is based on decentralizable technologies like OLED, storage devices (battery), capacitors *etc*. These technologies are advantageous for countries like India, where infrastructure is in demand for the technology transfer and implementation process.

Herein, we devoted for developing a new generation organic materials like PAH, hetero-doped graphene material through bottom-up approach for green renewable and sustainable energy production through water splitting (HER, OER),[5] perovskite solar cells (OPV), rechargeable sodium batteries,[6] and super capacitor *etc*.



Energy storage batteries (LIB,SIB)

Supercapacitors

Energy production (Hydrogen fuel) through water splitting

This work directly impacts our modern society, where extreme demand for green and sustainable energy is the biggest concern. In this regard, it is conspicuous to say that outcome of this research work slowly but surely will be an integral part of our "***Make in India***" project.

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P-55

Thiol-Capped Zinc Phthalocyanine Nanoparticles: Soft Aqueous Synthesis and Size-dependent Optical Properties

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Zinc-phthalocyanine (Zn-Pc) is an FDA-approved drug for photodynamic therapy [1]. However, it is insoluble in water and, therefore difficult to administer directly to cancer patients. This work aims to make molecular nanocrystals of Zn-Pc and modify the surface with suitable ambiphyllic ligands (to impart solubility in water). Few droplets of Zn-Pc solution in DMSO was added to deionized water at 10 ^{o}C and sonicated for few minutes, resulting in the formation of uncapped Zn-Pc nanoparticles. The effect of temperature on the synthesis process was also investigated. As the temperature increased from 10 to 60 ^{o}C, the hydrodynamic size increased linearly. Surface-capping of these nanoparticles was done with polyethylene glycol (PEG), and water-soluble thiols [2]. Different thiols chosen for capping are: Thioglycolic Acid (TGA), Mercaptopropanoic acid (MPA), Mercaptoethanol (ME), Cysteine (Cys), Cysteamine (Cya). FTIR spectroscopy confirmed that the thiol-end is bound to the nanoparticle while the other end-group remains free. Compared to bulk Zn-Pc, Q-band showed a blue-shift in all thiol-capped nanocrystals, and a maximum shift of 65 nm was observed for TGA. Upon formation of nanoparticle, a substantial increase in the extinction coefficient of the Q-band was also observed thereby making it suitable for photodynamic therapy. Zeta-potential measurements was done to estimate the surface charge and the relative stability of the particles. TGA-capped NPs were found to have negatively charged surface with a Zeta-potential of -34 mV. Cys- and Cya-capped exhibited interesting variation in surface charge depending on pH. At pH 6, Cys-capped NPs showed zetapotential of +21 mV which changed to -16 mV at pH 11. These thiol-capped ZnPc NPs with enhanced aqueous solubility, stability and optical properties can be better suited for photodynamic therapy.

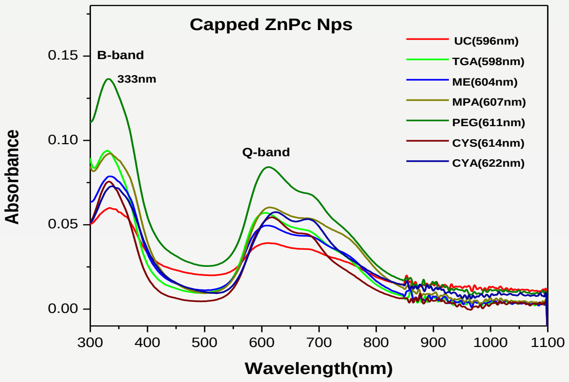

Figure 1: The UV-Vis absorption spectra of the ZnPc nanoparticles with different capping agents

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P-56

Ultrasound-assisted synthesis of Silver@Chitosan nanocomposites and its photocatalytic activity

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Photocatalytic degradation of methylene blue (MB) dye is reported by utilizing Silver@Chitosan nanocomposites (Ag@C NCs). Synthetic conditions for the Ag@C NCs were optimized by using ultrasonication and gallic acid. Different analytical techniques have been used to characterize the physico-chemical properties of Ag@C NCs. The synthesis of AgNPs was primarily identified by the appearance of yellow colour and confirmed by showing λ_{max} = 415 nm in UV-visible spectroscopy. All characterization techniques reveal that the generated Ag@C NCs were non-aggregated, quasi-spherical shape with an average size of 20-70 nm. Significant degradation (>70%) of MB dye was observed for 5 hrs in sunlight.

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P-57

Synthesis and Characterization of NiO nanoparticles

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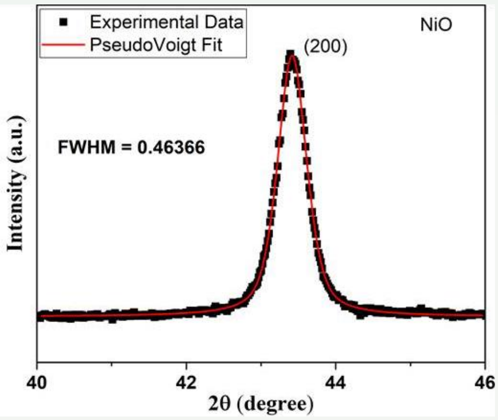
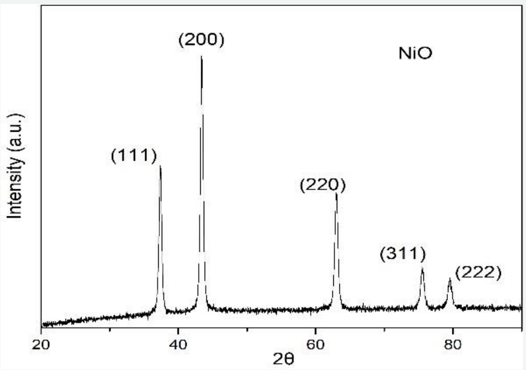
Properly controlling the size and phase purity of metal oxide nanoparticles are prerequisites for several applications. This work presents the modified sol-gel method based on propylene glycol for synthesizing NiO nanoparticles. The NiO nanoparticles were prepared using Nickel Acetate Tetrahydrate as a metal source and Propylene Glycol as a complexing agent, as reported earlier, with slight modification in the synthesis route Bonomo et al. & Wu et al. [1]. The NiO nanoparticles were synthesized with calcination temperature at 550°C for 2 hours. The XRD analysis confirms the formation of a crystallite size of 18 nm. The d-spacing was calculated using Bragg's equation.





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P-58

Colorimetric sensing of fluoride ion by 2-quinonimine functionalized gold nanoparticles

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Fluoride ion plays a vital role in biological and chemical processes. It plays a crucial role, particularly in the prevention of dental caries, and is widely studied for the treatment of osteoporosis. Fluorosis occurs due to an excess amount of fluoride, also known as fluoride toxicity, which leads to increased bone density. Also, diversity in fluoride ion function makes it essential for detection purposes. For successful analytical techniques, the principle themes are rapid, selective, and sensitive monitoring and measurement of hazardous materials as analytes. Colorimetric detection gives advantages of on-site applicability, ease of analysis, avoid complicated instrumentation and usage. Colorimetric detection also allows ease of monitoring and cost-effectiveness of toxic ions. A gold nanoparticle is a vital ingredient of these sensors. Due to having an intense surface Plasmon resonance absorption (SPR) band in the visible region, including a large surface area, the stability of gold nanoparticles has attracted much attention as a unique and advantageous optical platform for fluorine, colorimetric sensing for many practical applications like biosensors [1], medical diagnosis [2], environmental management [3], etc. This work is based on the easy synthesis and details characterizations of the 2-quinonimine functionalized gold nanoparticles for colorimetric sensing of fluoride ions in water. The 2-quinonimine functionalized gold nanoparticles have been synthesized by chemical reduction of $HAuCl_4$ in a basic medium using 2-aminophenol as a reducing and stabilizing agent. These functionalized gold nanoparticles offered an enormous possibility of applications in the selective and sensitive detection of fluoride ions in water by colorimetric method. The sensing parameters like selectivity, sensitivity, pH dependence etc. have been correlated with the proposed sensing mechanism.

Keywords: Functionalized gold nanoparticles, Colorimetric sensing, Fluoride ion sensing

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P-59

Sol-gel based synthesis and characterization of bioactive silver doped hydroxyapatite: effect on morphology, corrosion activity, in-vitro thrombogenicity and antimicrobial activity.

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An important bioceramic renowned for its strong osteoconductive qualities, non-toxic makeup, high bioactivity, and good biocompatibility is hydroxyapatite (HAp) with the chemical formula $Ca_{10}(PO_4)_6(OH)_2$. It is also said to resemble natural bone. Despite having many benefits, HAp also has some drawbacks, including poor mechanical characteristics, brittleness, a lack of an inhibitory impact on microorganisms, and taking long period to resorb in the body [1]. Using dopants, such as cations, anions and polymers, can mitigate these drawbacks. These are well enough known to enhance the hydroxyapatite's characteristics. In the body, silver is regarded as a micro-essential element. Since many years ago, silver (Ag^+) ions have been recognised for their antibacterial and sterile qualities. Study demonstrates that silver ions, metallic silver, and silver nanoparticles can be used in medical applications for treating burns, coating dental materials, coating stainless steel materials, treating water, treating textile fabrics, and making sunscreen lotions etc. It has little toxicity to human cells, excellent thermal stability, low volatility. Because the use of antibiotics is restricted, practitioners are turning back to silver wound dressings with varied silver content [2]. In the current investigation, different weight percent of Ag^+ ions are doped into the HAp matrix while changes in morphology, corrosion behaviour in Ringer's solution, blood clotting tendency and antibacterial activity are monitored.

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P-60

Selective sensing of ammonia in aqueous medium by core-shell hybrid of poly(*m*-aminophenol)/silver

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The source of ammonia emission is either the metabolic decomposition of organic nitrogen like manure from agriculture, wildlife, leaves etc. or the deposition of added ammonium and nitrate salts to the cultivated soil in the form of fertilizer. The agricultural sector has enhanced the addition of large amounts of fertilizer containing ammonium ion. However, the problems associated with this are eutrophication, acidification, change in vegetation, increased atmospheric ammonia concentration, etc. Sensing ammonia in aqueous phase should be helpful to protect plant, human and animal health. This communication develops a core-shell hybrid of poly(m-aminophenol)/silver for chemiresistive sensing of ammonia selectively in aqueous medium. Uniformly distributed silver nanoparticle as core was formed inside the shell of poly(m-aminophenol) by the thermal reduction of silver mono-positive complexes with the functional groups of polymer. Amount of silver nanoparticles within the poly(m-aminophenol) matrix was optimized in respect of size, dispersion of the nanoparticles present inside the polymer and the conductivity of the hybrid. The hybrid with ~10 % silver loading was found to have the highest DC-conductivity of 10^{-4} Scm^{-1} range, even without the usage of any other dopant. This poly(m-aminophenol)/silver hybrid have shown chemiresistive type effective sensing responses toward ammonia in aqueous medium. The selectivity of the ammonia sensing by the hybrid was also confirmed over the ammonium salts like ammonium sulphate, ammonium chloride, sodium nitrate and urea in aqueous medium. The sensing performances, e.g., response time, recovery time, reproducibility, repeatability, resistance, linearity, sensitivity and selectivity) of poly(m-aminophenol)/silver hybrid were also evaluated. The sensing mechanism was also proposed in the report.

Keywords:
Poly(m-aminophenol); conducting polymers; silver nanocomposites; functional nanocomposites, sensors

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P-61

Synthesis of Pectin based hybrid material for environmental remediation

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The aim of this work is the removal of pollutants and emerging contaminants from waste water [1]. A hybrid material pectin crosslinked poly(acryl amide-co-itaconic acid) functionalized with silica grains [Pec-cl-(PAM-co-IA)-fn-silica] was prepared. Different grades of this hybrid material were synthesized and characterized. The removal of kaolin suspension was performed by flocculation process and efficiency has been studied in terms of turbidity. The functionalization of crude material with silica grains to novel nanocomposite material has the flocculation [2] efficiency of 91.27% at 8ppm, showing good flocculation efficiency. [Pec-cl-(PAM-co-IA)-fn-silica] as a flocculant in synthetic and industrial effluent show that it will be very efficient in waste water [3] remediation.

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P-62

Sunlight-promoted green synthesis of silver nanocube by Xanthan gum

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In the present investigation, we reported the synthesis of cube/bar shape silver nanoparticles (AgNCs) using xanthan gum (XG) under sunlight. During the reaction, XG was used as both a reducing and capping agent. The optical property, size, structure, morphology, and composition of XG-AgNCs were determined using UV-visible spectroscopy, Dynamic light scattering (DLS), Scanning transmission electron microscopy (STEM) and X-ray diffraction techniques. UV-Visible spectrum and STEM images confirm the existence of cubic shape XG-AgNCs by showing their characteristic surface plasmon peaks at 354 and 444 nm. DLS showed mean particle size of 365 nm and XRD confirmed the purity of XG-AgNCs. The formed XG-AgNCs showed excellent catalytic activity of 4-nitrophenol reduction. This work provided a feasible method to synthesize AgNCs without using harsh chemicals.

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P-63

Approach towards a circular economy: Chemicals packaging waste as an emerging scavenger for neutral red from water and waste water

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Organic dyes removal from wastewater is a global concern for environment and human health. Using batch technique, a chemical packaging vermiculite as filler waste has been demonstrated for neutral red (NR) dye adsorption. The filler material was characterized by FTIR, pH_{ZPC}, and FESEM. FTIR suggests the presence of silicate functionalities. Maximum adsorption capacity was found to be 121.21 mg/g at 328 K. Optimizing parameters such as contact time, initial concentration, solution pH, and temperature suggests that the adsorption is more suitable at neutral pH and elevated temperature (318 K). Adsorption kinetics follows a combination of pseudo-second-order, second-order, and intra-particle diffusion kinetics. Langmuir adsorption isotherm model stands best fit model with R^2=0.967, suggesting a monolayer homogenous adsorption. 50% material was regenerated by using methanol and can be reused for a couple of cycles. The industrial effluent containing NR was tested and 43.8% removal efficiency was achieved. The adsorption of NR onto filler waste is attributed by combination of electrostatic interaction through silicate moieties coupled with weak hydrogen bonding via lattice water. This investigation indicates the practical application of filler wastefor dye removal from wastewater and water purification.

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Synthesis and application of Ni-Cr bimetallic composite fabricated with Ethylenediamine for sequestration of Malachite Green from waste water

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To assess the feasibility of eliminating malachite green from an aqueous solution, a batch study was conducted to examine the adsorption of malachite green on ethylenediamine mixed metal oxide composite (MMC). Co-precipitation-induced grafting was used to create MMC, which was then examined using FTIR spectroscopy, scanning electron microscopy, BET surface area, and point of zero charge (pHzpc). The surface area of MMC was found to be 26.592 m^2/g. Malachite green dye adsorption was improved with regard to crucial physio-chemical factors such temperature, pH change, contact duration variation, and concentration variation. The process follows a Freundlich isotherm model ($R^2 = 0.996$) and pseudo-second-order kinetics ($R^2 = 0.999$). It was determined that the highest adsorption capacity was 574.71 mg/g. The adsorption of dye onto MMC was found to be endothermic with a value of ($\Delta H° = 15.72$ kJ/mol and spontaneous ($\Delta G° = 4.84$ kJ/mol). Methanol/water solution was used as regenerating agent.

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P-65

Design, Synthesis and Medicinal Chemistry Exploration of New Pyridone Analogs

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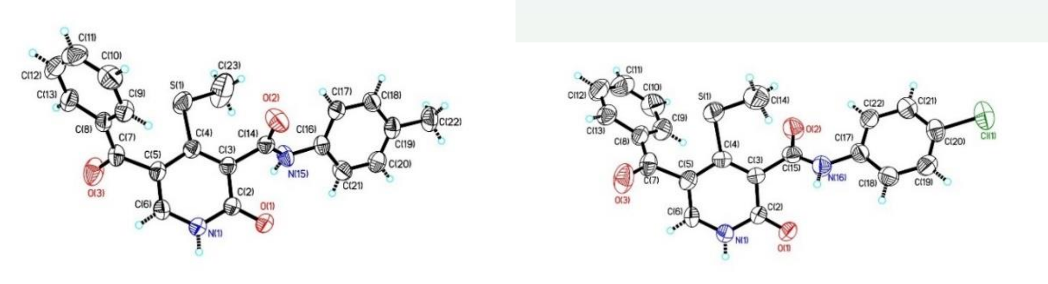
Synthesis and biological activity of 2-pyranone carboxamides analogues by intramolecular ring transformation was carried out. These compounds contained: 1) Di-ketone pyridone carboxamides analogs; 2) N-substituted pyridone analogs; 3) N-substituted pyridone acids analogs; 4) N-substituted pyridone ester analogs and conformation of obtained structure through by 1D&2D and 3D NMR along by X-ray single crystal diffraction with HRMS and inhibitory effect of above derivative of 2-pyridone on SARS-CoV-2 replication in VeroE6/TMPRSS2 cells give good result in anti-viral study.



2a 2b

Figure 1: The X-ray crystal structure of compound **2a** (CCDC No: 2178512) and **2b** (CCDC No: 2178513) respectively through ORTEP diagram using 50% ellipsoidal plot.

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P-66

Hydro-decarboxylation of 2*H*-Pyran-3-Carboxylic Acid Derivatives Under Both Basic and Acidic Conditions

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Despite the availability of several methods for decarboxylation, this area remains exploratory and requires new development. Here, we develop a convenience method both in acid/base and testified hydro-decarboxylation of pyranone-containing compound report a highly efficient decarboxylation of 4-(methylthio)-2-oxo-6-aryl-2*H*-pyran-3-carboxylic acids under basic. Besides all the condition microwave assisted condition is most suitable Owing to this step of the process may help in the synthesis of the bioactive compound in the future and also plays an imperative role in the synthesis; all compounds were characterized by spectroscopic analysis.

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P-67

Synthesis and Anti-HIV Activity of a New Isoxazole Containing Disubstituted 1,2,4-Oxadiazoles Analogs

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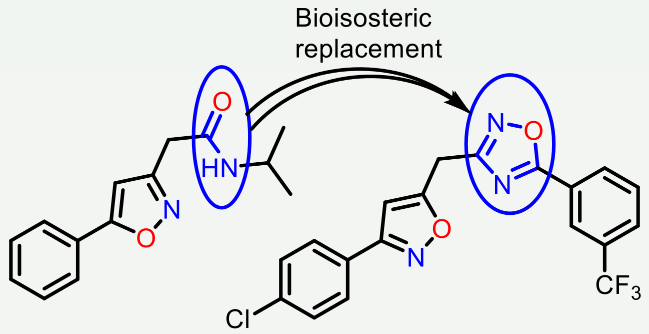
Continuing our anti-viral drug discovery research, we intended to diversify our lead anti-HIV-1 inhibitor by non-classical isosteric replacement of amide to 1,2,4-oxadiazoles [1]. The resulting molecules isoxazole-1,2,4-oxadiazole analogs were synthesized using mild bases in ethanol under microwave irradiation. The anti-HIV [2] potential was checked in human CD4$^+$ reporter cell lines, TZM-bl and CEM-GFP, at the highest non-cytotoxic concentration (HNC), demonstrating that 3-((3-(p-tolyl)isoxazol-5-yl)methyl)-1,2,4-oxadiazole and 3-((3-(4-chlorophenyl)isoxazol-5-yl)methyl)-1,2,4-oxadiazole inhibit HIV-1 replication significantly and could be considered as a new lead candidate against HIV-1.



anti-HIV-1 lead candidate
IC$_{50}$: 39.48 ± 2.36 nM
CC$_{50}$: 65.56 ± 2.48 nM

1,2,4-Oxadiazole Lead
IC$_{50}$: 85.7 ± 1.91 nM
CC$_{50}$: 13.28 ± 1.26 nM

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P-68

Synthesis and Single Crystal Structural Studies of Isoxazole Analogs

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Derivatives of isoxazoles can be obtained by scaffold transformation of pyranone carboxamide group present in the pyranone-3-carboxamide. The intramolecular attack of oxygen at C-6 carbon that attacked at the carbon bearing has been replaced efficiently using sodium bicarbonate. Further the hydroxylamino carboxamide cyclizes into five membered ring as a result of rearrangement. X-ray quality single crystal was prepared by slow evaporation method using methanol as solvent. Packing pattern reveals the intermolecular packing in space. Packing system initiates the way to supramolecular chemistry. Crystal studies also acquaint with the distance between bond to bond and atom to atom [1]. The presence of isoxazole moiety is a major core in our molecular designing process and crystal packing of molecules [2].

Isoxazole is a five membered ring compound that can be subjected to changes to develop new scaffold. Isoxazole ring enhances the efficacy of a compound decreasing the toxicity and increasing its pharmacokinetic profiles [3]. The approved drugs containing isoxazole ring such as Acivin, Pleconaril, Leflunomide, Sulfisoxazole [4], Oxacillin [5] appeared to be lifesaving drugs. Moreover, due its small size in comparison to six membered ring it experiences less hinderance. Its small size facilitates excellent binding properties with protein and other molecules.

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P-69

Interaction of Luminol with Spherical Metallic Nanoparticles

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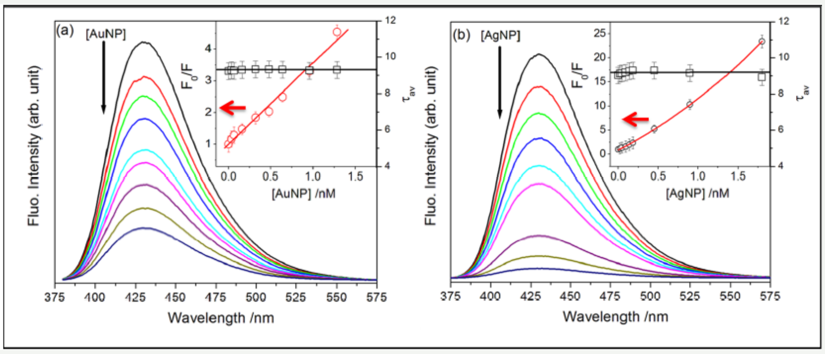
Chemiluminescent (CL) property of luminol (3-aminophthalic hydrazide, LH_2) has wide application in different fields like forensic science, biological and curative science, quantification and detection of macro and micro molecules such as proteins, carbohydrates, DNA, and RNA [1]. The application of luminol is also found in environmental monitoring as biosensors, in the pharmaceutical industry for cellular localization and as biological tracers, in reporter gene-based assays and several other immunoassays [2]. Literature reports suggest that the CL of LH_2 in H_2O_2 can be catalyzed by different metals nanoparticles (NPs) like silver, gold and platinum, metal oxide NPs like ZnO, ferric oxide, cerium oxide including gold/silver alloy and $CoFe_2O_4$ magnetic nanoparticles etc. [3]. These NPs catalyze the decomposition of H_2O_2 to produce some reactive oxygen species, thus enhancing the CL from the reaction between LH_2 and H_2O_2. Normally, metal NPs are used as efficient energy acceptor due to the strong overlap of their absorption band with donor emission.



Quenching of Luminol fluorescence in presence of varying concentration of Au (a) and Ag (b) NPs. Inset shows the Stern-Volmer analysis of the quenching data (circles). The variation in LH_2 average lifetime is shown by empty squares in both the cases.

These all findings motivate us for further study of the binding mechanism of these nanoparticles with LH_2. Luminol fluorescence is found to quench extremely efficiently in presence of both Ag and AuNPs. The non-variance of LH_2 fluorescence decay time with addition of quenchers indicates that a static type mechanism towards the formation of ground state complex between the fluorophore and the quencher is responsible for the quenching phenomenon.

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P-70

Interaction of Theobromine with Human Serum Albumin, a Combined Spectroscopic and Molecular Docking Study

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The obromine belongs to the xanthine group of drugs and are principle component of tea or coffee with important pharmacological activities and clinical applications. The N-methyl derivatives of xanthine like theobromine (3,7-dihydro-3,7-dimethyl- 1Hpurine-2,6-dione), is an alkaloid which has different biochemical effects and is widely distributed in plant product and beverage in different ratio [1]. Human serum albumins (HSA) are the most commonly studied proteins in biochemical studies, human blood mostly contains HSA, which acts as drug carrier to different parts of our body [2] The interaction of theobromine with human serum albumin proteins were investigated for the first time by using a series of biophysical techniques and molecular modelling calculations. Time resolved fluorescence measurements confirm that theobromine quench the intrinsic tryptophan fluorescence of the proteins through a static mechanism. Irrespective addition of drugs decreases α-helicity of the proteins. The binding mechanisms of psychoactive stimulating drugs THB with human serum albumins were investigated by spectroscopic methods in combination with molecular docking calculation.

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Interaction of Caffeine with Human Serum Albumin

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Protein-ligand interactions are important in distributing and transporting small drug molecules in living systems. Therefore, understanding the molecular basis of these interactions is indispensable towards designing of new and more efficient specific therapeutic agents for improved drug action. Caffeine (1,3,7-trimethyl-1H-purine 2,6(3H,7H)- dione 3,7-dihydro-1,3,7-trimethyl-1H-purine-2,6-dione, CAF) is a bitter, white crystalline xanthene. Caffeine is the world's most widely consumed psychoactive substance, particularly in the Western countries, and believed to stimulate central nervous system. In fact, caffeine and its derivatives are known antagonists for both A1 and A2 – adenosine receptors in brain preparations; although with varying degree of effectiveness [1]. Caffeine influences the body water excretion mechanism when consumed in sufficient doses.

The modular structural domain of human serum albumin [HSA] to bind a series of exogenous drugs led to intense research towards understanding the forces responsible as well as comparative thermodynamic parameters for drug binding etc. HSA is a protein with the molecular weight of 66,500 containing 585 amino acid residues. However, there is only a single Tryptophan residue within HSA at the position of 214 in domain II, which makes it very convenient to study the protein intrinsic fluorescence [2,3]. Fluorescence spectroscopy is one of the most widely used techniques to achieve this goal because of its high sensitivity coupled with easy operational procedure. The results confirm that CAF binds preferentially to sub-domain IIA in the binding domain of the protein, this knowledge can lead to better understanding towards the mechanism of the binding processes as well as transport properties of caffeine in human plasma at the molecular level.

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P-72

Studies On The Synthesis Of Fluorinated Diazo Compounds And Their Electronic And Biological Effect

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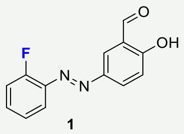
The introduction of a fluorine atom to organic compounds severally changes physical, chemical, and biological properties and due to this fluorinated compound have been widely used in different fields viz development of drugs, agrochemicals, and useful materials. Also, azo compounds have been widely used in drug designing since various of its analogs show promising anti-viral, anti-microbial, anti-biotic, and anti-cancer activities. So, here we are presenting our effort to the synthesis of fluorinated analogs of fluorinated diazo compounds and their studies on electronic properties, and physical and biological properties. To investigate we synthesized fluorinated and non-fluorinated analogs and compared their UV-vis absorption, thermal properties, and contact angle measurement. Further, we also investigated their anti-cancer activities. Here we observed that the presence of fluorine has a significant role in the few properties. All synthesized compounds are thoroughly characterized by different analytical techniques. To evaluate anti-cancer activity the cytotoxicity effect of these analogs was studied on both HCT-116 and A549 cells, and determined by MTT assay, which showed potent inhibitory activities in both cancer cell lines, A549 (7.01 ± 1.06) and HCT-116 (4.01 ± 1.06).



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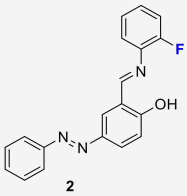

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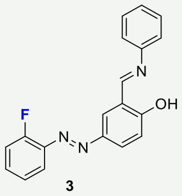

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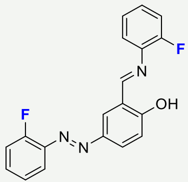

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P-73

Imino-phosphanamidinate and their Chalcogenide Derivatives as Potential Ligands to Synthesized Aluminum Complexes and their Utilization Towards Catalytic Hydroelementation Reactions

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Amidinate ligands have been used enormously in the field of coordination chemistry to stabilize different main group metals, transition metals, and lanthanides complexes as their steric and electronic property can be tuned by introducing different substitutions on the ligand backbone. [1] Recently, we developed various N-heterocyclic imine-based unsymmetrical imino-phosphanamide [NHI^{R}P(Ph)NHDipp] [R = Dipp (**1a**), Mes (**1b**), ^{t}Bu (**1c**), Dipp = 2,6-diisopropylphenyl, Mes = mesityl, and ^{t}Bu = *tert*-butyl] ligands which are structurally resemble with amidinate ligand. We also developed three aluminum alkyl complexes, [κ^2-{NHI^{R}P(Ph)NDipp}AlMe$_2$] [R = Dipp (**2a**), Mes (**2b**); ^{t}Bu (**2c**),], supported by imino-phosphanamide ligands (**1a**, **1b,** and **1c**) and investigated their catalytic efficiency towards catalytic guanylation reactions of carbodiimides with arylamines. [2]

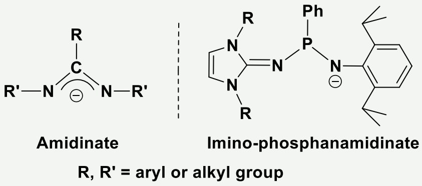

Figure 1. Amidinate ligand and imino-phosphanamidinate ligand.

Next we prepared the chalcogenide derivatives of imino-phosphanamide [NHI^{R}P(Ph)(E)NHDipp] [R = Dipp, E = S (**4a**), Se (**4b**); R = Mes, E = S (**4c**), Se (**4d**); R = ^{t}Bu, E = S (**4e**), Se (**4f**)] which give us a new set of ligand systems and can act as N, N- or N, E- donor monoanionic ligand (E = S or Se). Further we synthesized their corresponding aluminum complexes [κ$^2_{NN}$-{NHI^{R}P(Ph)(E)NDipp}AlMe$_2$] [R = Dipp, E = S (**5a**), Se (**5b**); R = Mes, E = S (**5c**), Se (**5d**)] or [κ$^2_{NE}$-{NHI^{R}P(Ph)(E)NDipp}AlMe$_2$] [R = ^{t}Bu, E = S (**5e**), Se (**5f**)]. All the compounds were characterized by multinuclear NMR spectroscopy and single-crystal X-ray diffraction analysis. Then the aluminum complexes **5a-5f** were tested as pre-catalysts for the hydroboration reaction of nitriles, alkynes and alkenes.

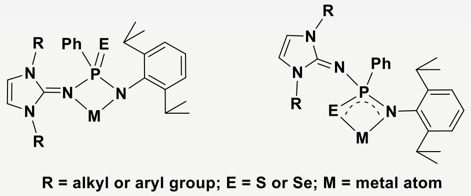

Figure 2. Different coordination modes of chalcogenide derivatives of imino-phosphanamidinate as ligand.

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P-74

Synthesis of a novel graft copolymer of plant peptone (Polymethylmethacrylate grafted plant peptone) and study of its flocculation characteristics in kaolin and coal fine suspensions

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A novel graft copolymer of plant peptone (PPEP) was synthesized by grafting methyl methacrylate monomer onto PPEP through microwave assisted technique. The synthesized graft copolymer was characterized by Intrinsic viscocity study, FTIR Spectroscopy, Elemental analysis, TGA-DSC and Scanning Electron Microscopy (SEM). Flocculation properties (Jar test and Settling test) of the grafted PPEP were performed in coal fine and kaolin suspensions for application as a flocculant in mineral ore processing.

P-75

Modulating the Electronics of Palladium Complexes Supported by Iminopyridine Ligands as The Catalysts in Suzuki-Miyaura and Heck-Mizoroki Cross-Coupling Reactions

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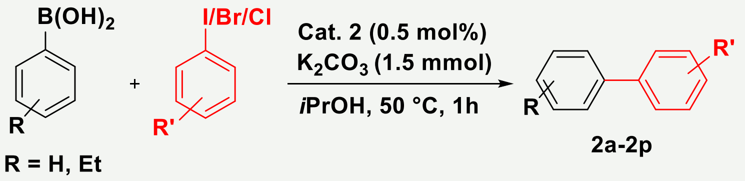
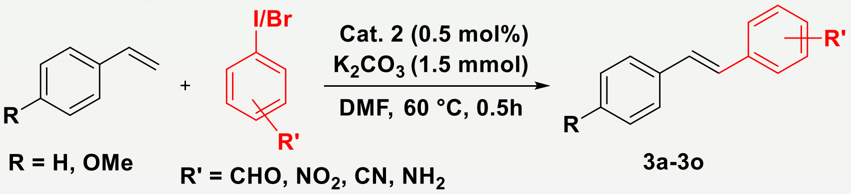
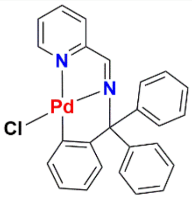
Two Bench stable palladium(II) complexes [κ^2-(PyCH=N(CHPh2)PdCl2)] (**1**) and [κ^3-(PyCH=N(CH(Ph2)(C6H4))PdCl)] (**2**) supported by iminopyridine ligands (PyCH=NR) [R = CHPh$_2$, (**L1**) and R = CPh$_3$, (**L2**)] were synthesised and utilised as the competent catalysts in the formation of C-C coupling products for Suzuki-Miyaura and Heck-Mizoroki reactions. The palladium complex **1** was obtained by the κ^2- coordination of the ligand **L1** to the palladium precursor whereas complex **2** was achieved by ortho-metallation of one of the phenyl groups present in ligand **L2** with the Pd metal under reaction conditions making the ligand κ^3-ligation to the metal center. Complex **2** exhibited an excellent catalytic efficiency at very low catalyst loading (0.5 mol%). The C-C bond formations of the desired products were obtained in high yield with low catalyst loading at mild reaction conditions. Wide varieties of substrate scopes were explored for the C-C bond cross-coupling reactions.

Suzuki-Miyaura coupling



Heck-Mizoroki cross-coupling





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References:

[1] (a) Suzuki *Angew. Chem., Int. Ed.*, 2011, **50**, 6723 —6737. (*b*) I. P. Beletskaya, F. Alonso and V. Tyurin, *Coord. Chem. Rev.*, 2019, **385**, 137 —173.

[2] C. Chong and R. Kinjo, *ACS Catal.*, 2015, **5**, 3238 —3259.

P-76

Titanium(IV) Complex as Promoter for Hydroboration of Esters and Nitriles

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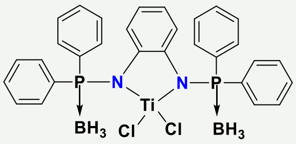
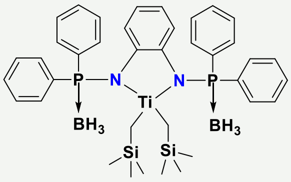
The reduction of carbonyls is among the most important and well-known transformations in organic synthesis, with ester functionalities being the most challenging to reduce when compared to aldehydes, ketones, and imines. The steric and electronic properties of ester moieties make their reduction more difficult. Titanium is largely present in the Earth's crust. This metal is inexpensive, easily accessible, biocompatible, and has low toxicity, owing to which it has found several uses in different catalytic reactions. The chemistry and catalytic activity of $TiCl_4$, $TiBn_4$, and Cp_2TiMe_2 are structurally known and they are relatively more pyrophoric and thus hard to handle.

Our group has a long-standing interest in amidophosphine ligands and their borane and chalcogen derivatives. For instance, their main group metal and early transition metal complexes have found many applications in homogeneous catalysis. The treatment of bis-borane ligand $[\{Ph_2P(BH_3)NH\}_2C_6H_4]$ in the presence of titanium tetrachloride ($TiCl_4$) [**1a**] in toluene followed by the addition of 2 equivalents of lithium hexamethyldisilazide $[LiN(SiMe_3)_2]$ furnished the Ti^{IV} complex $[\{Ph_2P(BH_3)N\}_2C_6H_4TiCl_2]$ [**1b**] as a dark red solid in 80% isolated yield. For the first time, we present the efficient reduction of alkyl and aryl esters, using a convenient titanium catalyst with excellent chemoselectivity and unique functional group tolerance.

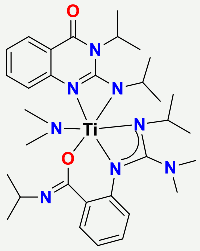


[**1a**]



[**1b**]

- 23 substrate scope
- Solvent free
- Room temperature
- Chemselectivity
- Yield up to 98%



Detailed kinetic studies are provided to determine the rate dependence on the concentration of catalyst, HBpin, and ester and proposed a plausible mechanism.

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P-77

o-Phenylene diamine based Schiff Base Complex of Cobalt as Electrocatalyst for Water Oxidation

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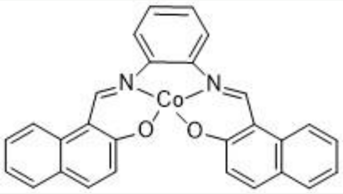
Earth abundant transition metal complexes may be a game changer in context of renewable energy production. Production of green energy has found a way in terms of Artificial Photosynthesis that mimics the process of energy production by green plants. extensive study in this regard has established the fact, that along with the CO_2 reduction, water oxidation is the major bottle neck of artificial photosynthetic energy production. Here in we report, one Cobalt-Schiff base complex which have shown promising results as an electrocatalyst for water oxidation. Different electrochemical techniques, e.g., Cyclic voltammetry, Linear sweep voltammetry, Differential pulse voltammetry, were studied for complex **1** to detect it's ability as a WOC. The ligand [*1,1'-((1E,1'E)-(1,2-phenylenebis(azaneylylidene)) bis(methaneylylidene)) bis(naphthalen-2-ol)*] and it's Cobalt complex were characterized by spectroscopic techniques such as FTIR, Mass Spectroscopy, UV-Vis Spectroscopy. Complex **1** was screened for the electrocatalytic water oxidation, proton reduction and carbon dioxide reduction. Results obtained from the CV, LSV and DPV indicates that the molecule is good electro catalyst for the water oxidation. pH dependence electrochemistry shows that the catalyst is highly active at pH 13.5.



Complex 1

REFERENCES:

[1] S.Sengupta,S.Naskar et.al Polyhedron 191 (2020) 114798

P-78

Extraction of Natural Dyes from Waste Flower and its Application as pH Indicator and pH Sensing

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India has a rich cultural and religious heritage wherein flowers such as marigolds, aster and roses are widely used in various ceremonies. As a result, floral waste is generated in large quantities and dumped into water bodies or improperly disposed [1]. This leads to breeding of harmful microbes since flowers have high carbon/nitrogen ratio and moisture content. Hence, these floral wastes can be utilized to relieve harmful effects from waste flower pollution. Again, the uncontrolled discharge of synthetic dyes into the aquatic ecosystem is a global environmental concern due to their negative Eco toxicological effects . Dyes obtained from different natural sources have emerged as an important alternative to synthetic dyes. Due to synthetic dyes' harmful effect, effort is now made to replace these dyes with natural dyes from waste flowers[2]. In this study, natural colorant were extracted from Gleblonis segetum (sample 1), Papaveraceae (sample2), Bouganvillea glabra (sample 3) and they were used as natural indicator in acid-base titration. The titration was performed separately using standard synthetic indicators such as phenolphthalein and methyl red. The end points obtained using natural and synthetic indicators were compared. Natural dyes extracted from sample1, sample2, sample3 produced visually distinct colour change at the end points of the titration. The present study displayed a practical procedure for obtaining suitable extract from waste flower as economic, accurate and environment friendly replacement for synthetic pH indicators in titrimetric analysis. Further, as the extract showed different colors at different pH, they could be used as a potential natural materials for pH sensing applications in different food industries or biomedical fields.

Reference:

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P-79

In vitro anti-cancer activities of Mn(II), Co(II) and Ni(II) complexes against K562, MCF-7 and DL cancer cells: Synthesis, characterization, crystal structures, and molecular docking studies

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Three new complexes [Mn(pfth)$_2$(o-phen)] (**1**) (Fig.1), [Co(pfth)$_2$(en)] (**2**) and [Ni(pfth)$_2$(en)] (**3**) based on a 4-phenyl-(2-furoyl)-thiosemicarbazide (Hpfth) ligand containing 1,10 phenanthroline (*o*-phen)/ ethylenediamine (en) as secondary ligands have been synthesized. The synthesized complexes have been characterized by various techniques. The tumoricidal potential of Mn, Co, and Ni salts, ligand Hpfth, and their complexes was evaluated against K562, MCF-7 (Fig.2), and DL cancer cell lines. Complexes **1** and **3** induce more growth inhibition as compared to complex **2** against all cancer cell lines. Complex **3** demonstrated impressive tumoricidal properties in a clonogenic assay in comparison to complexes **1** and **2**. These studies establish the role of metal centers in antiproliferative activities and reveal that Ni(II) complex exhibits more potent anti-tumoricidal activity. Molecular docking studies of Hpfth and complexes **1–3** were also performed against three target proteins.

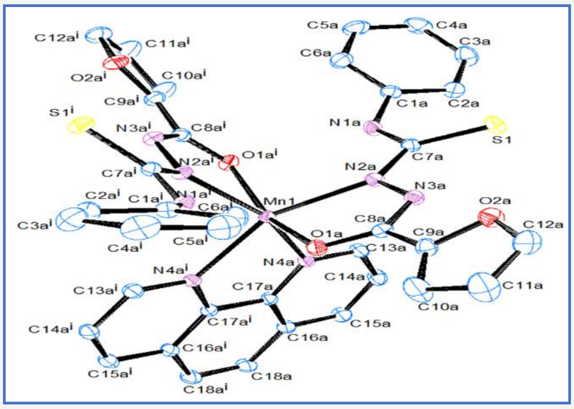

Fig. 1. ORTEP diagram of [Mn(pfth)$_2$(o-phen)] (**1**)

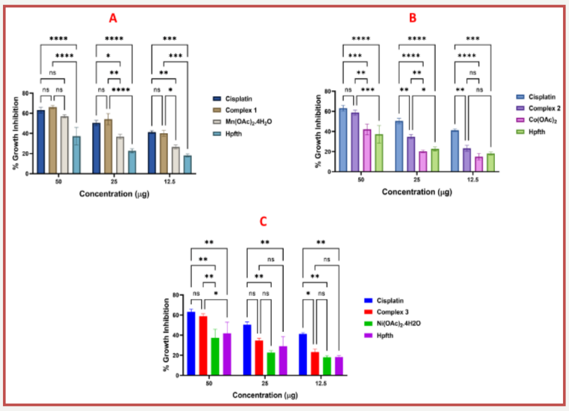

Fig. 2. Growth inhibition of MCF-7 cells

Keywords: *Antiproliferative activity, MTT Assay, XTT Assay and Molecular docking studies*

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P-80

Enhancing Chemotherapeutic Delivery to Tumor Cells with Surface-Coated Cerium Nanoparticles

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Cerium oxide nanoparticles have been more sought-after as a nanocarrier to enhance anti-cancer medications' delivery and therapeutic efficacy due to their antioxidant properties. Here, we present the production of alginate-coated ceria nanoformulations (ceria NPs) and their FTIR, Raman, and X-ray diffraction characterisation. When evaluated against the MDA-MB-231 breast cancer cell line at greater particle concentrations, the produced ceria NPs exhibit little inherent in vitro toxicity. We demonstrate a potential synergistic cytotoxic effect mediated by the drug and the ceria NPs after dosing these particles with doxorubicin (Dox) and paclitaxel (PTX), which leads to improved killing capacity as well as reduction of cell migration against the MDA-MB-231 cell line. Additionally, we coated the drug-loaded ceria NPs with the membrane of MDA-MB-231 cells using the extrusion approach in order to confirm the immune-escaping capacity before targeting cancer cells. The resulting delivery system demonstrated preferential in vitro uptake by the MDA-MB-231 cell line and demonstrated reduced uptake by the murine macrophage cell line (RAW 264.7), indicating its potential application as non-immunogenic personalized therapy in the targeting and killing of cancer cells.

P-81

Effects of Sintering on Hydroxyapatite at Different Temperatures

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The effect of sintering conditions on the microstructure, phase composition and mechanical properties of hydroxyapatite (HAp) was investigated at different temperatures 500 °C, 700 °C, 900 °C and 1200 °C. HAp powder was synthesized using calcium nitrate tetrahydrate and diammonium hydrogen phosphate as calcium and phosphorous precursor respectively. Then HAp pellets of 13mm diameter were prepared using Hydraulic press. Microwave sintering is reported to produce dense sintered HAp body with fine microstructure and improved mechanical properties [1]. The sintering time and sintering temperature both are known to show an effect on the morphology and particle size of HAp powders [2]. Various characterization was done; which includes phase analysis and compound formation using X-ray diffraction (XRD) studies, morphology analysis and elemental studies using Field Emission Scanning Electron Microscopy (FESEM), functional group detection using Fourier Transform Infrared Spectroscopy (FTIR), corrosion resistance in ringer solution, optical contact angle (OCA) and Brunauer-Emmett-Teller (BET).

From the characterization it was seen that as the temperature increases there was decrease in the pore size of the HAp pellets, the compactness and hardness also increased. All of these parameters indicated that HAp became more stable with the rising of sintering temperature.

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P-82

Warped Polycyclic Aromatic Hydrocarbons (PAH's): A Major Evolution in the field of Opto-electronic appliances

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Polycyclic aromatic hydrocarbons (PAHs) have been the subject of interdisciplinary research in the fields of chemistry, physics, materials science, and biology. These can effectively serve as model compounds of Graphene-Nanoribbons (GNR's) to understand how the structural features (e.g., size, edge configuration, and heteroatom incorporation) influence the electronic properties of GNRs.[1] Their application is also used in the making of nanowires, nanotubes, nanofibers; especially in nanoscience and nanotechnology.

The natural sources for most of the PAHs are found in coal, oil deposits, and thermal decomposition of organic matter. For example, in engines and incinerators or biomass burnt in forest fires. [2] Burning of coal and tobacco are also the sources of polycyclic aromatic hydrocarbons. In Laboratory, PAH's can be synthesized through chemical reaction via top down or bottom-up approach. The aromaticity of PAHs has been of great importance. [3]

All the opto-electronic applications requires a tunable semi-conducting material by tuning their molecular HOMO-LUMO gap. This property is much effectively exhibited by PAH which makes it an excellent material to be used in the organic electronic devices. PAHs are used as organic semi-conductors and they are the promising candidates in organic devices such as light emitting diodes (LEDs), Photo-voltaic cells and Field Effect Transistors.[4]

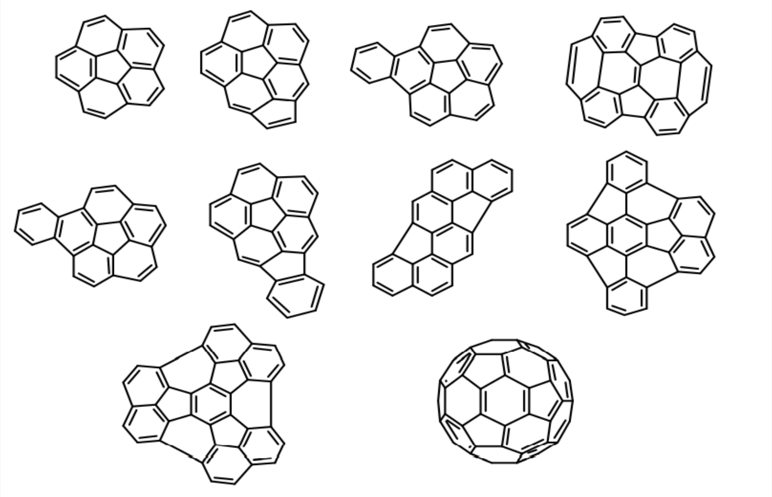

Figure1: *Examples of Geodesic Polyarenes*

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P-83

Green Chemistry Approach: Sodium Fluoride-Catalysed Highly Efficient One-pot Multicomponent Microwave Irradiation-Assisted Synthesis of Substituted Chromene Derivatives in Aqueous Medium

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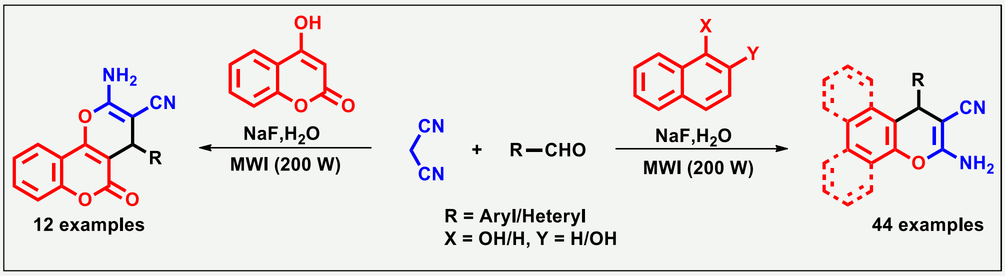
2-Amino-4*H*-benzo[*h*]chromene-3-carbonitrile and 2-amino-5-oxo-4*H*,5*H*-pyrano[3,2-*c*]chromene-3-carbonitrile are two important pharmacophores with extensive applications in medicinal chemistry. The multicomponent Knoevenagel-Michael reaction is one of the most efficient strategies to construct these two scaffolds. Previous efforts have been made in converting the traditional organic solvents to eco-friendly solvents including H_2O generally in the presence of complex catalysts. Here we present our work of using sodium fluoride (NaF) as catalyst to synthesize a wide scope of the two types of substrates starting from α- or β-naphthol or 4-hydroxycoumarin. Using NaF as a catalyst under microwave irradiation conditions, the reactions were completed within a short period with excellent yield. The reaction products were purified simply by washing with H_2O and can be further purified by crystallization with MeOH. The analysis of green chemistry-related parameters suggested that the current method was highly environmentally benign, highlighting the potential of this method in the use of drug discovery and development.



Keywords: Chromene, Green Chemistry, Microwave irradiation, Sodium fluoride, Water

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P-84

11-(4-(dimethylamino)phenyl)-3,3-dimethyl-2,3,4,5,10,11-hexahydro-1H-dibenzo[b,e][1,4]diazepin-1-one As Turn-Off Fluorescent Receptor for Detection of Picric Acid

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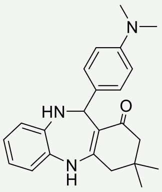
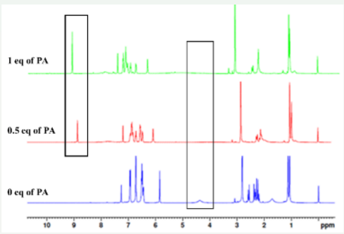
We have synthesized 11-(4-(dimethylamino)phenyl)-3,3-dimethyl-2,3,4,5,10,11-hexahydro-1H-dibenzo[b,e][1,4]diazepin-1-one (SPR) and demonstrated as turn-off fluorescent receptor for the detection of picric acid (PA). Compared with typical nitro explosive compounds of picric acid, the receptor SPR shows a great sensitivity for picric acid over other nitro aromatic explosive compounds. Moreover the detection limit toward picric acid was calculated to be low as 7.56×10^{-7} M in solution. Further it was demonstrated the receptor SPR in ^{1}H NMR Titration.



Receptor SPR



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P-85

Study of Microplastics as Emerging Pollutant and Development of Silica Functionalized Guar Gum Grafted Polyacrylamide For its Removal

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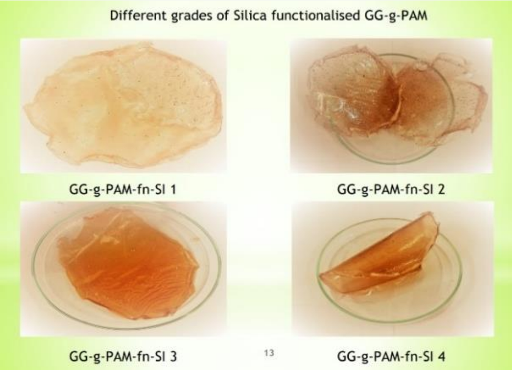
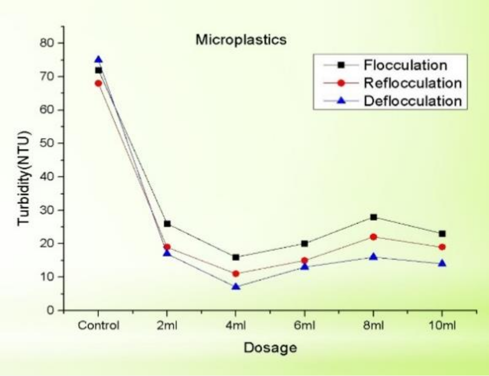
Plastic has become of the most concerning pollutants today. Not only is it a non-biodegradable and potentially carcinogenic pollutant, but it also leads to the generation of microplastics which is categorised as an emerging pollutant. Microplastics are plastic particles which are smaller than 5 microns in size. They are reported to have been found in various parts of the biosphere including human blood and tissues of various organs (1). Industrial and domestic effluents are two major contributing sources of microplastics in the ecosystem. Researchers are in search of an effective removal method for these microplastics as a large amount of microplastics escape from the various filtration processes of wastewater treatment plants (2).

This research is focused on the study of microplastics as an emerging pollutant and synthesizing guar gum grafted polyacrylamide functionalised with silica grains using a microwave-assisted grafting process as a flocculant for the removal of microplastics. Guar gum is a gum derived from the seeds of the guar plant (*Cyamopsis tetragonoloba*). Its polysaccharide chains are grafted on the polyacrylamide chain in a non-toxic and eco-friendly way using microwave radiations and ceric ammonium nitrate as a free radical initiator. For the flocculation process, 4 ppm of best grade flocculant in solution form was added to 500 ml of microplastic suspended water. It underwent a flocculation-electrocoagulation process under normal room temperature and pressure to achieve a removal efficiency of 92.64%. This indicates that modified polymers from plant-based polysaccharides can be used as effective biodegradable flocculants for the removal of microplastics.





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P-86

Base Catalyzed Sustainable Synthesis of Dihydroquinazolinones and Quinazolinones

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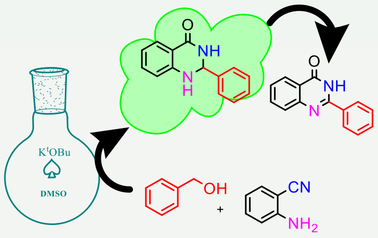
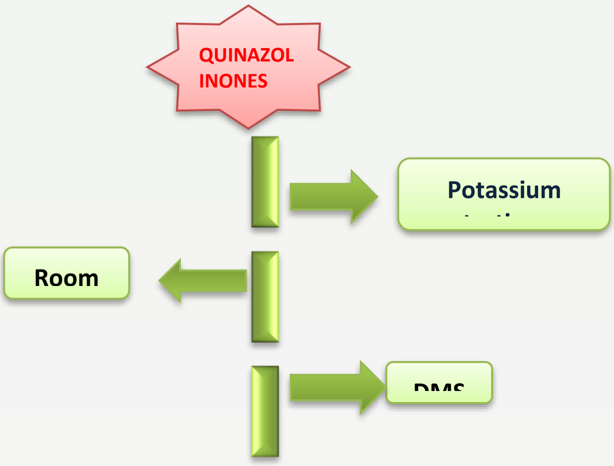
Quinazolinone is a principle part in various natural alkaloids and pharmaceuticals and has versatile biological activities. In contrast to the previous studies[1-4],we have modernized our synthetic pathway using metal-free and room-temperature reaction. Understanding the good monetary value, pKa value, and hygroscopic nature in the domain of bases, potassium tertiary butoxide[5] performed better compared to cesium hydroxide[4], revealing good productivity of quinazolinones. The reaction of benzyl alcohol and 2-aminobenzonitrile in the presence of K^{t}OBu in open air at room temperature afforded the quinazolinones, and in the absence of O$_2$ afforded the dihydriquinazolinones at rt. Mechanistically 2-aminobenzonitrile and benzyl alcohol were initially converted to 2-aminobenzamide and benzaldehyde respectively and further cyclization afforded the dihydroquinazolinones in the absence of O$_2$ and quiazolinones under oxidative conditions.





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P-87

Electrochemical Quantification of Hepatoprotective drug using CuO decorated Chitosan based Non-enzymatic Immunosensor

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This study discusses about the electrochemical quantification of Metadoxine (MTD) at Copper Oxide/Chitosan based nanocomposite modified glassy carbon electrode (CuO/CH/GCE). The electroactive surface was produced by drop-casting a CuO/CH nanocomposite suspension in DMF onto the non-enzymatic electrode surface. The nanocomposite was characterised by XRD, XPS, EDX, TEM, Raman and FESEM techniques. EIS technique was utilised to study the enhanced charge transfer phenomenon occurring at the surface of modified sensor. A one-electron/proton oxidation process of MTD at CuO/CH/GCE was dependent on pH of supporting electrolyte, scan rate and concentration of MTD. The optimised voltammetric response is observed in the BR buffer at pH 2.5, with an occurrence of an irreversible diffusion-controlled phenomenon. The anodic peak current is proportional to the MTD concentration within the range of 1.99 µg/L to 19.95µg/L, with a LOD 0.64 µg/L and LOQ 2.14 µg/L. The applicability of proposed method to determine MTD in pharmaceutical formulation and human blood serum was successful. This study was conducted first time with a high detection limit and MTD have no interference with common ions, carbohydrates and heavy metals. Thus, this is a novel sensor and it can be used for the detection of different electroactive compounds.

Keywords: Metadoxine, Voltammetry, CuO, Chitosan, Immunosensor, non-enzymatics

P-88

One-Pot Synthesis of Dihydropyrimidin-ones/-thiones catalyzed by Magnesium Perchlorate Hexahydrate Catalyzed and Mechanistic Study via DFT calculations

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The 3,4-dihydropyrimidin-2(1H)-one (DHPMs) are admirable scaffolds for a wide range of physiologically significant compounds. Biginelli's reaction is a simple example of a multi-component reaction from which DHPMs can be produced. [1] Herein we described a simple and efficient method to synthesize a series of dihydropyrimidin-ones and thiones through Biginelli's one-pot multicomponent condensation reaction. [2] We explored $Mg(ClO_4)_2.6H_2O$ as a Lewis acid catalyst to promote the Biginelli reaction. Indeed, the results showed that the catalyst plays a crucial role in synthesizing biologically active dihydropyrimidin-ones/thiones due to the stabilization of the polar intermediates via coordinating carbonyl functionalities. The reaction mechanism was studied using the Mass spectroscopy [3] and DFT Calculations. [4] The reaction is very efficient and afforded a variety of dihydropyrimidin-ones/thiones with good to excellent yield in a shorter reaction time.

Keywords: Magnesium Perchlorate, One-pot synthesis, Biginelli's synthesis, DFT Calculations

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P-89

^{89}Zr-Radiolabelled monoclonal antibody as diagnostic biomarker: Synthesis and In-vivo studies

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Molecular biomarkers can be used to monitor, image, and measure biological processes at molecular or cellular level. Different types of biomarkers are known, including diagnostic, prognostic, and predictive biomarkers, or a combination of these. Specific uptake of molecular biomarkers can be achieved using radiolabeled targeting agents such as antibodies, directed against tumor-associated antigens like epidermal growth factor receptor (EGFR), human epidermal growth factor receptor 2 (HER2), and many others. The high specificity and affinity of radiolabeled antibodies make them attractive candidates as an imaging agent such as ^{89}Zr-labeled antiHER2 antibodies can be used to differentiate between HER2^{+} and HER2^{-} tumors, also appreciating intra and inter-tumoral heterogeneity. For antibody based PET imaging ^{89}Zr has several advantages as ^{89}Zr has a half-life of 78.4 h which matches the pharmacokinetics of antibodies.

Produced ^{89}Zr via ^{89}Y (p, n) ^{89}Zr was purified using Hydroxamate based solid phase media and isolated in the form of ^{89}Zr-oxalate. The ^{89}Zr-oxalate was chelated with modified mAb (Rituxmab) via DFO-Squaric acid linker and purified using size exclusion column (PD10 column). The radiolabelled mAb's quality assurance was performed and its in-vitro stability was analysed its chelation stability. The in-vivo studies were performed to study the pharmacokinetic as well pharmaco-dynamic profile in healthy Wistar rat at different intervals.

The cyclotron produced^{89}Zr via ^{89}Y (p, n) ^{89}Zr was isolated in good radionuclidic purity and chelate with modified DFO tagged mAb (DFO-Sq-Rituxmab) in good yield with high specific activity. All the QC analyses (HPLC, iTLC, ϒ-well counter) were performed and qualify. The in-vivo studies were performed and bio-distribution among different organs at different point of time were analysed.

Key Words: Zirconium-89, Radioisotope, biomarker, Immuno-PET

P-90

Efficient Utilization of Rice-Wheat Straw to Produce High Value Biofuels

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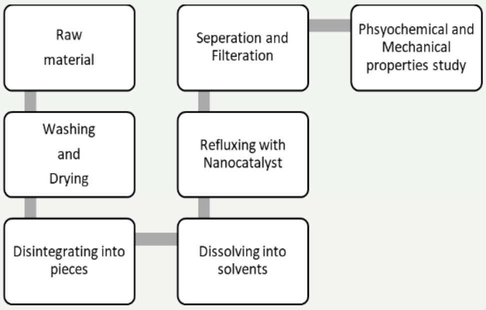
Today when we live in an era where our primary source of energy, fossil fuels is on the verge of depletion and the impact they had been creating in the environment is almost ineradicable. Biofuels as a proficient solution are renewable source of energy which has less carbon footprint and can be used without any modification or can be blended with the conventional fuels in required ratios. According to a survey based on Food and Agriculture Organization grain production data of 2009 we produce 727,400 Kton of straw/a and 583,776 Kton of straw/a in the cultivation of rice and wheat worldwide respectively which are of very less importance and are eventually discarded. Through this we aim to study the efficient conversion of superfluous rice-wheat straw to valuable biofuels. Among various nanocatalysts such as metal oxides based nanocatalyst, nanozeolite, magnetic nanocatalyst we aim to design an optimized pathway for high yield production of biofuels. With the help of oxide based nanocatalyst we aim to conduct a comparative study on better productivity and better selectivity. Along with the efficient production of the biofuel its physiochemical and mechanical properties studies have to be performed. Measurement of density, viscosity, cetane number, saponification value, acid value, iodine value, flash point has been done (1). For better productivity and optimization of the process effects of methanol to oil ratio, reaction temperature, reaction time, particle size, solvent, catalyst weight and moisture content have been evaluated (2). Through this we aim to study the efficient conversion of superfluous rice-wheat straw to valuable biofuels.



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P-91

Synthesis and Characterization of Pd-Co Bimetallic Anode Catalyst for Direct Ethanol Fuel Cells

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Sustainable energy development is a major challenge, particularly when considering population increase, rising energy demands resulting from the excessive use of non-renewable fossil fuels, and growing consequences on global pollution and climate change. It is critical to continue to develop new sources of renewable and clean energy. Direct alcohol fuel cell (DAFC) represents a technological approach that meets all the requirements in terms of energy conversion with good electrical efficiency and lower emissions of pollutants. The use of low molecular weight alcohols as energy sources has many advantages: they are liquids, which simplifies their storage and transport. They have high energy densities, which means that small amounts of these compounds provide large quantities of energy compared to conventional fuels. However, it largely suffers from the poisoning of the anode catalyst caused by the accumulation of intermediate products. Propanol oxidation reaction on Pt catalyst has been widely studied. Development of anode materials using nanostructured conducting polymers-based support plays a vital role in reducing catalyst loadings. In a nutshell, this review will give readers a thorough understanding of the principles of direct alcohol fuel cells.

Key Words: Direct propanol fuel cell, Electro oxidation, Electro catalyst, Palladium-Cobalt, Bimetallic

P-92

Storage and stabilization of biomolecules in nanotubular ionic covalent organic framework

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Covalent organic frameworks (COFs) are an emerging class of crystalline porous material synthesized by linking organic building blocks through dynamic linkages. Ordered structure, permanent porosity, tunability, and high chemical stability have made COFs a highly interesting class of materials with potential applications in gas storage, molecular separation, catalysis, energy storage etc., with new horizons being explored regularly [1]. In this work, we have studied the applicability of COFs as a potential medium for storage and stabilization of sensitive biomolecules. Various classes of biomolecules like Ribo-nucleic acids (RNA) are prone rapid degradations in extracellular environments. Traditionally these are preserved by storing in cryogenic condition, in liquid nitrogen or at -20 ^{o}C to -80 ^{o}C. A more convenient approach will be their storage at room temperature. Recent studies have shown that ionic liquids (ILs) can be used as an efficient solvent for storing various proteins, biopolymers and enzymes [2]. Tulsiyan *et al.* in an recent mechanistic study showed that RNA is stabilized in choline amino acid based ILs through an interaction with the cationic charge of the IL [3]. But ILs suffer from various drawbacks like toxicity and high vapor pressure, which makes recovery of the biomolecules from the IL solution a hectic process. Herein, we have prepared an imine linked ionic COF with nanotubular morphology. Encapsulation of the biomolecules inside the COF and favorable interaction with the positive charge leads to their preservation in room temperature. The loading activity of the ionic COF is compared with another non-ionic COF with similar pore size. The ionic nanotubular COF exhibited higher loading capacity and extended stabilization compared to the non-ionic COF.

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P-93

Identification of pharmacological agents that enhance energy expenditure to counter metabolic diseases

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Adaptive thermogenesis can increase energy expenditure as well as help to counter metabolic disorders such as type II diabetes, obesity, cardiovascular disease and fatty liver disease. There are numerous reports focus on UCP1 driven thermogenesis, but little is known regarding UCP1-independent thermogenesis in muscle and adipose tissue. Our study focused on capsaicin derived analogues, because capsaicin has a good interaction with SERCA revealed by molecular docking. So we are trying to check whether capsaicin derived analogues can increase energy expenditureby decreasing the palmitate-induced insulin resistance in C2C12 cells and improved insulin sensitivity in nicotinamide-streptozotocin induced mice. Mechanistically, capsaicin derived analogues treatmentsignificantly increased PI3K/AKT and AMPK phosphorylation, which helps in enhancing glucosetransporter 4 expression. Capsaicin derived analogues lowered fasting glucose, insulin, leptinlevels, and markedly reduced the impairment of glucose tolerance in nicotinamide-streptozotocin induced mice.In conclusion, our data can unveil the unknown mechanism of capsaicin derived analogues in myotube and suggest a possible therapeutic molecule that can reduce insulin resistance.

P-94

Utilizing serum metabolites as indicators of metabolic disease status in mouse model of sedentary lifestyle

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As advancement of technology, people are adapting to sedentary life style not only in developed but also in developing countries. These changes influence the social behavior, mental well-being and more over metabolism of our body. As per the latest National Family Health Survey (NFHS-5) data in 2019-21, obesity is prevalent in Indians with one out of four people being overweight and heading to metabolic disease such as diabetes and vascular disease. Most of the metabolic researchers focus on the effect of diet, exercise and drug to balance the metabolism, but a few researchers focused on the kinetics of metabolites in body. So, from a classical standpoint, we can propose that metabolites have role in progression of metabolic diseases due to obesity. Towards this hypothesis, we have tried to gain insight about metabolic pathways involved in two contrasting life style adaptation (restricted sedentary and endurance physical exercise) model. Metabolic profiles of sera were obtained using high-resolution 1D 1H CPMG NMR spectra. The metabolic profiles were compared using multivariate statistical analysis to identify the disease specific metabolic disturbances associated with obesity and, therefore, the perturbed biochemical pathways in this condition. Many metabolites are deviated from the control group specifically amino acids and the results will be explained in the conference.

P-95

Cnaphalocrocismedinalisinfestations in Oryzasativa (L.) and its control through cationic polymer based RNAi technology

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Rice is a major crop widely cultivated in the south-east Asian countries including India. It is a staple food for majority of the Indian populations and holds economic, social, and cultural values. Pest infestations in the crop are a major hindrance in agriculture thereby leading to a large scale loss in the yield. Cnaphalocrocismedinalis is a common pest in the rice plant that has led to huge losses in rice yield in several countries. Use of chemical pesticides offers short term solution and is also accompanied with several adverse effects on the crop as well as the environment. The current work aimsto develop a cationic polymer (CP) based formulation to control C. medinalis infestations in rice crops via RNAi mechanism. The cationic co-polymer was synthesized under oxygen limiting conditions followed by guanylation [1]. Oligonucleotides (GapmeR) were designed to specifically target the hexokinase gene in C.medinalis through post-transcriptional gene silencing. The GapmeR was able to silence the hexokinase gene in cell lines of SF9 confirmed through qPCR studies.The CP was used for complexation with the GapmeR at varying concentrations (N/P ratio). DLS studies indicated an N/P ratio of 8:1 and 16:1 as suitable for the complexation process. The data was successfully cross-verified by running the complexes in a 1.5% agarose gel. The GUMA at a concentration of 10 ppm was applied on soil collected from the rhizosphere of the rice plants grown under greenhouse conditions. Chemical parameters such as pH, E.C, O.C, N, P, and K were studied after 5 days of application. The results showed no substantial changes in the chemical profile of the soil thus implying no harmful effects of the GUMA on the soil environment. Impact of the GUMA on different plant biochemical parameters was analysed. The polymer was found to have no significant effect on the plant. The work further aims to use the final formulation via conducting feeding assays on C. medinalisin vivo.

Keywords: Cationic polymer, Pest control in rice plants, Post-transcriptional gene silencing, RNAi mechanism, Sustainable agricultural practice

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P-96

Exploring molecular machinery of interaction between Sarcoplasmic Reticulum and mitochondria as targets to reduce the pace of sarcopenia

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Sarcopenia is aging-related muscle loss that is very gradual and most prominent is the skeletal muscle. Muscle loss not only impairs mobility of the individual but also it is closely associated with (may be predisposes to) variety of metabolic diseases. Research mostly focused on the effect of diet and exercise to promote healthy aging and retard the process of muscle loss but the interplay of skeletal muscle organelles and their role in aging has been not been studied in details. We are targeting two of the key players in muscle metabolism and function: Mitochondria and Sarcoplasmic Reticulum (SR). In this study, we focused on the development of SR, mitochondria, and their interplay through aging by using neonates and old rats as models. We used histological techniques to elucidate the position of the mitochondria in relation to the SR and using a technique called Proximity Ligation Assay (PLA) as a tool to study the developmental regulation of propinquity between SR-mitochondria. For PLA we have used mitofusin 1 (located predominantly in SR) and 2 (located predominantly in mitochondria) as our baits to analyze developmental regulation of SR-mitochondria proximity. Based on SDH (Succinate Dehydrogenase) staining we find that neonates don’t have a clear distinction of fiber types and have evenly distributed SDH expression pattern but adults have specific arrangements of glycolytic and oxidative fibers, the SDH expression is mostly seen in the peripheral region of oxidative fibers. These studies will open the door to targeting SR-mitochondria interaction to deter aging-related muscle loss.

P-97

Design, Synthesis and *In silico* Studies of Substituted Dibenzopyrrocolines Alkaloids: A Promising Scaffold as Anti-Alzheimer's Agents

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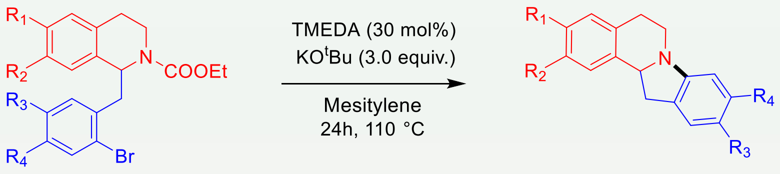
Alzheimer's disease (AD) is a prevalent irreversible neurological disorder and seen in age dependent dementia which results in cognitive impairment.[1] Currently, the potent treatment agent for AD is acetylcholinesterase inhibitors (AChEIs), which increases the cholinergic neurotransmission in the synaptic cleft by inhibiting degradation of ACh.



1

2

Dibenzopyrrocolines
(Upto 88% yield)

Herein, we report a new, highly efficient TMEDA-catalyzed decarboethoxy C-N bond forming methodology for selective synthesis of substituted dibenzopyrrocolines from precursor **1**. *In silico* studies of various analogues of **2** were carried out against the protein **4ey7** present in the binding pocket of AchE enzyme. The docking studies revealed that the analogues of **2** were found to be more potent than the standard drug Donepezil. The details of the study will be presented.

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P-98

Domino Synthesis of Novel 3-Alkenyl Benzofuran Derivatives- Base Mediated Condensation Cascade Reaction: A Greener Approach.

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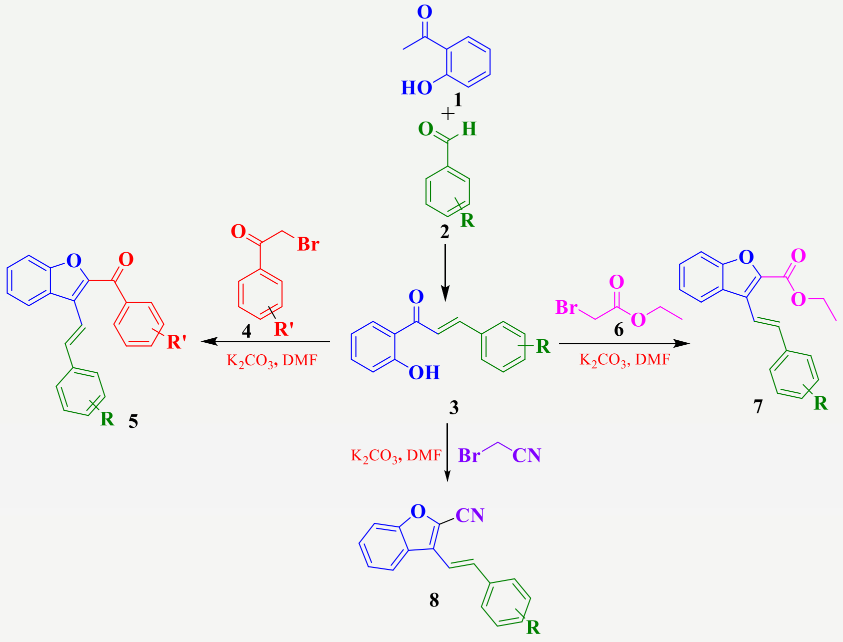
Choice of mode - Poster Presentation
Name of Presenter – Surbhi
DOB – 8TH June, 1994

Abstract: Benzofuran is a well-known oxygen-containing fused heterocyclic scaffold and a key part of many natural and therapeutically important synthetic molecules. A one-pot and an efficient construction method for pharmacologically relevant molecular structures, 3-alkenyl benzofuran with excellent yields, has been developed using a greener approach. Products are obtained from 2-hydroxy chalcone with phenacyl bromide, Bromo acetonitrile, and/or ethyl-2-bromo acetate via an alkylation followed by a condensation reaction. This methodology features faster condensation over Michael addition, transition metal or catalyst-free medium, and an environmentally friendly synthetic route toward the synthesis of substituted 3-alkenyl benzofurans.



No additives/catalysts/oxidant
Mild, with broad substarte scope
Synthesis of Novel 3-Alkenyl Benzofuran Derivatives
Synthesis of bioactive molecules
37 examples

P-99

Characterization of Electrochemically Deposited Palladium-Cobalt Bimetallic Anode Catalyst for Direct Ethanol Fuel Cells

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The growing energy and climate crisis inspires one of the greatest challenges of the 21st century—developing novel power sources. The direct ethanol fuel cell (DEFCs) is a portable device and has the potential to produce much higher energy density than lithium-ion rechargeable batteries. The greatest drawback of this technology is the lack of electrocatalyst that would enhance reaction kinetics and good stability under process conditions. In this research, bimetallic palladium-cobalt (Pd-Co) anode catalysts were investigated as bifunctional anode catalysts with enhanced efficiency and stability toward the direct electrooxidation of ethanol in an alkaline medium. X-ray diffraction, field emission scanning electron microscopy and energy-dispersive spectroscopy were employed for the in-depth characterization of the nanocatalysts synthesized by galvanostatic electrodeposition technique. Electrochemical analysis like cyclic voltammetry (CV), chronoamperometry (CA) and electrochemical impedance spectroscopy (EIS) revealed improved electrocatalytic activity, excellent stability and very low charge transfer resistance (R_{ct}) toward the anodic oxidation of ethanol. The superior catalytic activity is related to the reduced poisoning on the catalyst surface induced by the synergistic effect of the bimetallic catalysts and altered Pd electronic structure by the incorporation of Co.

Key Words: Direct ethanol fuel cell, Electrooxidation, Electrocatalyst, Palladium-cobalt, Bimetallic

P-100

A Novel Approach for the Syntheses of Thiocarbamates Employing Copper-Polyaniline Nano-composite

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Thiocarbamates are an important class of compounds, displaying a wide range of potential applications as pharmaceuticals such as anti-AIDS, anti-cancer, anti-fungal, antibacterial, analgesic, hypnotic, anti-diabetic agents and have also been emerged as potential agrochemicals such as herbicidal, pesticidal, bactericidal, fungicidal agents. Thiocarbamates also play a key role in biology as bioregulators, enzyme inhibitors and an excellent building blocks for the synthesis of the many pharmaceutically important drugs and natural occurring biologically active compounds. Thiocarbamates have also been employed as useful synthon for the synthesis of thiophenols, thiols and other important biologically important scaffolds and also serve as starting material for the Newman-Kwart rearrangement. Keeping the view of the great importance and wide potential applications, their syntheses has been become the focus of organic chemists worldwide.

Traditionally, thiocarbamates have been synthesized through a two-step reaction of phosgene/triphosgene with amines and thiols and by direct carbonylation of amines using carbon monoxide(CO) and disulfides or elemental sulfur. In recent years, many methods for the syntheses of thiocarbamates have been reported employing disulfides, isocyanides, thiols, thiosulfonates, N-substituted formamide, sulfonyl chloride, sodium sulfinates etc. acting as starting materials in different type of reaction medium either catalyst or catalyst-free conditions. However, the reported methods have been associated with several drawbacks like harsh reaction conditions, longer reaction times, uses of strong bases, costly and toxic reagents, less atom economy, industrially unfavourable conditions etc. Therefore, there is continued interest in developing novel methods for their syntheses. In the present paper, we are reporting an efficient and novel approach for the synthesis of thiocarbamates through the reaction of amines, alkyl halides, carbonyl sulfide employing Cu-polyaniline nanocomposite catalyst

(**Scheme 1**).

Scheme 1

P-101

Design and docking studies of Phenothiazine clubbed triazole compounds

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Cancer is a worldwide issue and needs a good therapeutic agent. Phenothiazine is heterocyclic ring with a wide range of activities and triazoles are well known moiety present in many biologically active molecules. Clubbing both the moieties together could produce better active molecules. We in this work have designed twenty phenothiazine clubbed 1,2,3-triazole compounds and explored them for their *in silico* inhibition of cancer associated proteins human topoisomerase IIα and aromatase. Compounds a1, a2 and a12 produced best *in-silico* inhibition of both the proteins with binding energy (ΔG) less than -10 Kcal/mol. Further studies are necessary to explore the biological properties of these compounds.

Keywords: Docking, triazoles, phenothiazines, clubbing, designing

P-102

Click Chemistry and its Applications in Organic Chemistry

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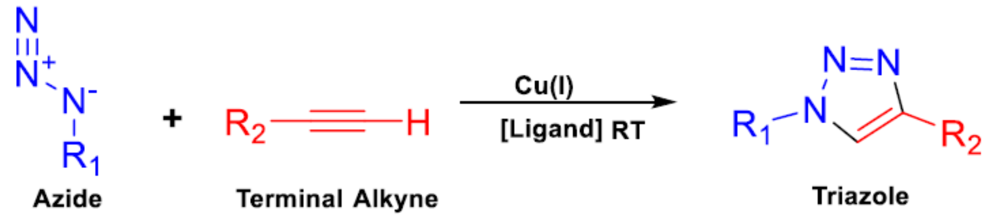
“Click chemistry” is a synthetic, modern approach to the assembly of new molecular entities. This powerful strategy is very convenient and relies mainly upon the construction of carbon heteroatom bonds using “spring-loaded” reactants which can be naturally available; otherwise, it can also be synthesized in the petrochemical industry in bulk quantities. Its growing interest in the field of chemistry has an immense impact and can be found in almost all areas from drug discoveries to bioconjugation; to electronic semiconductors and material science. The Cu(I) catalyzed- 1, 2, 3-Triazole formation by the reaction of an azide with a terminal alkyne has become a golden standard of Click chemistry due to its reliability, specificity and biocompatibility. In 1998, the term "click chemistry" was coined by K. Barry Sharpless, and to recognize the importance of click chemistry in modern days applications the Nobel Prize in Chemistry in the year 2022 was jointly awarded to Carolyn R. Bertozzi, Morten P. Meldal and K. Barry Sharpless, "for the development of click chemistry and bioorthogonal chemistry".



Scheme 1: The Cu (I)- catalyzed alkyne- azide cycloaddition (CuAAC) "Click" reaction

P-103

Molecular docking and anticancer studies of benzimidazole clubbed 1,2,3- triazole derivatives

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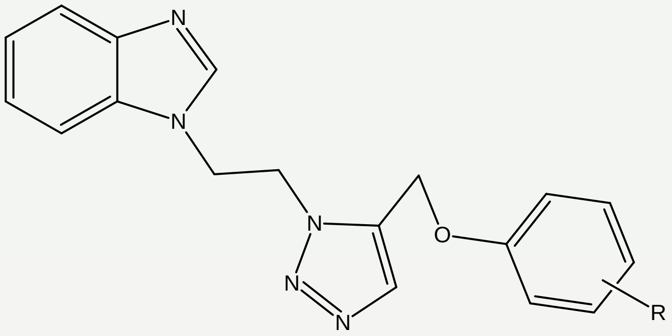
Cancer is a disease in which abnormal cells divide uncontrollably and destroy body tissue. The primary anticancer medications recently approved are antibody drug conjugates (ADCs), small molecule inhibitors of oncogenes, and antibodies. Due to its substantial applicability in numerous areas of chemistry, scientific community have paid attention to the 1,2,3-triazole fused heterocyclic compounds. A variety of biological activity, including antibacterial, anti-HIV, antiallergic, anti-fungal, cardiovascular, anti-leishmanial, and chemotherapeutic properties, have been reported in 1,2,3-triazole fused heterocyclic compounds. Novel compounds of 1,2,3-triazole fused benzimidazole derivatives were synthesized and then characterised using a variety of spectroscopic techniques including NMR, FTIR, and Mass Spectroscopy. All the new analogues for EGFR target cell lines underwent in silico studies. Molecular docking and ADME was performed for the most potent compounds in the active site of EGFR.

Keywords: Benzimidazole, 1,2,3- triazole, Click reaction, Molecular docking, EGFR



P-104

Molecular docking analysis of *Erigeron annuus* and *Nerium indicum* against MAPK pathway

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The proto-oncogene RAS, which generates the 21 kDa protein, is mutated in 20% of lung cancers (p21). Lung cancer survival prediction is still debated. Lung cancer remains a top killer despite advances in detection and treatment. Only 10% survive five years. However, patient or tumour circumstances may change the prognosis. Many cancer therapies are hazardous and cytological. Alongside cutting-edge cancer treatments, phytochemicals are being investigated. Many Indian and other nations use *Nerium indicum*, a valuable medicinal herb, as a folk treatment. *Nerium indicum's* flowers and leaves have been used in traditional Chinese medicine for its anti-cancer, anti-neoplastic, and anti-inflammatory effects. The local *Erigeron annuus* (E. annuus) plant may treat diarrhoea, epidemic hepatitis, enteritis, lymphadenitis, and haematuria. Thus, repurposing these two herbs for anti-cancer treatments may be novel. This study docked phytoconstituents from these two plants to RAS protein receptors. Our in-silico protein-ligand interaction may help discover the cell death induction threshold for repurposing medications to treat lung cancer.

Keywords: *Erigeron annuus*, *Nerium indicum*, RAS, lung cancer, *in-silico*, phytoconstituents.

P-105

Synthesis of benzofuran clubbed 1,2,3- triazole derivatives as an anticancer agent and it's in silico studies.

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Choice of mode: Poster presentation

ABSTRACT

Cancer is one of the deadly diseases, not a single disease but a combination of more than hundreds of diseases where the normal cells become abnormal, divide rapidly and invade other tissues. Benzene ring fused with five membered heterocyclic ring i.e.,furan collectively called Benzofuran. Triazoles are five membered ring with three nitrogen and two carbon atoms capable of forming hydrogen bonds. The structure possesses numerous biological activities viz antiviral,anti-fungal,anti-tuberculosis,anti-convulsant,anti-depressant,anti-inflammatory,anti-cancer activities.

We design and synthesize novel Benzofuran clubbed 1,2,3-Triazole derivatives 8a-8s(19 derivatives) and screened for their anticancer activity against four human cancer cell lines such as human lung carcinoma(A549), human breast carcinoma(MD-MB-231), human prostate carcinoma(DUI145) and normal human lung cell line(MRC5) by employing MTT colorimetric assay. These compounds showed good to moderate activity on tested cell lines. Among them, compound(8g)(N,N-diethyl-2-((2-(4-(isopropoxymethyl)-2,5-dihydro-1H-1,2,3-triazol-1-yl)(phenyl)methyl)benzofuran-6-amine)showed potent anticancer activities against A549, MD-MB-231, DUI145 and MRC5 cell lines with IC50 values of 2.9±0.84μM, 1.1±0.84μM, 3.3±0.80μM and 45.3±1.65μM respectively. These compounds could serve as basic template for anticancer drug development. The molecular docking was applied to explore the binding affinity and correlate its docking score at EGFR active site.

Keywords: Benzofuran, triazole, cancer cell lines, MTT assay, anti-cancer activity.

Symposium Theme: Synthetic/Medicinal Chemistry
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P-106

Structural Studies on the Hsp90-Cdc37-Cdk4 Modulator Using Molecular Dynamics

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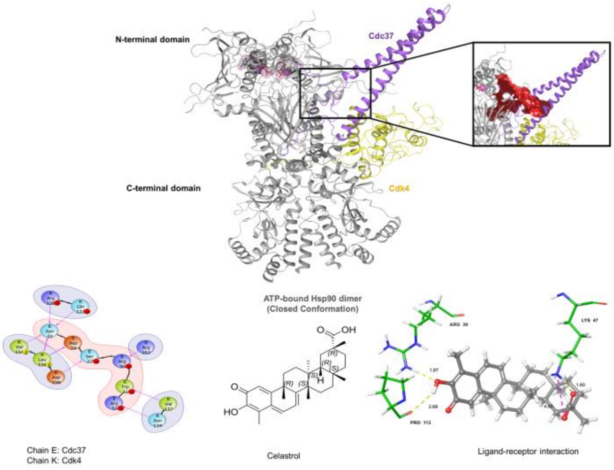
Abstract

The dynamic structure of Hsp90 allows it to bind to co-chaperones and client proteins, thus posing as a fundamental research target. Modulating interfacial interactions by drug-like molecules, thus causing instability in the Hsp90-Cdc37-Cdk4 complex, can inhibit Hsp90's ability to carry out its biological function. Celastrol, previously reported as a non-N-terminal ATPase inhibitor, has been investigated as an Hsp90-Cdc37 modulator. However, it is challenging to determine the precise binding location of celastrol as no co-crystal structures are available for other domains. Thus, we employed a computational approach to predict an active site, a new exploration at the interface of Hsp90 and Cdc37. The probable active site has been evaluated based on the site mapping parameters, followed by docking of the ligand at the site. Further, the binding of celastrol at the interfacial active site has been validated by performing molecular dynamics, yielding satisfactory results. Identification of the active the site, molecular docking, the study of non-covalent interaction in ligand-receptor docked complex and structural validation by molecular dynamics has been performed with Schrödinger Suite 2022.

Authors acknowledge the High-End Computation Facility and Schrodinger Software support from BIT Mesra.



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P-107

Study of agonistic behaviour shown by MeTC7 in Vitamin D receptor

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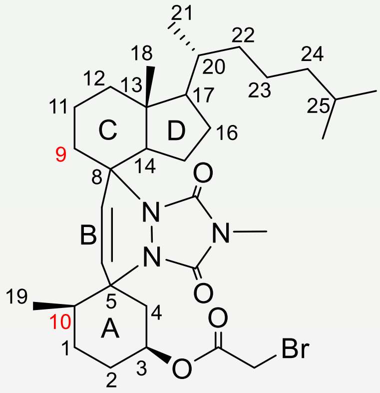
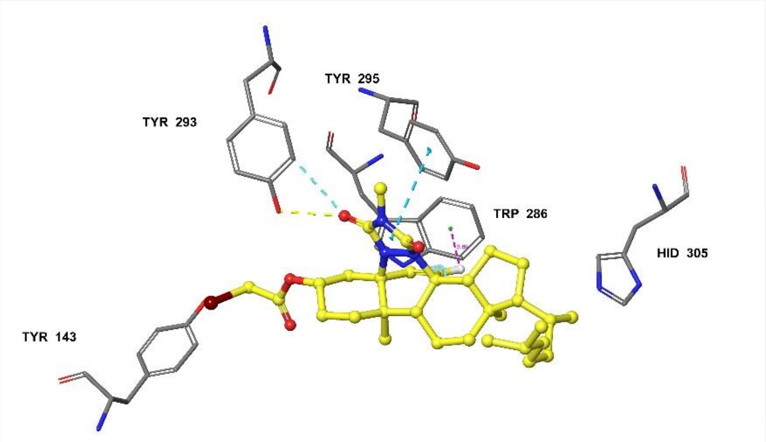
Abstract

The vitamin D receptor (VDR), a member of the nuclear receptor superfamily, mediates the biological activities of 1,25-dihydroxyvitamin D3, the active form of vitamin D. It controls calcium homeostasis, immunity, cellular differentiation, and a variety of other physiological functions. Calcitriol is the active form of Vitamin D in the body. A ring, a conjugated linker, as well as a flexible chain mediated by hydroxy groups is critical for Calcitriol's hyper agonistic behaviour. MeTC7's chemical structure is a structural equivalent of Calcitriol; however, it is bigger in size and has a more conformationally stiff system. The Induced Fit docking approach was employed to dock the MeTC7 to the calcitriol site in the VDR, followed by side-chain modification using Prime3 to provide receptor flexibility based on binding mode. Calcitriol's agonistic behaviour is heavily influenced by histidine and arginine residues. The loss of the conjugated linker system in MeTC7, followed by a reduction in the distance between rings in contrast to Calcitriol, is an important element in MeTC7 interactions and behaviour. Thus, the triazolidine-dione moiety and a hydrophobic N-methyl group occupy the same spatial location inside VDR as the hydrophilic hydroxy group of calcitriol. Thus, MeTC7 has carbonyl groups that engage with certain residues to enhance MeTC7's strong binding.

Authors acknowledge the High-End Computation Facility and Schrodinger Software support from BIT Mesra.





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P-108

Design, Synthesis, and Anticancer Activity of Benzoxazolone fused 1,2,3-triazoles derivatives

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Choice of mode- Poster presentation

ABSTRACT

Cancer is the uncontrolled growth and development of cells in the body and is one of the foremost reasons for death throughout the world. Triazoles and Benzoxazolone have received the most attention from researchers due to their favored chemotherapeutic and pharmacological use. Benzoxazolone fused 1,2,3 - triazole derivatives showed various biological activities such as analgesics, anti-inflammatory, and anti-cancer. In the present work, we have prepared benzoxazolone fused 1,2,3-triazoles using click chemistry and evaluated their cytotoxicities and anti-cancer properties in human cancer cell lines A549, MCF, as well as the normal cell line PC3. The basic benzoxazolone fused 1,2,3-triazole substitution pattern was maintained, allowing for the synthesis of derivatives with a wide range of various atoms and functional groups as substituents. A total of eight compounds were prepared and the structures of these compounds were characterized by FT-IR, elemental analysis, 1H NMR, and Mass spectrometry (EIMS). Cytotoxicities of all the target compounds were investigated by MTT assay. MTT results showed that compounds were effective in terms of reduction of cell viability. All cancer cell lines were shown to be most susceptible to compound C4. Furthermore, molecular docking studies were performed for the most potent compounds in the active site of EGFR. It could be concluded that benzoxazolone fused 1,2,3 - triazole derivatives increase potential anti-cancer effects and they could be promising novel therapeutic agents for chemotherapy.

Keywords: 1,2,3- Triazoles, Benzoxazolone, Anticancer activity, Click Chemistry, Molecular docking.

P-109

Design, Synthesis, and Evaluation of Purmorphamine Analogues for Structure-Activity Relationship Studies at Second Position of Purine Scaffold in Hedgehog Pathway

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Choice of mode- Poster presentation

ABSTRACT

Hedgehog (Hh) pathway is a developmental pathway that is involved in organogenesis, stem cell maintenance, tissue repair, and regeneration. The Hedgehog signaling pathway is a signaling pathway that transmits information to embryonic cells required for proper cell differentiation. It plays a significant role in embryonic development and the overall growth and morphology of insects and vertebrates. Inappropriate Hh signaling can result in developmental diseases. Diseases associated with the malfunction of this pathway include basal cell carcinoma (BCC). Somatic genomic modification in genes encoding members of the pathway supports the development and maintenance of several cancers, especially basal cell carcinoma and medulloblastoma. The study aimed to design, synthesize, and evaluate Purmorphamine analogs for structure-activity relationship studies at the second position of the purine scaffold in the hedgehog pathway. The structures of the products were characterized by IR, H^1NMR, and Mass spectroscopy. The synthesized compounds were evaluated for in-vitro cytotoxicity on A549 cells by MTT assay at a single concentration of 20μM. The structure-activity relationship of purmorphamine at the second position showed potent activity that induces osteogenesis, cell proliferation, cell repairing, and cell maintenance by activation of the hedgehog signalling pathway.

Keywords: Hedgehog, Purmorphamine, MTT Assay, Cytotoxicity, A549 cells.

P-110

Identification and Characterization of Genes Underpinning Heat Acclimatization in Wheat

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The unanticipated harsh weather conditions have a significant impact on wheat productivity during flowering and grain filling phase. As a result, heat acclimatization at a non-lethal high temperature may protect against subsequent high temperature stress. Heat acclimatization has been primarily studied in rice yet reports describing their molecular function in wheat progenitor species is still unexplored. The aim of the current work is to identify the potential heat acclimatization genes (HAGs) in progenitor species of wheat that were well known to adapt themselves in temperate regions. A total of seven genes were identified from *Triticum durum* L. and *Aegilops tauschii*. These genes were then characterized for their physiochemical properties, domain and motif analysis, cellular localization, exon-intron distribution, phylogenetic tree construction, nuclear localization signal and chromosomal localization. Plaza analysis indicated that all the HAGs have orthologous sequence in *Triticum dicoccoides*, *Secale cereale* and *Brachypodium distachyon* showing the presence of similar heat acclimatization domains in other monocot plants. Thirty-six *cis*-regulatory elements including hormone, stress and tissue specific regulation were detected in the upstream regions of HAGs. Gene ontology study revealed their participation in biological, cellular and molecular processes. The result furnishes the fundamental knowledge on characterization and molecular function of HAGs in *Triticum durum* L. *and Aegilops tauschii.* This will further help plant breeders in developing new wheat lines with high potential to express the desired heat stress tolerant phenotype under field conditions.

Keywords: Heat acclimatization, *Triticum durum* L., *Aegilops tauschii*, Wheat

P-111

Identification of circular RNA and their Targets in leaves of *Triticum aestivum L.* under leaf rust pathogenesis

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Abstract

Wheat (*Triticum aestivum* L.) is a major food crop that suffers significant losses due to leaf rust caused by the fungal pathogen *Puccinia triticina* Eriks. When this fungus attacks wheat plants, hundreds of genes are involved in stress (biotic and abiotic) response experience regulated expression. This regulation partly depends on the vital member of the endogenous non-coding RNAs (ncRNAs) family, viz. circular RNA (circRNA). These are covalently closed-loop single-stranded RNA molecules ubiquitously expressing in eukaryotes, associated with diverse biological processes, and interact with microRNA(miRNAs) or proteins. In this study, we performed a genome-wide identification of circRNAs using ribosomal-depleted RNA-sequencing (RNA-Seq) of susceptible (S) wheat cultivar HD2329 and its resistant (R) NIL (HD2329 +*Lr*28) at 0 h pre- inoculation and 96 h post-inoculation (as S0/S96 and R0/R96). In total, 73 circRNAs were identified through CIRI(circular RNA identifier) tool, in which 52 circRNAs are differentially expressed (DE) in susceptible wheat cultivars against resistant wheat cultivar. Still, only 31 circRNA targeted the disease responsive 22 miRNAs using the psRNATarget tool and act as miRNAs sponges. The BLAST2GO analysis of the targeted transcripts describes that the circRNAs were estimated to be presumed mostly in defense responsive process, response to external stimulus, response to molecule of fungal origin, auxin-activated signaling pathway, and regulation of transcription. These processes are directly responded through metal ion binding, hydrolase activity, DNA binding, ATP binding and protein kinase activity. Hence, here, we revealed the possible complexity of the regulatory circRNAs and may open a window for understanding the functions of circRNAs in plants, especially in wheat against biotic stress.

Keywords: *circularRNA, miRNA Sponge, Defense response, biotic stress.*

P-112

A proportional multivariate analysis of azoreductase enzyme: a combination based computational approach

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Azoreductases are azo dye degrading enzymes, widely present among bacterial and fungal species and in few plant species. Azo dyes are extensively used in textile and various dyestuff manufacturing industries, from where these are released into the environment as pollutants that are not readily degraded. Using azoreductase-based biodegradation of azo dyes has been considered as a potential sustainable method. However, detail studies on azoreductase enzyme in terms of diversity, structure and substrate binding ability are not yet available and thus much needed for better understanding and effective application. In present study, we have carried out a computational comparative study using coding gene sequences, amino acid sequences and three-dimensional structures of azoreductases from different bacterial, fungal and plant species. Evolutionary and structure sequence co-relation pattern analysis with the help of phylogenetic trees generated using coding gene and amino acid sequences, multivariate analysis of codon and amino acid usage, motif analysis, and molecular dynamic simulation was performed. Phylogenetic tree reveales numerous small clusters for discrete sequences of bacteria, fungi and plants, wherein half of the fungal species taken in consideration remained in one clade cluster while others were grouped among bacteria clade cluster. The results show presence of highly conserved amino acids F25, D42, L43, P49, N88, Y110, K122,G114, L118, Y146, F153, G155 and E165 among bacterial species and significant similarities in the active site of the enzymes among different species. These outcomes have good potential to design new enzymes using site-directed mutagenesis for better efficacy in industrial application.

P-113

Effect of Lead Substitution on Electronic and Charge Transport Properties in Low-Dimensionaluble Perovskites

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Over a decade, significant development has been seen in the application of organic-inorganic hybrid perovskite-based semiconductors in the field of optoelectronics. The power conversion efficiency (PCE) of perovskite-based solar cells has crossed the benchmark value of 25% whereas, in the case of green and red light-emitting diodes (LEDs), the external quantum efficiency (EQE) was recorded at over 20%. Even after showing such extraordinary performances the commercialization of perovskite-based devices is yet to be realised due to the degrading tendency of the material. The degradation can be induced by several external factors like moisture, applied voltage, heat, or even the electrode used. Subsequently, research has shifted from regular 3D perovskite materials of the type ABX_3 to quasi-2D materials of type $A'_2A_{n-1}B_nX_{3n+1}$ ($1 \leq n \leq \infty$), which of late gained a lot of attention to make environmentally stable perovskite material. This is because in quasi-2D perovskites the bulky and insulating A′ cation acts as an alternating barrier layer and thus creates multiple quantum-well structures which are in a way imparts significant structural tunability for optoelectronic applications. In this report, we have developed lead-based quasi-2D perovskite, $(BA)_2PbBr_4$ (BA= benzylammonium), and two other analogs by partially or completely replacing lead with monovalent silver (Ag) and trivalent bismuth (Bi) atoms in a double perovskite structure via mechanical grinding method. The structure and morphology of the as-prepared samples were fully characterized by powder X-ray diffraction (PXRD) and field-emission scanning electron microscopy (FESEM) techniques while optical properties were analyzed by UV-vis absorbance and photoluminescent (PL) spectroscopy. Further, the conductivity of all the samples was measured under ac and dc techniques. The nature of point defects present in these three samples varied with the composition as observed in positron annihilation spectroscopy (PAS).

Keywords: Perovskites, quasi-2D, quantum-well, defects, positron annihilation spectroscopy

P-114

Understanding the Structural Basis of Hsp90-Cdc37-Cdk4 Modulator

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Hsp90 has emerged as a potential research target due to its structural flexibility allowing it to bind to co-chaperones and client proteins, and its significance in the design of anti-cancer drugs. The co-chaperone, Cdc37, binds to the Cdk4 client protein and stabilizes the Hsp90-Cdc37-Cdk4 protein complex. Disruption of the stability of the protein complex may substantiate the hypothesis to prevent the folding of the misfolded conformation of Cdk4. Experimental studies have reported that celastrol modulates the Hsp90-Cdc37 interactions. Since, it is difficult to design drug-like molecules for targets involving protein-protein interactions due to many reasons, one of being highly hydrophobic, it is crucial to study the interfacial interactions present in the Hsp90-Cdc37-Cdk4 complex. The protein complex are computationally investigated for probable active site at the interface of Hsp90-Cdc37, followed by docking of the ligand at the site. The identified binding site, hotspot residues, and non-covalent interaction profile open the scope for drug candidate discovery to explore this new target. Investigation of the interfacial interactions, identification of the active site, molecular docking, and study of non-covalent interactions in ligand-receptor docked complex has been performed with Schrödinger Suite 2022.

Authors acknowledge the High-End Computation Facility and Schrodinger Software support from BIT Mesra.

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Design, Synthesis and Application of Novel fluorescent Bis-heterocycles Based on Imidazo[1,2-*a*] pyridine and Benzimidazole

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A novel fluorescent bis-heterocycle based on Imidazo[1,2-*a*]pyridine and Benzimidazole is designed, synthesized, and characterized. The benzimidazole moiety can serve as a multifunctional unit whereas imidazo[1,2-*a*]pyridine has been widely employed in drugs, few medicines in use: zolpidem for insomnia, alpidem for hypnosis, zolimidine for gastric protection, miroprofen as an analgesic. Both the moieties are merged in a single molecule bridged by a phenyl ring to obtain an extension of conjugation to enhance the fluorescent properties. For the synthesis of these fluorescent bis-heterocycles, a greener method has been employed involving green solvents, fewer by-products, no production of hazardous chemicals, and less time taking. Along with the greener method, microwave irradiation is preferred over conventional heating and refluxing. Microwave irradiation provides uniform heating at the molecular level and attains high temperatures safely in less time.[1] After achieving the desired molecules, they were characterized and progressed for photophysical studies. In photophysical studies, the behavior of molecules in different environments such as different solvents, aqueous medium, viscous environments and a broad range of pH was studied and found them pH sensitive, working at pH neutral to basic. The molecules are intended for application as pH-sensitive probes for conditions like alkalosis.[2]

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P-116

Synthesis and Structural Elucidation of Novel Indolizine Derivatives as an anti-tubercular Agent: *In-silico* Target Identification Through Molecular Modeling and Computational Approach.

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A novel series of diversely substituted indolizine were designed and will be synthesized and evaluated for their in vitro anti-mycobacterial activity against H37Rv. The series of Ethyl 3-Benzoyl-7-(Piperidin-1-yl) Indolizine-1-Carboxylate Analogue by reacting pyridine containing heterocyclic ring compound 4-(piperidin-1-yl)pyridine with phenacyl bromide forming quaternary pyridinium N-ylide in the presence of acetone and further these N-ylide reacts with different acetylenes underwent 1, 3-dipolar cycloaddition with potassium carbonate and N, N- dimethylformamide as a solvent at room temperature. The *H37Rv* strain will be tested against the substituted indolizine analogues. *In-Silico* Screening like drug likeness, pharmacokinetics, and toxicity prediction will be done for the novel synthesized indolizine scaffold. Molecular target identification by computational methods. Docking studies were performed for identification of binding affinities against proteins like 5OP9 which shows the designed molecules have good binding affinity compare to the reference Isoniazid. All the synthesized novel indolizine derivatives were characterized by Spectroscopic techniques such as 1H NMR, 13C NMR, Infrared spectroscopy, and mass spectroscopy.

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Magnetic nanocomposite and its dye removal kinetics

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Over the last decades, industrialization and urbanization have caused an increment in toxic contamination, such as dyes in water sources. The removal of such dye from water resources is required in the context of environmental remediation. The present work aimed to effective removal of aniline blue (AB, an anionic dye), magnetic nanocomposite of almond gum grafted poly acrylamide crosslink N, N'-methylene bis(acrylamide) (Amg-g-PAM-cl-MBA/Fe_3O_4) were synthesized Nezami et al. [1] and characterized. The Amg-g-PAM-cl-MBA/Fe_3O_4 nanocomposite was used as an efficient adsorbent for the removal of aniline blue from an aqueous solution. The impact of various factors such as contact time (0-3 hr), different dosage (0.01-0.4 gm), varying pH (2-12), different concentrations of dye solution (10 -60 mg/l), and the temperature (25-55°C) was investigated Saberi et al.[2] . The kinetic isotherms and thermodynamic parameters of adsorption were also studied. The magnetic nanocomposite hydrogel provides an effective tool for environmental remediation.

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P-118

Polymer hybrid MOFs for the treatment of mining effluents

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Metal Organic Frameworks (MOFs) are hybrid materials comprising of metal ions coordinated with organic ligands. MOFs are considered an efficient candidate for catalysis owing to their high surface area, tunable porosity and high stability. He et al. [1]. MOFs have been extensively investigated for numerous applications like gas storage, gas separation, sensing, drug delivery and water treatment. Li et al. [2]. Encapsulation of MOFs with hydrogels give rise to material with high absorptive capacity and hydrophilicity. Yang et al. [3]. In the present work we aim to synthesize polymer-based MOF hydrogels using Zr-fenugreek as a precursor and chelating Zr with 5-aminoisophthalic acid and its applications in water treatment for mine effluents and emerging contaminants.

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Hetero-doped poly aromatic hydrocarbons (PAHs) based next generation organic-electronic development

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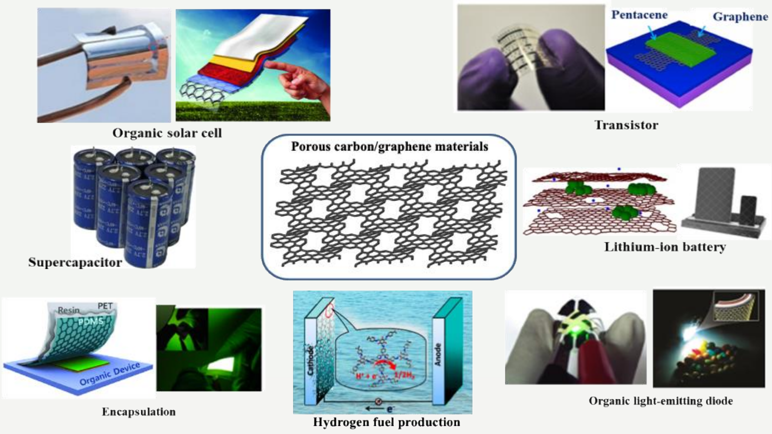
In the last quarter century, research on polycyclic arenes (PAs) [1] has seen a remarkable renaissance in the literature as compound accessibility and characterization have been made easier with the advent of modern synthetic methods and instrumentation, respectively. [2] One key motivation for this resurgence lies in PAs' unique optical and electronic properties due to their inherently high levels of π- conjugation, and delocalization. [3] These attributes make PAs useful for a variety of material applications, such as organic light-emitting diodes (OLEDs), field-effect transistors (OFETs), and photovoltaics (OPVs). [4] Devices such as OLEDs and OPVs are constructed around a donor-acceptor interface between an organic donor layer and an organic acceptor layer. Generally, acene-type molecules such as pentacene and anthradithiophene behave as organic p-type (electron-donating) compounds. There are considerably fewer organic n-type (electron-accepting) structures in the literature. Thus, there is a pressing need for new molecular frameworks that can transport electrons.



Top-down techniques give giant ribbons; bottom-up organic syntheses may lead to designed graphene nano ribbons of controlled geometries. The Scholl reaction is a special, yet not fully understood, chemical tool since it yields efficiently to the graphitization of long and flexible polyphenylene precursors. Even highly twisted structures may be obtained preferentially despite the possibility of forming less crowded isomers. After discovering this unexpected regioselectivity, we initially used it to create polyhelicenic species [5].

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