32nd ISCB International Conference ISCBC-2026

SUSTAINABLE ADVANCES IN CHEMICAL AND BIOLOGICAL SCIENCES

ABSTRACT BOOK

12 - 14 May, 2026

Department of Chemistry,
Indian Institute of Technology (BHU), Varanasi, India

Jointly Organized by:
Indian Society of Chemists & Biologists (ISCB)
Department of Chemistry, IIT (BHU) Varanasi

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ISCBC-2026

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आचार्य अमित पात्रा
निदेशक
Prof. Amit Patra
Director

Message

It is a matter of great pride and joy to learn that the Department of Chemistry, Indian Institute of Technology (BHU), Varanasi, is hosting the 32nd International Conference of Indian Society of Chemists and Biologists on Sustainable Advances in Chemical and Biological Science (ISCBC-2026) during May 12-14, 2026. This distinguished event reflects the department's continued commitment to advancing scientific knowledge and innovation in chemical biology and medicinal chemistry.

In recent years, chemical biology and medicinal chemistry have become increasingly important in overcoming the challenges posed by various health problems. Chemical biology and medicinal chemistry together have solved many of the health issues. Yet, challenges remain in overcoming the drug side effects and drug resistance problems.

ISCBC-2026 brings together leading researchers, industry experts, and young scholars from across the globe to exchange insights, discuss recent breakthroughs, and foster collaborations that will shape the future of drug development through optimized chemical biology and medicinal chemistry. Such interactions are vital for translating research outcomes into practical solutions that benefit society at large.

I extend my warmest congratulations to the organizing committee for their dedication in convening this important conference and curating a platform for rich academic and professional exchange. I am confident that the participants will find the discussions intellectually stimulating and that their stay in the ancient, spiritually vibrant city of Varanasi will be both memorable and inspiring.

I wish ISCBC-2026 grand success and look forward to its valuable contributions to the field of chemical biology and medicinal chemistry.

(Amit Patra)
Date: 30th April 2026

संस्कार ही शिक्षा Education is Character

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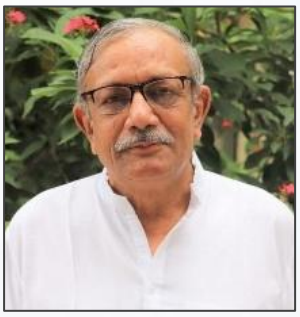

Prof. (Dr.) Anamik Shah
President, ISCB

Prof. (Dr.) PMS Chauhan
General Secretary, ISCB

Message

We are delighted to announce that the Indian Society of Chemists and Biologists (ISCB), Lucknow, is hosting the **32nd ISCB International Conference (ISCBC-2026)**. This prestigious event is being jointly organized by **Indian Society of Chemists and Biologists** and the **Department of Chemistry, Indian Institute of Technology (BHU), Varanasi**, and will take place at **IIT (BHU), Varanasi, India, from May 12 to 14, 2026**.

The central theme of ISCBC-2026 is "**Sustainable Advances in Chemical and Biological Sciences**." The conference will bring together researchers to discuss ground-breaking advancements in these fields, with a focus on fostering innovation to enhance healthcare practices and environmental sustainability.

Renowned scientists and researchers from across the globe will join as keynote and invited speakers, with over 100 senior scientists and professors presenting insights into cutting-edge developments and innovations in healthcare.

The scientific committee will compile an abstract book showcasing the diverse presentations featured during the conference. We extend our heartfelt gratitude to the organizing committee for their invaluable contributions in making this event possible. The conference aims to facilitate meaningful discussions on emerging trends, opportunities, and future directions in scientific research, creating a vibrant platform for collaboration and knowledge exchange.

The comprehensive program will include plenary lectures, invited talks, and panel discussions by eminent scientists from India and abroad. Young researchers will have the opportunity to present oral talks, and poster sessions will highlight the contributions of Ph.D. students and budding scientists.

We warmly welcome national and international delegates from research organizations, universities, academic institutions, and pharmaceutical companies. We hope all participants enjoy a memorable stay in Bhubaneshwar. In closing, we extend our sincere thanks to the members and office bearers of the organizing committee for their dedication to the success of ISCBC-2026.

ISCBC-2026

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SCIENTIFIC PROGRAMME

Tuesday, May 12, 2026

Venue: Dev & Vardhana Goswami Lecture Hall Complex, IIT (BHU)

7:30-8.30 AM	**Registration and Breakfast**
8.30 AM - 9.30 AM	**Inaugural Session** **Venue: HALL-IA**
9.30 AM – 9.50 AM	**High Tea**

Session – I
Venue: HALL-IA
Chairpersons: Dr. PMS Chauhan and Prof. Sundaram Singh

PL-1 9.50 PM - 10.25 PM	**Anamik Shah** President, ISCB Former Vice Chancellor, Gujarat Vidyapeeth, Ahemdabad, India Founder, National Facility for Drug Discovery Centre, Saurashtra University, Rajkot, India **Major API & Pharma Products through Flow Chemistry Processes: An untaped potential for Academic Research**
PL-2 10.25 AM - 11.00 AM	**Anil K. Singh** Professor (Ret.), Indian Institute of Technology Bombay, Powai, Mumbai, India **Sustainable Approaches and Strategies for Design and Development of Platform Chemicals and Novel Molecules**

Parallel Session – II A
Venue: HALL-IA
Chairperson: Dr. Manisha Malviya

KL-1 11.00 AM - 11.25 AM	**Rupam Dinda** Professor, Department of Chemistry, National Institute of Technology, Rourkela, Odisha, India **Anticancer Metallodrugs: Solution Stability, Protein Interaction, and Cellular Localization**
IL-1 11.25 AM - 11.45 AM	**Biswadip Banerji** Multidisciplinary Organic Synthesis Laboratory, Chief-Scientist, HOD, Central Instrumentation Facility (CIF), Indian Institute of Chemical Biology (CSIR-IICB), Jadavpur, Kolkata, India **Targeting Glioma with Hybrid PARP-1 Inhibitors via DNA Damage and ROS Generation**
IL-2 11.45 AM - 12.05 PM	**T. Kumaraguru** Senior Scientist, Biocatalysis Lab, CSIR-IICT, Hyderabad, India **Biocatalysis at the Chemistry–Biology Interface: Enabling Sustainable Technologies**
IL-3 12.05 PM - 12.25 PM	**Ananthalakshmy Sundararaman** Scientist C and Ramalingaswami Fellow, Rajiv Gandhi Centre for Biotechnology (RGCB), Thiruvananthapuram, Kerala, India **Mitochondria-derived Vesicles and Mito-nuclear Trafficking of Proteins in the Heart**
IL-4 12:25 PM - 12.45 PM	**Suman K. Barman** Department of Chemical Sciences, Indian Institute of Science Education and Research Mohali, Punjab, India **Asynchronous Transition State Tuned from Remote Site for Nitrite Reduction at Copper Centre**
IL-5 12:45 PM - 01.05 PM	**Sanjay Kumar** Professor, Department of Chemistry, Birla Institute of Technology and Science, Pilani, K K Birla Goa Campus, Goa, IndiaDrug discovery research in India: Current trends and analysis of Industry-Academia and Government collaborations
01:05 PM - 2.15 PM	**Lunch**

Parallel Session – II B
Venue: HALL-2A
Chairperson: Dr. Arindam Indra

KL-2 11.00 AM - 11.25 AM	**Nashreen S. Islam** Professor, Department of Chemical Sciences, Tezpur University, Tezpur, Assam, India **Highly Selective and Sustainable Oxidation of Biomass-Derived 5-HMF to HMFCA over Polymer-Supported Vanadium- and Tungsten-Based Catalysts**
IL-6 11.25 AM - 11.45 AM	**Anjali Patel** Head, Chemistry Department, Associate Director, M S University of Baroda, Vadodara, Gujarat, India **From Monotherapy to Dual Therapy: Engineered nMCM-48 based hybrid systems for controlled delivery of antidiabetic drugs**
IL-7 11.45 AM - 12.05 PM	**Biswarup Chakraborty** Associate Professor, Department of Chemistry, Indian Institute of Technology Delhi, New Delhi, India **Mechanistic Insight into the Electroreduction Pathway of Nitrate to Ammonia on Metal Oxides**
IL-8 12.05 PM - 12.25 PM	**Ashutosh Kumar Mishra** Associate Professor, Department of Chemistry, Indian Institute of Technology Hyderabad, Telangana, India **Tuning the functional properties of flavin entity for biological applications**
IL-9 12:25 PM - 12.45 PM	**Sarika Singh** Senior Principal Scientist, Toxicology & Experimental Medicine, CSIR-Central Drug Research Institute (CDRI), Lucknow, India **Natural Products as Dual-Target Agents: Bridging UPR and Redox Signaling**
IL-10 12:45 PM - 01.05 PM	**Ashoke Sharon** Professor, Department of Chemistry, Dean of Faculty Affairs (DoFA), Birla Institute of Technology, Mesra, Ranchi, India **Drug Discovery Approaches through Structure, Computation and Chemistry: A Case Study on Anti-CoVID Molecule Development**
01:05 PM - 2.15 PM	**Lunch**

Session – III : Wiley Sponsored
Venue: HALL-IA
Chairperson: Prof Anamik Shah

PL-3 2.15 PM - 2.50 PM	**Abhishek Dey** Professor, Indian Association for the Cultivation of Science (IACS), Kolkata, India **Functional Modelling of Cytochrome P450**
PL-4 2.50 PM - 3.25 PM	**Dibyendu Das** Associate Professor, Chemistry Sciences, Indian Institute of Science Education and Research, Kolkata, India **Non-equilibrium self-assembly for living matter-like properties**
PL-5 3.25 PM – 4.00 PM	**Sergii RUDIUK** CNRS researcher (CR), Associate Professor PSL/ENS, Department of Chemistry, Ecole Normale Supérieure, PSL University, Paris, France **Hybridization, Compaction and Coacervation of DNA : from photocontrol to applications in bio- and nanotechnology**
PL-6 4.00 PM - 4.35 PM	**Mariana Nadirova** Application Technology Manager, Apeiron Synthesis, Wroclow, Poland **Metathesis reaction in modern industry: A technical lense on sustainable and efficient synthesis**
4.35 PM - 4.50 PM	**Tea**

Session – IVA
Venue: HALL-IA
Chairpersons: Dr. Asha Gupta

IL-11 4:50 PM - 5.10 PM	**Biswajit Mondal** Department of Chemistry, Indian Institute of Technology Gandhinagar, Gujarat, India **Cooperative Catalysis in Electrochemical Ammonia Oxidation**
IL-12 5.10 PM - 5.30 PM	**Bhupesh Goyal** Associate Professor, Department of Chemistry & Biochemistry, Thapar Institute of Engineering & Technology (Deemed to be University), Patiala, Punjab, India **Computation-Driven Rational Design of Peptides as Inhibitors of Human Islet Amyloid Polypeptide Fibrillation in Type 2 Diabetes**
IL-13 5.30 PM - 5.50 PM	**Anirban Pradhan** Assistant Professor, Department of Chemistry, Birla Institute of Technology (BIT) – Mesra, Ranchi, Jharkhand, India **Metal Free Porous Carbon Materials Based Electrocatalyst for Sustainable Hydrogen Fuel Production**
IL-14 5.50 PM - 6.10 PM	**Pratibha Kumari** Associate Professor, Department of Chemistry, Deshbandhu College, University of Delhi, New Delhi, India **Application of cellulose-based nanomaterials in the sensing of pesticides**
IL-15 6.10 PM - 6.30 PM	**Abha Mishra** Professor, School of Biochemical Engineering, IIT BHU
6:30 PM onwards	**Poster session**

Parallel Session – IV B
Venue: HALL-2A
Chairpersons: Dr. V. Ramanathan

IL-16 4:50 PM - 5.10 PM	**Ravi Prakash Singh** Professor, Department of Chemistry, Indian Institute of Technology Delhi, New Delhi, India **Atropisomerism in the Realm of Pharmaceutically Relevant Compounds**
IL-17 5.10 PM - 5.30 PM	**Ganesh Venkataraman** Associate Professor, Department of Chemistry, Indian Institute of Technology Kharagpur, West Bengal, India **Transition Metal-Catalyzed Annulation Platforms for Pharmacologically Relevant Tetralone and Chromanol Frameworks**
IL-18 5.30 PM - 5.50 PM	**Deepti Goyal** Assistant Professor, Department of Chemistry, DAV College, Chandigarh, India **Rational Design of Phenol–Triazole Derivatives as Modulator of Aβ/ Cu^{2+}–Aβ Aggregation and Cytotoxicity**
IL-19 5.50 PM - 6.10 PM	**Chandana Rath** Associate Dean (Faculty Affairs), School of Materials Science and Technology, Indian Institute of Technology (Banaras Hindu University), Varanasi, India **Synergistic Effect of $CoFe_2O_4$-85S Nano Bio-glass Composites for Hyperthermia**
SIL-1 6.10 PM-6.25 PM	**Raju Bej** Assistant Professor, BM School of Health Sciences and Technology, IIT Guwahati **Mucin-Inspired Filamentous Amphiphilic Copolymers Effectively Inhibit Human Respiratory Syncytial Virus (hRSV) Infectivity**
6.30 PM-8.00 PM	RSC-sponsored poster sessions Poster Number P-1 to P-32 Venue: HALL-2C Poster Number P-33 to P-64 Venue: HALL-2D Chairpersons: Dr Moni Sharma, Dr Mrunal Ambasana
8.00 PM-9.30 PM	**Conference Dinner**

Wednesday, May 13, 2026

Registration
Venue: Dev & Vardhana Goswami Lecture Hall Complex

7.30 AM-9:00 AM	**Registration and Breakfast**

Session – V
Venue: HALL-IA
Chairpersons: Dr. Samya Banerjee

PL-7 9.00 AM - 9.35 AM	**Ganesh Pandey** Distinguished Professor, Department of Chemistry, Institute of Science, Banaras Hindu University, Varanasi, India **Abstract Awaited**
PL-8 9.35 AM - 10.10 AM	**Arindam Mukherjee** Professor, Department of Chemical Sciences, Indian Institute of Science Education and Research, Kolkata, India **Strategic Therapeutic Methodologies using Metal complexes: From Enzyme Modulation to High-Efficiency Phototherapy**
10.10 AM - 10.45 AM	**Session with Wiley**
10.45 AM - 11 AM	**Tea**

Parallel Session – VI A
Venue: HALL-IA
Chairpersons: Dr. Gyan Prakash Modi

KL-3 11.00 AM - 11.25 AM	**N. B. Singh** Department of Chemistry and Biochemistry & Department of Computer Science and Electrical Engineering, University of Maryland, Baltimore County (UMBC), Baltimore, MD, USA **Morphological transition in synthetic bone materials**
IL-20 11.25 AM - 11.45 AM	**Indu Bhusan Deb** Senior Principal Scientist, Organic & Medicinal Chemistry Division, CSIR-Indian Institute of Chemical Biology, Kolkata, West Bengal, India **Access to Functionalized N-Heterocycles via Electrochemical Synthesis and Annulation Reactions**
IL-21 11.45 AM - 12.05 AM	**Anuradha Gupta** Senior Scientific Officer, Biologics Division, Indian Pharmacopoeia Commission, Ministry of Health & Family Welfare, Govt. of India, Ghaziabad, India **Environmental sustainability approaches: Indian Pharmacopoeia Perspective**
IL-22 12.05 AM - 12.25 PM	**John J Georrge** Head, Department of Bioinformatics, University of North Bengal, Raja Rammohunpur, District-Darjeeling, West Bengal, India **AI-Driven *Camellia sinensis* Inhibitors of P-Glycoprotein: From Nature to Market**
IL-23 12.25 PM - 12.45 PM	**Harish C. Upadhyay** Department of Applied Sciences, Rajkiya Engineering College (Affiliated with Dr. A.P.J. Abdul Kalam Technical University, Lucknow), Churk, Sonbhadra, India **Advancing Therapeutic Strategies for Microbial Resistance Through Multitargeting Hybrid Molecules**
IL-24 12.45 PM - 1.05 PM	**Asha Jain** Professor & Former Head, Department of Chemistry, University of Rajasthan, Jaipur, India **Preparation and Structural Characterization of Organometallic Complexes with Potential Biological Applications**
1.05 PM-2: 15 PM	**Lunch**

Parallel Session–VI B
Venue: HALL-2A
Chairperson: Prof. Dhanesh Tiwari

KL-4	**Subhas Chandra Pan**

11.00 AM - 11.25 AM	Department of Chemistry, Indian Institute of Technology Guwahati, Assam, India **Importance of Chirality and Asymmetric Synthesis of Cyclic Molecules**
IL-25 11.25 PM - 11.45 PM	**Amit Shard** Associate Professor, Department of medicinal Chemistry, NIPER-Ahmedabad, India **Sustainable Design, Synthesis and Biological Evaluation of Novel Ferrocene Derivatives as Pyruvate Kinase M2 Modulators for Oral Cancer Therapy**
IL-26 11.45 AM - 12.05 AM	**Namrata Rastogi** Principal Scientist, Medicinal & Process Chemistry Division, CSIR-Central Drug Research Institute, Lucknow, India **Organophotoredox-mediated Sustainable Chemical Synthesis**
IL-27 12.05 AM - 12.25 AM	**Tharamani C.N.** Professor and Former Head, Department of Chemistry, Indian Institute of Technology Ropar, Rupnagar, Punjab, India **Designing greener energy conversion system for a sustainable future**
IL-28 12.25 AM - 12.45 AM	**Jeyakumar Kandasamy** Associate Professor, Department of Chemistry, Pondicherry University, Kalapet, Pondicherry, India **Advancing Carbohydrate Chemistry through Aryl Diazonium-Mediated Transformations**
IL-29 12.45 PM - 1.05 PM	**Dinesh Kumar** Associate Professor, Department of Medicinal Chemistry, National Institute of Pharmaceutical Education & Research (NIPER), Ahmedabad, Gujarat, India **Introducing Sustainability in Allylic Cross-Animations**
1.05 PM-2: 15 PM	**Lunch**

Session – VI.C
Venue: HALL-2B
Chairperson: Prof. Indrajit Sinha

KL-5 11.00 AM - 11.25 AM	**Priyankar Paira** Associate Professor, Vellore Institute of Technology, Department of Chemistry, School of Advanced Science, Vellore, Tamilnadu, India **Mechanistic Sights of Organometallics in Mitochondria for Cancer Therapy**
IL-30 11.25 AM - 11.45 AM	**K. D. Mandal** Professor (HAG), Department of Chemistry, Indian Institute of Technology (BHU), Varanasi, Indi **Synthesis and Characterization of Complex Perovskite Oxides**
IL-31 11.45 PM - 12.05 PM	**Rakesh Kumar Parashar** Professor, Department of Chemistry University of Delhi, Delhi, India **Design, synthesis and applications of Chemosensors for the Naked Eye Detection of metal ions, anions and amino acids**
IL-32 12.05 AM - 12.25 PM	**Krunalkumar Ramanlal Mehariya** Research and Development Chemist, Natara Global Ltd, Hartlepool, United Kingdom **What does 'natural' mean anyway…?**
IL-33 12.25 PM - 12.45 PM	**M.A. Quraishi** Professor, Department of Chemistry, I.I.T.(B.H.U.), Varanasi, India **Green Corrosion Inhibitors: A Sustainable Journey from Fundamentals to Industrial Applications**
IL-34 12.45 PM - 1.05 PM	**Mrunal Ambasana** Assistant Professor, Department of Chemistry and Forensic Science, Bhakta Kavi Narsinh Mehta University, Junagadh, India **Molecular Design Strategies for Selective and Sensitive Chemosensing of Ions, Environmental Pollutants, and Bioactive Compounds**
1.05 PM-2: 15 PM	**Lunch**

Parallel Session – VII A
Venue: HALL-IA
Chairpersons: Prof. Yogesh Chandra Sharma

IL-35 2.15 PM - 2.35 PM	**Surendra Singh** Professor, Department of Chemistry, University of Delhi, Delhi, India **Design and Synthesis of Recoverable Chiral Catalysts for Asymmetric Organic Transformations**
IL-36 2.35 PM - 2.55 PM	**Satpal Singh Badsara** Associate Professor, Department of Chemistry, Institute of Science, Banaras Hindu University (BHU), Varanasi, India **Electro-catalyzed Functionalization of Indolizine Frameworks**
IL-37 2.55 PM - 3.15 PM	**Shuvomoy Banerjee** Assistant Professor, School of Biotechnology and Bioengineering, Institute of Advanced Research (IAR), Gandhinagar, Gujarat, India **Pre-clinical evaluation of phytosterol-ionic liquid conjugated-derivatives shows enhanced anti-cancer activities in colon cancer cells**
IL-38 3.15 PM - 3.35 PM	**Sumit Mishra** Professor & Head, Department of Chemistry, Birla Institute of Technology Mesra, Ranchi, India **Flaxseed Mucilage based composite material as a sustainable flocculant for treatment of mining and Industrial Effluents**
IL-39 3.35 PM - 3.55 PM	**Pravinkumar M. Patel** Head & Associate Professor, Industrial Chemistry Department. V. P. & R. P. T. P. Science College, Affiliated to Sardar Patel University, Vallabh Vidyanagar, Gujarat, India **Formulation Innovation for Health: Triazine Dendrimers**
IL-40 3.55 PM - 4.15 PM	**Vikas Tyagi** Associate Professor, Department of Chemistry and Biochemistry, Thapar Institute of Engineering and Technology, Patiala, Punjab, India **Harnessing Electricity and Enzymes for Sustainable Organic Synthesis**
4.15 PM - 4.30 PM	**Tea**

Parallel Session – VIIB
Venue: HALL 2A
Chairperson: Dr. Pandeeswar Makam

IL-41 2.15 PM - 2.35 PM	**Sudhir K Shukla** Scientific Officer F & Asst. Prof. Homi Bhabha National Institute, Biofouling and Biofilm Processes Section, Water and Steam Chemistry Division, BARC Facilities, Kalpakkam, India **DEVELOPMENT OF A MULTISPECIES BIOFILM BIOFILTER: MICROBIAL INTERACTIONS, COMMUNITY DYNAMICS, AND HEAVY-METAL REMOVAL EFFICIENCY**
IL-42 2.35 PM - 2.55 PM	**Ranjan C. Khunt** Professor, Department of Chemistry, Saurashtra University, Rajkot, Gujarat, India **Tetrazole-Embedded Scaffold via Ugi Four-Component Reaction: Efficient Synthesis and Drug -Likeness Evaluation**
IL-43 2.55 PM - 3.15 PM	**Subhendu Naskar** Department of Chemistry, Birla Institute of Technology, Mesra, Ranchi, India **Transition metal Complexes as Molecular Electrocatalysts for OER, HER and CO2RR**
IL-44 3.15 PM - 3.35 PM	**Roop Shikha Singh** Assistant Professor, Department of Chemistry, Institute of Science, Banaras Hindu University, Varanasi, India **Engineering Charge Transfer in AIE Systems: From Molecular Design to Targeted Theranostic Applications**
IL-45 3.35 PM - 3.55 PM	**Ved Prakash Singh** Professor & Head, Department of Industrial Chemistry, Mizoram University, Aizawl, Mizoram, India **Drug Design, Synthesis and Study of Novel Series of Bio-active analogues**

IL-46 3.55 PM - 4.15 PM	**Satyendra K. Pandey** Organic Chemistry, Department of Chemistry, Institute of Science, Banaras Hindu University, Varanasi, India **Metal- and Reagent-Free Approaches for the Synthesis of Bioactive Molecules**
4.15 PM - 4.30 PM	**Tea**

Parallel Session – VII C
Venue: HALL 2B
Chairpersons: Dr. Rosy

IL-47 2.15 PM - 2.35 PM	**Sourav Chakraborty** Associate Professor, Department of Chemistry, Indian Institute of Technology, Tirupati, Andhra Pradesh, India **Redox-active Interlocked Molecules for Energy Storage Applications**
IL-48 2.35 PM - 2.55 PM	**Sabbasani Rajasekhara Reddy** Professor, School of Advanced Sciences, Department of Chemistry, Vellore Institute of Technology (VIT), Vellore, India **Carbohydrates and Copper for Sustainable Catalysis, Health Care and Environment**
IL-49 2.55 PM - 3.15 PM	**Debasish Mandal** Associate Professor, Department of Chemistry and Biochemistry, Thapar Institute of Engineering and Technology, Patiala, Punjab, India **Computational Exploration of Ligand-Directed C–H Activation in Bio-Inspired Metal–Oxo Complexes**
IL-50 3.15 PM - 3.35 PM	**Bichismita Sahu** Professor and Head, Department of Medicinal Chemistry, NIPER-Ahmedabad, Gandhinagar, Gujarat, India **Epigenetic modulation through nucleobase ispired scaffolds: Discovery of anti-cancer compounds targeting LSD1**
IL-51 3.35 PM - 3.55 PM	**Rinku Chakrabarty** Head, Department of Chemistry, Alipurduar University, Aipurduar, West Bengal, India **Rhodamine Based Cu(II) Complexes: Application as PDT Agent**
IL-52 3.55 PM - 4.15 PM	**Dina Nath Singh** Professor, K.S. Saket PG College, Dr. Ram Manohar Lohia Avadh University, Ayodhya, India **Current Approaches for the Search of New Bioactive Leads from Medicinal Plants**
4.15-4.30 PM	Tea

Parallel Session – OP-1
Venue: HALL-1A
Chairperson: Prof Neelima Gupta

O-1 4.35 PM- 4.45 PM	**Pratibha Yadav** Center for Rural Development and Technology, IIT Delhi, Hauz Khas, New Delhi, India 110016 **Biosynthesis of Rutinose from Broccoli flower head pulp using F. monilliforme MTCC-2015**
O-2 4.45 PM - 4.55 PM	**Prakriti Sharda** Department of Biotechnology, Thapar Institute of Engineering Technology, Patiala-147001, Punjab, India **Sensitive electrochemical detection of ciprofloxacin using a GO/LDH composite-modified screen-printed electrodes**
O-3 4.55 PM - 5.05 PM	**Vishal Agarwal** Department of Chemistry and Biochemistry, The University of Arizona, USA **Expanding Optochemical Ligation Chemistry through Cation–Cation Photosensitization**
O-4 5.05 PM - 5.15 PM	**Shikha Pandey** Department of Chemistry, Indian Institute of Technology (BHU), Varanasi, Uttar Pradesh -221005, India **Visible-Light-Mediated S-C Bond Cleavage for the Synthesis of Amides**
O-5	**Nidhi Sikri**

5.15 PM - 5.25 PM	Department of Biotechnology, Thapar Institute of Engineering and Technology, Patiala, India **Horseradish Peroxidase immobilized GO-SWCNT Hybrid Biocatalytic Platform for Efficient Degradation of Bisphenol A**
O-6 5.25 PM - 5.35 PM	**Harshita Pandey** Department of Chemistry, Indian Institute of Technology (BHU), Varanasi-221005, India **Visible-light-driven photocatalytic esterification of thioesters involving radical pathway via sigma bond cleavage**
O-7 5.35 PM - 5.45 PM	**Priya Mahaur** Department of Chemistry, IIT BHU, Varanasi, Uttar Pradesh, India **Synthesis of Imidazo[1,2-a]pyridine via Sustainable Photocatalytic C (sp)3–H Functionalization of Ethylarenes and Their Luminescence Investigations**
O-8 5.45 PM - 5.55 PM	**Amod Kumar** Chemical& Material Sciences Division, CSIR-Indian Institute of Petroleum, Haridwar Road, Mohkampur, Dehradun, India **Synthesis of cyclic carbonates from CO_2 and epoxides under ambient conditions**

Parallel Session – OP-2
Venue: HALL-2A
Chairperson: Dr Gurpreet Singh Minhas

O-9 4.35 - 4.45 PM	**Priyadarshini R** Department of Life Sciences, School of Natural Sciences, Shiv Nadar Institution of Eminence, Delhi NCR, Greater Noida 201314, India **Small organic metabolites produced by *Lactobacillus rhamnosus* with anti-biofilm properties against *Streptococcus mutans* biofilms**
O-10 4.45 PM - 4.55 PM	**Parikh Kaushik** Department of Biotechnology, Thapar Institute of Engineering & Technology, Patila-147001, Punjab, India **Development of Sodium Alginate-Based Microcapsules for Controlled Release of Coenzyme Q_{10}**
O-11 4.55 PM - 5.05 PM	**Rashmi D** Department of Biochemistry, JSS Medical College, JSS Academy of Higher Education & Research, Mysore, India **IN VITRO ANTI-INFLAMMATORY AND ANTI-CANCER ACTIVITY OF FERMENTED FRUIT EXTRACT IN LIPOPOLYSACCHARIDE-STIMULATED RAW 264.7 MACROPHAGES AND $CaCO_2$ CELLS**
O-12 5.05 PM - 5.15 PM	**Yogita Rani** Department of Chemistry, Indian Institute of Technology (BHU), Varanasi-221005, U.P. India **Polarity-Tunable Curcumin-Derived Carbon Quantum Dots for Multifunctional Liposomal Theranostics**
O-13 5.15 PM - 5.25 PM	**Ram Pratap Pandey** Department of Medicinal Chemistry, Institute of Medical Sciences, Banaras Hindu University, Varanasi-221005, India **Lewis Acid-Controlled Divergent Transformations of Glycals: Stereoselective Access to Fused Pyran Frameworks, C-Glycosides, and Glycoconjugates**
O-14 5.25 PM - 5.35 PM	**G.K. Mohan Krishna** Division of Biochemistry, School of Life Sciences, Mysuru, JSS Academy of Higher Education & Research, Mysuru 570 015, Karnataka, India **Sustainable Synthesis of Silver nanoparticles (AgNPs) using *Kanchanara guggulu* extract: Antioxidant, and Cytotoxic Potential**
O-15 5.35 PM - 5.45 PM	**Samanmitha S** Centre of Excellence in Molecular Biology and Regenerative Medicine (CEMR), Department of Biochemistry, JSS Medical College, JSS Academy of Higher Education and research, Mysuru -570015, Karnataka, India **Quercetin induces BMAL1 and targets METTL3/m^6A–SND1–Mediated Epitranscriptomic novel Axis to Attenuate Hepatocellular Carcinoma under**

	Circadian Disruption
O-16 5.45 PM - 5.55 PM	**Sandeep Chovatiya** Department of Biosciences, Saurashtra University, Rajkot, Gujarat, India **Cytotoxic and Genotoxic Effects of Aluminum Oxide (Al_2O_3) Nanoparticles on Human Haematocytes: An In Vitro Study**

Parallel Session – OP-3
Venue: HALL-2B
Chairperson: Dr Mohan Prasad

O-17 4.35 - 4.45 PM	**Anjisha Maharshi** Department of Microbiology, Faculty of Science, Marwadi University, Rajkot-Morbi Road, Rajkot 360 003 Gujarat, India **Bioprospecting of Endophytic Aspergillus niger Associated with Withania somnifera for Pharmacologically Active Metabolites**
O-18 4.45 PM - 4.55 PM	**Tanima Debnath Sarkar** Department of Zoology of Annamalai University, Tamil Nadu, India **Green Biologics and Mechanistic Toxicology: Advancing Sustainable Pharmaceutical Development**
O-19 4.55 PM - 5.05 PM	**Vinay Kumar Pandey** Department of Chemistry, Institute of Science, Banaras Hindu University, Varanasi, India **Design, Synthesis and Antiviral Activity of Pyrazole-linked Fused Curcumin Glycoconjugates against Influenza A Virus (H3N2)**
O-20 5.05 PM - 5.15 PM	**Yashika Mehta** Department of Biotechnology, Thapar Institute of Engineering and Technology, Patiala-147001, Punjab, India **Microalgal consortia-derived biogenic fluorescent carbon dots exhibiting multispectral emission**
O-21 5.15 PM - 5.25 PM	**Chaitanya H.S** Department of Zoology, Vijayanagara Sri Krishnadevarya University, Ballari, Inida **Evaluation of single and combined effects of Dimethyl phthalate and Bis (2-ethyl hexyl) phthalate on Reproductive and Neural health in Sprague Dawley rats**
O-22 5.25 PM - 5.35 PM	**Koushik Barman** Kolkata, India **Beyond Bulk Measurements: Decoding Nanoscale Electrocatalysis with Scanning Electrochemical Microscopy**
O-23 5.35 PM - 5.45 PM	**Shuchi O C** Centre of Excellence in Molecular Biology and Regenerative Medicine (CEMR), Department of Biochemistry, JSS Medical College, JSS Academy of Higher Education and research, Mysuru -570015, Karnataka, India **Unravelling the Novel Mechanism of Anti-Tumor Role of Sodium Butyrate: SND1-mediated Telomerase and miR-155 Pathway Suppression in HCC**

Parallel Session – OP-4
Venue: HALL-2C
Chairperson: Dr Keshav Deo

O-24 4.35 PM - 4.45 PM	**Shweta Srivastava** Lucknow, India **Fostering Environmental Responsibility at secondary school level through NCERT Chemistry Kits**
O-25 4.45 PM - 4.55 PM	**Ranjana Das** Department of Pharmaceutical Engineering and Technology, Indian Institute of Technology, (BHU) Varanasi, India **An integrative approach combining computational simulation and spectroscopic analysis elucidates the stability of L-asparaginase on the nanocomposite surface**

O-26 4.55 PM - 5.05 PM	**Akanksha Singh** Biofuel Research Laboratory, School of Biochemical Engineering, Indian Institute of Technology (BHU), Varanasi, India **DESIGN OF A BATCH BIOREACTOR UTILIZING A DEVELOPED MICROBIAL-NANOCOMPOSITE BEAD SYSTEM FOR SCALE-UP OF HEAVY METAL REMEDIATION PROCESS FROM AQUEOUS SYSTEMS**
O-27 5.05 PM - 5.15 PM	**Smriti Dogra** Department of Chemistry, Dr B. R. Ambedkar National Institute of Technology, Jalandhar-144008 (Punjab), India **Ultrasensitive Electrochemical Sensor for Nitroaromatics Using C_3N_4-MoS_2-Au Nanocomposite with Pendimethalin as a Real Sample**
O-28 5.15 PM - 5.25 PM	**Pooja Kumari** Department of Chemistry, Indian Institute of Technology (BHU), Varanasi, Uttar Pradesh – 221005, India **Visible-light-initiated *N*-arylation of hydrazones with diazonium tetrafluoroborate via EDA complex formation**
O-29 5.25 PM - 5.35 PM	**Aswathi C Narayanan** Department of Chemistry, Indian Institute of Technology (BHU), Varanasi, Inida **Synthesis of cinnamic esters and acids *via* palladium-catalyzed reactions of aryl diazonium salts and their biological evaluation**
O-30 5.35 PM - 5.45 PM	**Khushi Malaybhai Mehta** Department of Microbiology, Faculty of Science, Marwadi University, Rajkot-Morbi Road, Rajkot 360 003 Gujarat, India **Bioprospecting of *Endophytic Aspergillus niger* Associated with *Withania somnifera* for Pharmacologically Active Metabolites**
O-31 5.45 PM - 5.55 PM	**Pratikshya Das Pattanayak** Department of Chemistry, NIT Rourkela, Rourkela, India **V^{IV}-TSC-based Metallodrugs: Solution Chemistry, Cytotoxicity, and Cellular Internalization**

Poster Session – II (Wiley-sponsored)
Venue:
Chairpersons: Dr Babita Malik, Dr Rinku Chakrabarty, Dr Jaybir Singh

6.15 PM – 7.30 PM	Poster Number P-64-P96 (Wiley-sponsored) (Room no. 2D) P-97 to P-128 (Thieme-sponsored) (Room no. 2E)
8.00 PM	**Dinner**

Thursday, May 14, 2026

Parallel Session – VIII A (IDAPT sponsored)
Venue: HALL IA
Chairpersons: Dr. Prabhat Tripathi

IL-53 9.00 AM - 9.20 AM	**Ashim K. Mukherjee** Retired Professor, Department of Chemistry, Indian Institute of Technology, Banaras Hindu University, Varanasi, India **Abstract Awaited**
IL-54 9.20 AM - 9.40 AM	**Devdutt Chaturvedi** Head, Department of Chemistry, Mahatma Gandhi Central University, Motihari (East Champaran), Bihar, India **Versatility of heteroallenes: An easy access for the syntheses of biologically potent scaffolds**
IL-55 9.40 AM - 10.00 AM	**Meenakshi Singh** Assistant Professor, Department of Medicinal Chemistry Institute of Medical Sciences, Banaras Hindu University (BHU), Varanasi, India **Replisome-Targeted Antimicrobials: Harnessing Indole Chemistry to Combat Drug Resistance**
IL-56 10.00 AM - 10.20 AM	**Hitesh D. Patel** Professor & Head, Department of Chemistry, Gujarat University, Ahmedabad, Gujarat, India **IPR for Natural Products – Scope & Boundaries**

Parallel Session – VIII B (IKS in Chemistry)
Venue: HALL 2A
Chairpersons: Dr. Saravanakumar Elangovan

IL-57 9.00 AM - 9.20 AM	**V. Ramanathan** Associate Professor, Chemistry, IIT (BHU)
IL-58 9.20 AM - 9.40 AM	**Dr. Amita Sinha** Full Time on Contract Professor, Department of Architecture, Planning and Design, IIT (BHU)
IL-59 9.40 AM - 10.00 AM	**Chandan Upadhyay** Professor and Coordinator of the School of Materials Science, IIT BHU, Varanasi, India

Parallel Session – VIII C
Venue: HALL 2B
Chairpersons: Dr. Bhuvaneshwari B

IL-60 9.00 AM - 9.20 AM	**Ram Sagar Misra** Professor of Chemistry, School of Physical Sciences, Jawaharlal Nehru University (JNU), New Delhi, India **Efficient Synthesis of 2-Deoxy Sugars: A Route to Substituted Chiral Quinoline-based Glycohybrids and Indole-C-glycosides**
IL-61 9.20 AM - 9.40 AM	**Neeraj Kumar Mishra** Associate Professor, Department of Chemistry, Faculty of Science, University of Lucknow, Lucknow, India **Late-Stage C–H Activation–Functionalization of Heterocyclic Drug Candidates: An Annulative Pathway**
IL-62 9.40 AM - 10.00 AM	**Chandan Singh** Assistant Professor, Department of Biochemistry, Institute of Science, Banaras Hindu University, Varanasi, India **Intricate Interaction of Microbiome and its Reflection in Metabolome of ALS patients by NMR**

IL-63 10.00 AM - 10.20 AM	**Mayank K. Pandya** School of Science, Dr. Subhash University, Junagadh, Gujarat, India **A Fast, Sensitive, and Validated Analytical Method for Quantitation of Imidacloprid Pesticide Residual in *Mangifera indica* Matrix by LC-Tandem Mass Spectrometry (LC-ESI-MS/MS)**

Parallel Session – OP-5
Venue: HALL 1A
Chairpersons: Prof Shailesh Rajanikant Shah

O-32 10.20 AM – 10.30 AM	**Varshini Manjunath** Centre of Excellence in Molecular Biology and Regenerative Medicine (CEMR) laboratory, (a DST-FIST Sponsored Centre) Department of Biochemistry (a DST-FIST Sponsored department), JSS Medical College, JSS Academy of Higher Education & Research (JSS AHER), Mysuru – 570015, Karnataka, India **Targeting Breast Cancer Progression with Taurine: Inhibition of Proliferation, Metastasis, EMT, and RISC-Mediated Regulatory Pathways**
O-33 10.30 AM – 10.40 AM	**Madhusmita Mishra** Department of Biotechnology and Medical Engineering, National Institute of Technology (NIT), Sector-1, Rourkela, Odisha, India **Investigating the Emerging Neurotoxic Potential of Acetonitrile-d3 in a Zebrafish Model: Implications for Human Mental Health**
O-34 10.40 AM – 10.50 AM	**Harshitha Marla** Biotechnology Division, Department of Life Sciences, School of Science, GITAM (Deemed to be University), Visakhapatnam- 530045, Andhra Pradesh, India **EXPLORING MARINE DERIVED FUNGI FROM THE VISAKHAPATNAM COAST: AN ECO-FRIENDLY APPROACH TO MICROPLASTICS DEGRADATION**
O-35 10.50 AM – 11.00 AM	**Srikrishna Kedlaya Herga** Department of Public Health Genomics, Manipal School of Life Sciences, Manipal Academy of Higher Education, Manipal, Karnataka, India **Streptococcal Surfaceome-Host Interactions Drive Adhesion, Invasion, and Divergent Inflammatory-Apoptotic Signaling in Oral Cancer Cells**
O-36 11.00 AM – 11.10 AM	**Vijaykumar B. Malashetty** Molecular Reproduction and Mechanistic Toxicology Lab, Department of PG Studies and Research in Zoology, Gulbarga University, Kalaburagi-585106, India **Alpha-Terpineol: From Human Exposure to Molecular Toxicity - Mechanistic Insights into Reproductive and Developmental Effects**
O-37 11.10 AM – 11.20 AM	**Hanamantray** Department of studies in Zoology, Vijayanagara Sri Krishnadevaraya University, Ballari-585105, India **Effect of Polyethylene terephthalate (PET) micro plastics on pre- and post-natal development, including maternal function in Wistar rats**

Parallel Session – OP-6
Venue: HALL 2A
Chairperson: Dr Harish C. Upadhyay

O-38 10.20 AM – 10.30 AM	**Surajit Pradhan** Department of Chemistry, Indian Institute of Technology (BHU), Varanasi-221005, India **Sustainable production of biodiesel from waste frying oil using biowaste-derived CaO/K_2CO_3 nanocomposite catalyst: RSM optimization and E-metrics study**
O-39 10.30 AM – 10.40 AM	**Pakkiresha Goravara** Department of Zoology, Vijayanagara Sri Krishnadevaraya University, Ballari-583105, Karnataka, India **Mechanistic Insights into α-Terpineol-Induced Reproductive Toxicity in Male Rats: Evidence from Molecular, Genotoxic, and Ultrastructural Analyses**

O-40 10.40 AM – 10.50 AM	**Arif Ali Mandal** Department of Chemistry, Indian Institute of Technology (BHU), Varanasi-221005, India **Ru(II)-Based Photoantibiotics: Light-Driven Eradication of Bacterial Biofilm and Rapid Healing of Infective Wounds in Wistar Rat**
O-41 10.50 AM – 11.00 AM	**Nandita Kushwaha** Department of Chemistry and Environmental Science, M.M.M. University of Technology, Gorakhpur (273010), Uttar Pradesh, India **β-Cyclodextrin Xanthate-Acrylamide Hydrogel as a Sustainable Adsorbent for Cu^{2+} and Ni^{2+}: Adsorption and Biodegradability Assessment**
O-42 11.00 AM – 11.10 AM	**Neha Chaurasiya** Department of Chemistry and Environmental Science, Madan Mohan Malaviya University of Technology, Gorakhpur (273010), Uttar Pradesh, India **Eco-Friendly Novel Gum Ghatti Xanthate-Based Hydrogel for Removal of Cu^{2+} and Co^{2+} Ions from Synthetic and Real Water**
O-43 11.10 AM – 11.20 AM	**Bharti Singh** Department of Chemistry, Indian Institute of Technology (BHU) Varanasi, Uttar Pradesh, India **Computational Investigation of Sulphur-Centred Hydrogen Bonds in Ethanedithiol-Solvent Clusters**

Parallel Session – OP-7
Venue: HALL 2B
Chairperson: Prof S.K. Singh

O-44 10.20 AM - 10.30 AM	**Praveen Kumar** Department of chemistry and environmental science, M.M.M. University of Technology, Gorakhpur (273010), Uttar Pradesh, India **Optimization of Acrylic Acid/Acrylonitrile functionalized Gg-based Hydrogel for Synthesis Eco-friendly, Cost-effective and Efficient Removal of Heavy Metal Ions**
O-45 10.30 AM - 10.40 AM	**Prerna Shekhawat** Department of Chemistry, IIS (deemed to be) University, SFS, Mansarovar, Jaipur, Rajasthan, India **From Synthesis to Simulation: Multicomponent-Derived Compounds Evaluated via Computer-Aided Drug Design, Molecular Docking, and ADME Profiling**
O-46 10.40 AM - 10.50 AM	**Riya Sharma** Department of Chemistry and Environmental Science, Madan Mohan Malaviya University of Technology, Gorakhpur (273010), Uttar Pradesh, India **Allyl Mannitol Crosslinked Pectin-Based Hydrogel for Efficient Adsorptive Removal of Cu^{2+} and Ni^{2+} Ions from Aqueous Solutions**
O-47 10.50 AM - 11.00 AM	**Hardik L. Varu** Department of Chemistry, School of Science, Dr. Subhash University, Junagadh, 362001, Gujarat, India **Sunlight Mediated Yellow Fluorescence Detection of Mercury and Copper**
O-48 11.00 AM - 11.10 AM	**Kausha P. Bhatt** Department of Chemistry and Forensic Science, Bhakta Kavi Narsinh Mehta University, Junagadh, 362001, Gujarat, India **Colorimetric detection of cations and anions with eosin y-quinoxaline motif**
O-49 11.10 AM - 11.20 AM	**Belal Ahamad** Department of Chemical Engineering and Technology, Indian Institute of Technology (Banaras Hindu University), Varanasi, India **Studies on modified montmorillonite as catalyst to produce upgraded fuel oil from the pyrolysis of waste extended polystyrene**

Parallel Session – OP-8
Venue: HALL 2C
Chairperson: Dr Ved Prakash Singh

O-50 10.20 AM - 10.30 AM	**Sumit Kumar Jaiswal** Department of Microbiology, Faculty of Science, Marwadi University, Rajkot 360 003 Gujarat, India **Development of Biocompatible Carbon Quantum Dots as Sustainable Alternatives to Traditional Sunscreen Ingredients**
O-51 10.30 AM - 10.40 AM	**Ramya P R** BRIC- National Institute of Animal Biotechnology (NIAB), Hyderabad-500032, Telangana, India **Epitope-Level Insights for Immuno-Recognition of JEV NS1 via Gold Nanoflower-MXene Composite**
O-52 10.40 AM - 10.50 AM	**Aman Singh** Department of Chemistry, Indian Institute of Technology (BHU), Varanasi– 221005, U.P., India **Visible light-induced C(sp2)-N bond-formation from diazonium tetrafluoroborates and secondary amines via Electron Donor–Acceptor Complex Formation**
O-53 10.50 AM - 11.00 AM	**Mansi Srivastava** Department of Chemistry and Environmental Science, Madan Mohan Malaviya University of Technology, Gorakhpur (273010), Uttar Pradesh, India **Development of Neem-Mediated Phytonanoparticle-Based Nanocomposites for Enhanced Adsorption of Toxic Dyes from Wastewater**
O-54 11.00 AM - 11.10 AM	**Vadivel Ganapathy** Department of Cell Biology and Biochemistry Texas Teach University Health Sciences Center Lubbock, TX 79430 USA **Newly found biological targets for the anti-helminthic drug niclosamide in cancer cells, highlighting its potential in cancer therapy**

Insight Forum: Engaging Minds Through Dialogue
Venue:

Panel Discussion 11.30 AM – 12.00 PM	**Collaboration Among Industry, Academia, and Government: Driving Sustainable Innovation in India** Moderator: Prof. Sanjay Kumar, BITS Pilani, K K Birla Goa Campus

Valedictory Session
Venue:

12.00 PM – 1.00 PM	**Valedictory Session**

1.00 PM	**Lunch**

- End of Programme -

PL = Plenary Lecture | KL = Keynote Lecture | IL = Invited Lecture | SIL = Short Invited Lecture | O = Oral Presentation | P = Poster Presentation

ISCBC-2026

PLENARY

PL-1

Major API & Pharma Products through Flow Chemistry Processes: An untaped potential for Academic Research

Anamik Shah

President, ISCB
Former Vice Chancellor, Gujarat Vidyapeeth, Ahemdabad, India
Founder, National Facility for Drug Discovery Centre, Saurashtra University, Rajkot, India

Abstract

Abstract Awaited

PL-2

Sustainable Approaches and Strategies for Design and Development of Platform Chemicals and Novel Molecules

Anil K. Singh

Professor (Retd.), Department of Chemistry, Indian Institute of Technology Bombay, Powai, Mumbai – 400 076, India
(E-mail: retinal@chem.iitb.ac.in)

Stagnation in petrochemicals and limited availability of petrochemical intermediates hugely constrain the potential for further development and production of chemicals/ chemical products, and energy. Hence, a great deal of attention is now towards discovering, developing and promoting alternate approaches and strategies. This talk will uncover a few of these strategies, which focus on shifting from traditional 'take-make-dispose' linear models to circular chemistry frameworks.

One of the imminent strategies envisions the use of bio-privileged molecules (BMs), which are biotic chemical intermediates, endowed with a diversified group of desirable chemical functionalities beyond those available in the petrochemicals or *via* conventional synthetic means. BMs are abundantly available from bio-resources and can serve as a sustainable and versatile source of various kinds of chemical entities, be it direct replacements for petrochemicals, platform chemicals, or specialty chemicals. This strategy, together with fast-advancing chemical and biochemical technologies greatly facilitates expansion of BMs to almost any molecular framework that one could visualize. This strategy provides a new basis for the diversity-oriented synthesis leading to design and development of various kinds of chemical products such as agrochemicals, antimicrobials, drugs and pharmaceuticals, nutraceuticals, polymers, etc.

Light-induced chemical processes, which are inherently connected to sustainability, provide another valuable strategy for achieving chemical reactions not accessible through conventional thermal chemistry. Such approaches have great potential to simplify chemical synthesis, unlock diverse chemical possibilities, and create novel molecules for various applications. Today, developing environmentally safe and economically viable photochemical processes is an important and critical area for many researchers worldwide. This talk while briefly uncovering these aspects, will demonstrate how photochemical strategies enable efficient synthesis of intricate organic structures and significantly expand the chemical space for drugs and pharmaceuticals, agrochemicals, speciality chemicals, and novel molecules like the molecular photo triggers and photo switches for dynamic studies in biology, chemistry, physiology, and medicine, particularly for precise spatiotemporal drug activation and targeted delivery. Also, will be highlighted ways of achieving clean and high chemical yield in photochemical reactions by proper mechanistic understanding of the photo-process, judicious functional group manipulations, and appropriate reactor design, for scale-up operations.

Smart photoactive nano-org microbial bio-factories provide yet another potentially very useful approach for low-cost carbon sequestration and eco-friendly manufacturing of chemicals. Different core–shell quantum dots, with excitations in UV to near-IR range, when coupled with targeted enzyme sites in certain bacteria have been found to efficiently catalyze light-induced air–water–carbon dioxide reduction to isopropanol, 2,3-butanediol, C_{11}–C_{15} methyl ketones, H_2 and chemicals such as formic acid, ammonia, ethylene, bioplastics, polyhydroxybutyrate, etc.

Another new strategy is based on what is now known as the 'Methanol Economy'. This strategy offers great potential for replacing fossil-based fuels and chemical products technology for sustainable production of platform chemicals, and energy security. Essentially aimed at utilization and repurposing CO_2 to produce CH_3OH and CH_3OCH_3, this strategy is a promising solution for sustainable fuels requirements and to produce various kinds of platform chemicals such as hydrocarbons, olefins, propylene, gasoline, aromatics, etc.

Finally, considering the emergence of many new challenges and exciting opportunities, the talk will conclude by emphasizing the essentiality of integrating sustainability principles into chemistry-allied sciences education, research and practice, thus bringing it in alignment with the emerging growth and development trajectories, and technology requirements. Illustrations and examples will be drawn from the research and academic journey of the speaker as well as from the efforts and contributions of other researchers.

PL-3

Functional Modelling of Cytochrome P450

Abhishek Dey

IACS, Kolkata

The versatile reactivity of cytochrome P450 has long enticed the community to try to create small molecule mimics of the enzyme active site. Erstwhile attempts to use synthetic iron porphyrins with axial thiolate ligands, while arduous, have not been very successful. In particular, the use of molecular oxygen as the oxidant has eluded the community. In this lecture, a curious case of valence tautomerism, inherent to thiolate co-ordinated iron porphyrins, and how this leads to the degeneration of such entities in the presence of oxygen will be discussed. Understanding the origin of this phenomenon led to the discovery of the crucial role played by the hydrogen bonding interactions in stabilizing the "air stable" ferric thiolate form; a crucial breakthrough in using these as catalysts! Transferring these synthetic systems to aqueous conditions, which offer abundant hydrogen bonding, on electrodes allowed accumulation of ferric superoxide, ferric peroxide (compound 0) and compound I analogues (detected using in-situ resonance Raman spectroscopy) via reductive oxygen activation under different experimental conditions which attenuates the electron transfer steps involved in catalysis. This resulted in catalytic dioxygenase, aldehyde dehydrogenase and monooxygenase reactivity using molecular oxygen as the oxidant with turnovers $>10^4$ in the same catalytic construct.

Selected References:

1. PK Das, S Samanta, AB McQuarters, N Lehnert, A Dey Proc. Natl. Acad. Sci. 2016, 113, 6611-6616
2. A Rana, S Amanullah, PK Das, AB McQuarters, N Lehnert, A Dey J. Am. Chem. Soc. 2019, 141, 5073-5077
3. M Mukherjee, A Dey ACS Central Science 2019, 5, 671-682
4. M Mukherjee, A Dey Inorg. Chem. 2020, 59, 7415-7425
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PL-4

Non-equilibrium self-assembly for living matter-like properties

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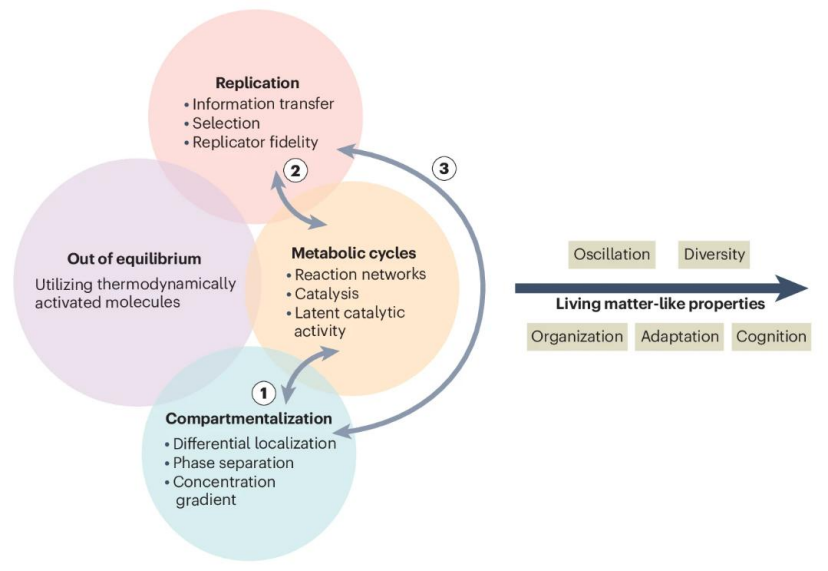
Life's soft and wet machinery arose from spatially confined assemblies of biomolecules capable of replication, integrated with metabolic reaction cycles that function far from equilibrium.[1] By methodically synthesizing and integrating these key elements, i.e. replication, metabolism, and confinement under non-equilibrium conditions, we can begin to explore how chemically constructed systems might acquire life-like, evolving properties.[2-5] This ambitious goal lies at the heart of systems chemistry. In this talk, I will outline recent insights into how reaction networks, self-reproduction, and compartmentalization can be brought together under non-equilibrium settings.[1-6] I will also delve into the interplay between reaction dynamics and transient compartmentalization, and explore the development of self-replicating systems capable of sustained operation in far-from-equilibrium conditions.



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PL-5

Hybridization, Compaction and Coacervation of DNA : from photocontrol to applications in bio- and nanotechnology

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Nucleic acids represent one of the most fundamental biological macromolecules, not only because they encode genetic information, but also due to their remarkable binding specificity and catalytic capabilities in a wide range of biological processes. From a physicochemical perspective, however, DNA can be simply considered as a negatively charged, semiflexible polyelectrolyte, whose behavior is governed by relatively simple interactions. This enables DNA and DNA-based nanomaterials to be manipulated through their physicochemical properties using a variety of external stimuli, such as light, temperature and ionic strength.

In this talk, I will highlight three key physicochemical properties of DNA, namely hybridization[1–3], compaction[4–7], and coacervation,[8] and demonstrate how, by combining electrostatic interactions, the hydrophobic effect, and hydrogen bonds, DNA can be put under external control in a predictable and tunable manner. Particular emphasis will be placed on how these interactions can be modulated to achieve dynamic and reversible responses.

I will present strategies for the photocontrol of DNA hybridization to control the formation of nanostructures such as hairpins and DNA origami, enabling precise spatial and temporal regulation. Photocontrol of DNA compaction will be shown as a means to selectively regulate gene expression, offering potential applications in synthetic biology and gene delivery. In addition, photocontrol of DNA coacervation provides a novel approach for sequence-selective DNA purification and separation.

Together, these results underline the importance of understanding DNA at the physicochemical level and illustrate new ways of controlling nucleic acid systems in advanced nano- and biotechnological applications, opening perspectives for the design of responsive and programmable biomolecular materials.

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PL-6

Metathesis Reactions in Modern Industry: Sustainable and Efficient Synthesis Enabled by Advanced Ruthenium Catalysts

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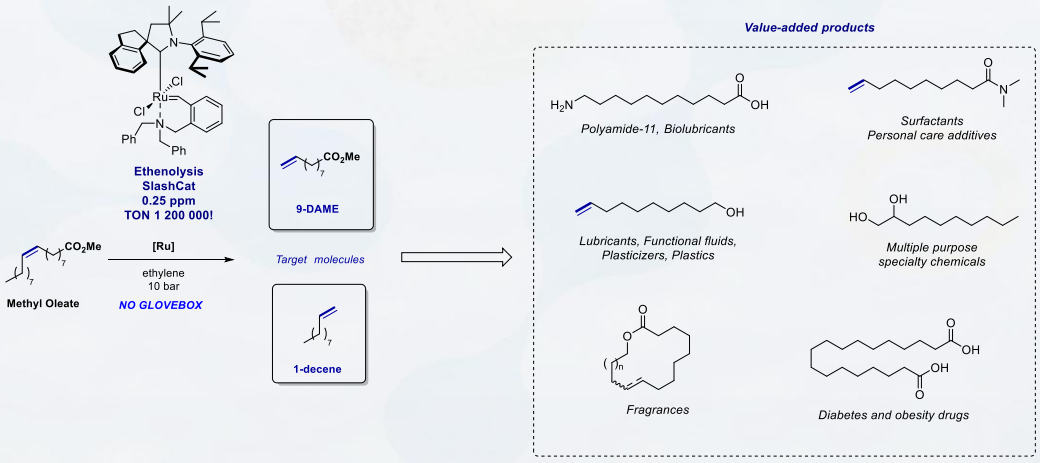
Olefin metathesis has emerged as one of the most transformative tools in modern synthetic chemistry, offering unparalleled versatility across pharmaceuticals, fine chemicals, polymer science, and agrochemicals.

In the pharmaceutical domain, CM-based ethenolysis of renewable plant oils yields key intermediates such as 9-DAME and 1-decene, which serve as starting materials for the long-chain fatty acid moieties (C18–C20) incorporated into next-generation GLP-1 agonists including semaglutide and tirzepatide. Apeiron's proprietary CAAC-based catalysts — SlashCat and UltraCat — demonstrate exceptional selectivity (up to 98.5%) and turnover numbers exceeding 1200 000, significantly outperforming conventional Grubbs-type systems. In the fragrance and agrochemical sectors, RCM enables macrocyclization for musk synthesis and stereoselective pheromone production with improved atom economy over classical Wittig and Julia routes.

A recurring theme across all applications is the critical role of catalyst engineering in overcoming process limitations: reducing ruthenium loading, minimizing isomerization side reactions, broadening functional group tolerance, and enabling efficient ruthenium removal from final products. These advances collectively position olefin metathesis not merely as a laboratory curiosity but as a scalable, green, and economically viable platform for next-generation industrial synthesis.



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PL-7

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Abstract

Abstract Awaited

PL-8

Strategic Therapeutic Methodologies using Metal complexes: From Enzyme Modulation to High-Efficiency Phototherapy

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Cancer progression is driven by dysregulated signalling networks and persistent genetic mutations that promote inflammation, malignancy, cellular plasticity, and immune evasion. Metal-based therapeutics, most notably platinum(II) complexes, remain central to chemotherapy, with additional metals increasingly expanding this paradigm. A persistent challenge, however, is the design of metal complexes that retain biological efficacy after metal dissociation, relying on ligands with intrinsic targeting or therapeutic functions. Addressing this challenge is the central focus of our group (@SMTL_IISERK). Our early studies identified cellular thiol sequestration as a major mechanism underlying the deactivation of metal-based drugs. We subsequently developed strategies to overcome this limitation and redirect metal reactivity toward biologically relevant targets.[1-3]

In particular, we have investigated imidazole- and benzimidazole-based ligands by conjugating them with drugs in clinic or in clinical trials to modulate their properties and dose tolerance. Our results demonstrate that the –NH functionalities play a critical role in modulating cytotoxicity through variation in stimuli. Building on this foundation, we have developed BODIPY and Ir(III) based complexes that can downregulate peroxiredoxin or generate suproxide/excited-state proton-coupled electron transfer (ES-PCET). The subtle changes in the structure and electronic properties makes them exhibit distinct killing mechanism. Collectively, this work expands the scope of metal-based anticancer therapeutics and enables the rational design of dual-targeting, stimuli-responsive agents with enhanced precision and efficacy.

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KEYNOTE

KL-1

Anticancer Metallodrugs: Solution Stability, Protein Interaction, and Cellular Localization

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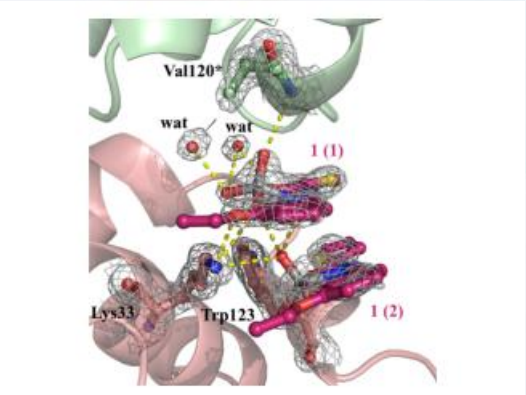
Metal-based luminescent drugs are in high demand today for diagnostics and therapeutics. In anticancer research, a fluorescent compound with low cytotoxicity, high fluorescence properties, and organelle specificity would be useful for diagnosing physiological disorders related to that organelle. In short, it can act as a real-time tracking bioimaging agent. Similarly, fluorescent compounds with high cytotoxic properties help evaluate the cell death mechanism more accurately. Therefore, nowadays the design of anticancer metallodrugs has received great attention, which exhibits the combined modalities of therapy and diagnostic imaging as so-called "theranostics" agents. As an alternative to platinum-based anticancer drugs, many metal-based compounds have been studied. However, their mechanistic pathways of cell death are still less explored. Again, main-group metal probes are rare in bioimaging. Thus, encouraging findings from the pharmacological investigation of metal complexes offer an opportunity to explore how these transition and main group metal complexes can be used in "biomedical molecular imaging." Our group has begun investigating the metal-based anticancer and bioimaging agents based on transition and main group metals with various bioactive ligands [1-11]. During this presentation, I will discuss luminescent metal-based chemistry and its biomedical applications.



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KL-2

Highly Selective and Sustainable Oxidation of Biomass-Derived 5-HMF to HMFCA over Polymer-Supported Vanadium- and Tungsten-Based Catalysts

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The increasing demand for sustainable alternatives to fossil resources has intensified research on the valorization of biomass as a renewable feedstock for the production of high-value chemicals. Among biomass-derived platform molecules, 5-hydroxymethylfurfural (5-HMF) has emerged as an important intermediate for the synthesis of valuable bio-based products. Its selective oxidation to 5-hydroxymethyl-2-furancarboxylic acid (HMFCA) is a significant yet challenging transformation. HMFCA has attracted considerable attention as it serves as a versatile precursor for the production of bio-based polymers, pharmaceuticals, and biofuels. The majority of reported methods for HMFCA synthesis typically employ expensive noble-metal-based catalysts [1].

In our recent work, we developed a series of heterogeneous catalysts consisting of peroxido complexes of non-noble metals, namely vanadium (V), niobium (Nb), and tungsten (W), immobilized on functionalized polystyrene resin. These catalysts exhibited excellent performance in the selective oxidation of HMF, achieving complete conversion with over 99% selectivity toward HMFCA, using environmentally benign hydrogen peroxide (H_2O_2) as the oxidant and water as the solvent. Moreover, these supported catalysts efficiently mediated other selective oxidative transformations, including olefin epoxidation, thioether sulfoxidation, and phenol hydroxylation, under eco-friendly, organic-solvent-free conditions. Operational simplicity, easy recyclability with consistent activity–selectivity profile are notable advantages of these catalytic systems. This presentation will provide an overview of these findings and highlight the potential of polymer-supported peroxido-metal catalysts for sustainable organic oxidation processes.

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KL-3

Morphological transition in synthetic bone materials

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Hydroxyapatites single crystals have been investigated for more than past half century for laser host applications. However, the tremendous need for the implantation materials to replace the metals in human body and teeth propelled researchers to explore hydroxyapatites for bonding to tissues and their growth. Both glassy and crystalline hydroxyapatites which affect metabolic processes such as tissue growth and healing are affected by the electrical, electrochemical and optical properties investigated in this study. We have experimentally observed that impurities play very important role in morphological transition of kidney stones also. Hench et al. [1-2] proposed that bioactive glasses of this class have great potential and developed several compositions and their research demonstrated that several compositions of bio glasses such as "45S5 Bioglass" have good properties for bonding to bones and soft tissues. Commercial materials listed as "45S5", "13-93B3" and "1605" have been developed and discussed by them for very good activities. It has been realized that more than 65% bone is some form of hydroxyapatite. We synthesized several hydroxyapatite silicates and phosphor borate bio active glasses by using carbonates, oxides, borate, phosphate, and silicates source materials to study the effect of high energy radiation. SEM morphology and EDX for each bio active glass showed that a significant time (>80 hours) for processing was required to achieve the homogeneous materials. This was needed for bio glasses in which we added gallium and titanium for their dissolution. The electrical properties, including capacitance decrease significantly for the silicate glasses. However, the electrical resistivity increases significantly. Bioactive glasses showed very good stability at the bias voltage of 50 mV to 1000 mV. Capacitance and resistance were constant for a particular frequency. Several compositions of hydroxyapatites were studied and development of mechanism for phase transition from crystalline to glass materials were proposed. We observed that during transition hexagonal morphology is formed which changes to glassy phase depending on the cooling conditions and compositions. Irradiation of silicate bio glasses showed huge effects on the electrical characteristics such as dielectric constant (hence polarity) and resistivity of the materials while optical properties showed small changes. The IR and Raman spectra for irradiated glasses exposed for 24 hours showed very small change. Morphological results showed that substitution of gallium, magnesium and /or titanium affect the transition to glass formation. The addition of selenium showed great potential to improve the mixing and glass formation without titanium and gallium precipitates in the matrix. We also demonstrated that bioactive glassy materials can be processed using organic media at much lower temperature. These results have great potential to understand the design of bone materials and morphology and control of kidney stones.

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KL-4

Importance of Chirality and Asymmetric Synthesis of Cyclic Molecules

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Chirality can be defined as the potential of a molecule to occur in two asymmetric forms that are non-superimposable mirror images of each other without changing the atomic composition, atom-atom connections, or bond orders. This phenomenon generally occurs due to a difference in the three-dimensional orientation of four different substituents attached to a single central atom, creating what can be considered left-hand and right-hand versions of the same molecule. These two versions of the molecule are referred to as enantiomers. As of 1992, governmental regulations on drug safety and efficacy have become stricter with regard to compounds that have stereochemistry. This has added complexity to the drug discovery process from initial virtual and experimental screening, through the rational design and synthesis, to clinical trial data analysis and manufacturing quality controls. When a compound can exist in several different stereochemical configurations, experimental work must be able to identify the stereoisomers present and ascribe biological effects to each of the stereochemical entities present since one stereoisomer may have quite different effects compared to another.

Cyclic compounds, because of the unique shapes, reactivities, properties, and bioactivities that they engender, are the majority of all molecules involved in the biochemistry, structure, and function of living organisms, and in man-made molecules such as drugs, pesticides, etc. Our group is interested to develop asymmetric synthesis of cyclic molecules.

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KL-5

Mechanistic Sights of Organometallics in Mitochondria for Cancer Therapy

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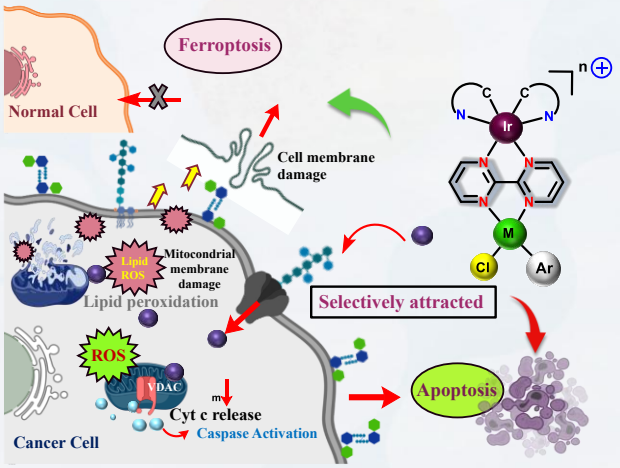
Mitochondria, the 'powerhouse of the cell' or 'local energy gradients' serve as highly dynamic organelles and arbitrators of cell's life and death. Incessant proliferation and undaunted growth of cancer cells are nourished by the immensely exploitation of the mitochondria. The design of mitochondria-demolishing anticancer agents can, therefore, be the significant weapons for efficiently treating the cancer. But chemoresistance and systemic toxicity are inexorable issues associated with the traditional chemotherapy. To securely cut-off the energy source of the cancer cells, contriving of the mitochondria-targeting prodrugs will be "kill of two birds with one stone" strategy, where prodrugs remain inactive at the outset and liberate active form of the drugs either by internal stimuli like copious thiols, acidic pH, and reactive oxygen species (ROS) in tumour tissue microenvironment or by external stimuli like localised light, ultrasound, electric impulse, magnetic field and radiation after reaching at the target-site. To abate the world-wide rampant prevalence of cancer, recently we have developed organelle targeted Ru(II)/Ir(III)/Re based half-sandwich and cyclometallated complexes for ROS mediated selective dynamic therapy with or without visible light irradiation (CDT or PDT) enhancing the therapeutic potential against the distinct tumour microenvironment (TME) (**Figure 1**).[1]

Keywords: CDT, PDT, Bioorganometallics, ROS, Heterobimetallic complex, Cancer theranostic



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INVITED

Targeting Glioma with Hybrid PARP-1 Inhibitors via DNA Damage and ROS Generation

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Glioma represents the most common class of malignant primary brain tumors in adults, with Glioblastoma multiforme (GBM) being the most aggressive subtype[1]. Despite advances in treatment, including surgical option followed by radiotherapy and chemotherapy, patient outcomes remain poor. This highlights the urgent need for more precise and effective therapeutic strategies. Poly(ADP-ribose) polymerase-1 (PARP-1)[1], a key enzyme involved in DNA repair, is overexpressed in glioma and represents an important therapeutic target. However, the major hurdle lies in developing compounds capable of crossing the blood–brain barrier[2]. In this work, a series of fused hybrid heterocycles were designed and synthesized as novel PARP-1 inhibitors (PARPi). The most potent compound in the series, induced apoptosis in glioma cells by promoting PARP cleavage, triggering DNA damage, and elevating reactive oxygen species (ROS) levels, offering a promising scaffold for future drug development.

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IL-2

Biocatalysis at the Chemistry–Biology Interface: Enabling Sustainable Technologies

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Abstract:

Biocatalysis has emerged as a powerful tool at the interface of chemistry and biology, offering transformative solutions for sustainable chemical synthesis. By integrating the principles of green chemistry with enzyme-driven selectivity, biocatalytic processes enable environmentally benign, energy-efficient, and highly selective routes for the production of valuable chemicals.[1] This synergy between chemical and biological sciences is redefining modern process development, particularly in the pharmaceutical sector.[2,3]

This invited lecture will highlight our contributions at CSIR-IICT toward the sustainable production of API intermediates using biocatalytic and chemo-enzymatic strategies. Emphasis will be placed on the development of robust enzymatic platforms, addressing challenges such as substrate inhibition, solubility limitations, and process scalability. Case studies on the synthesis of L-phenylalanine derivatives and steroid biotransformations will be presented to demonstrate the practical implementation of green and sustainable methodologies (Figure 1).[4]

Figure 1:

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IL-3

Mitochondria-derived Vesicles and Mito-nuclear Trafficking of Proteins in the Heart

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Abstract: Mitochondria, in addition to being central energy producers of the cell, act as signalling hubs interacting with several other organelles directly and indirectly. Since most mitochondrial proteins are encoded in the nucleus, mitochondria must signal the nucleus to alter metabolism or gene expression in response to external stimuli. These signals, known as retrograde signalling from mitochondria to nucleus, determine mitochondrial functionality at the basal state and in response to stress. Cardiac cells rely heavily on mitochondrial oxidative phosphorylation for >95% of cellular ATP production. Additionally, mitochondria in healthy adult hearts are ovoid and do not undergo fission-fusion events characteristic of other cell types. Nevertheless, the genes regulating mitochondrial dynamics are abundantly expressed in the heart, suggesting that these proteins may be utilised in alternative quality control pathways. One recently identified pathway involves mitochondria-derived vesicles (MDVs) that carry damaged mitochondrial proteins to lysosomes for degradation. Mitochondria-derived vesicles (MDVs) are a set of small single or double-membrane vesicles of sizes 70-150 nm originating from the mitochondria. Our lab is interested in understanding MDV biology – biogenesis, cargo selectivity and trafficking–in the cardiac system and its role in mitochondrial quality control during cardiac pathophysiology.

Recent studies indicate that mitochondrial proteins, such as Pyruvate dehydrogenase (PDH), can be directly transferred to the nucleus to perform moonlighting roles. We show that the direct transit of large protein complexes to the nucleus in the heart is mediated by MDVs, establishing a novel mito-nuclear trafficking route. Following an unbiased proteomic approach to detect cargo proteins in cardiac MDVs, we screen for the presence of MDV cargo in the nucleus. Pyruvate dehydrogenase complex (PDH) and Cytochrome c oxidase subunit IV isoform 1 (COX4I1) are packaged into MDVs in cardiomyocytes. However, only PDH is targeted to the nucleus in this cell type, demonstrating that a subset of cargo-selective MDVs fuse with the nucleus. Using in vitro reconstitution approaches, we show that MDV docking and PDH nuclear delivery are NEM-sensitive. In rat cardiomyoblasts, this pathway of mito-nuclear PDH shuttling is enhanced under pyruvate supplementation. Mitochondrial stress increases MDV biogenesis but decreases its nuclear targeting. We envisage cargo triage in which functional proteins are directed to the nucleus basally and perform dual roles, while damaged proteins in MDVs are directed to lysosomal degradation. Mito-nuclear trafficking thus represents a basal physiological pathway in cardiac cells that enables cargo shuttling from mitochondria to the nucleus.

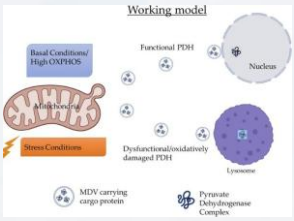

Figure 1. Differential trafficking of PDH in health and pathophysiology- working model

Keywords: Mitochondria-derived Vesicles (MDVs), Pyruvate Dehydrogenase (PDH)

Acknowledgement: This work was supported by DBT Ramalingaswami Fellowship (BT/RLF/Re-entry/51/2019) and SERB POWER grant (SPG/2021/003267)

IL-4

Asynchronous Transition State Tuned from Remote Site for Nitrite Reduction at Copper Centre

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Nitrite (NO_2^-) is known as reseorviour for nitric oxide (NO) which is involved in several important biological functions e.g. vasodilation and neurotransmission. In biology, Cu-nitrite reductase performs NO_2^- to NO conversion while alternatively NO_2^- can be chemically reduced to NO at copper centre via oxygen atom transfer (OAT) to phosphines or proton coupled electron transfer (PCET) by phenol. This work demonstrates systematic stabilization of LUMO energy of a series of Cu^{II}-NO_2^- complexes by remote site modification which results in anodic shift in $Cu^{II/I}$ redox potential and enhanced OAT and PCET activity. The observed increase in OAT and PCET reactivity is attributed to an increase in the extent of asynchronicity in the corresponding transition states which was controlled from remote site modification.

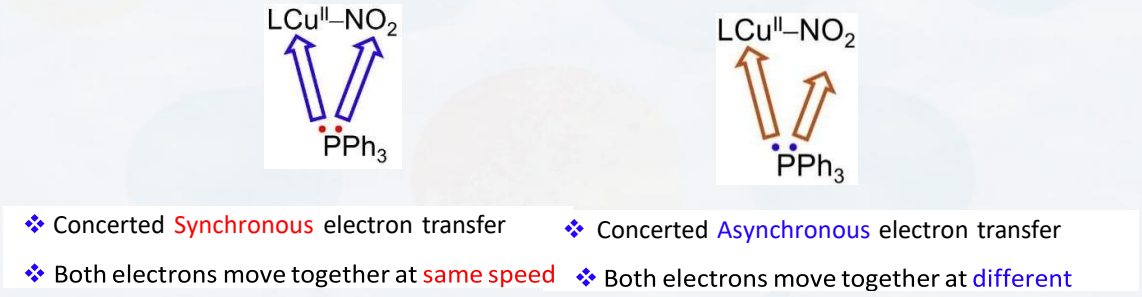

Figure 1. Synchronous and Asynchronous electron transfer

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IL-5

Drug discovery research in India: Current trends and analysis of Industry-Academia and Government collaborations

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Abstract:

India has long been recognized as the "pharmacy of the world," owing to its stronghold in the generics and biosimilars market. However, its contributions to innovative drug discovery, particularly in the development of new chemical entities (NCEs), have been relatively modest. This talk will provide a critical overview of the current trends in drug discovery research in India, highlighting both the scientific advancements and systemic challenges that define the landscape. Recent years have witnessed a growing emphasis on next-generation drug delivery strategies, including antibody–drug conjugates (ADCs), nanoparticle-based formulations, bioconjugates designed to enhance therapeutic efficacy and reduce systemic toxicity. One such innovation is our Exa-HSA-Nanoparticle, which demonstrates promising potential as a novel delivery system for oncology applications. These advances underscore the importance of multidisciplinary collaboration among industry, academia, and government agencies. Despite these scientific strides, India's NCE output remains limited. A key reason lies in the industry's preference for low-risk, high-reward generics, coupled with fragmented collaboration frameworks and limited translational funding. This presentation will analyze the evolving role of government initiatives such as the Anusandhan National Research Foundation (ANRF) and explore how academia–industry partnerships can be restructured to incentivize innovation.

By presenting a comprehensive analysis that blends technical progress with policy insights, this talk aims to foster dialogue on how India can transition from a generics-dominated ecosystem to a globally competitive hub for innovative drug discovery.

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From Monotherapy to Dual Therapy: Engineered nMCM-48 based hybrid systems for controlled delivery of antidiabetic drugs

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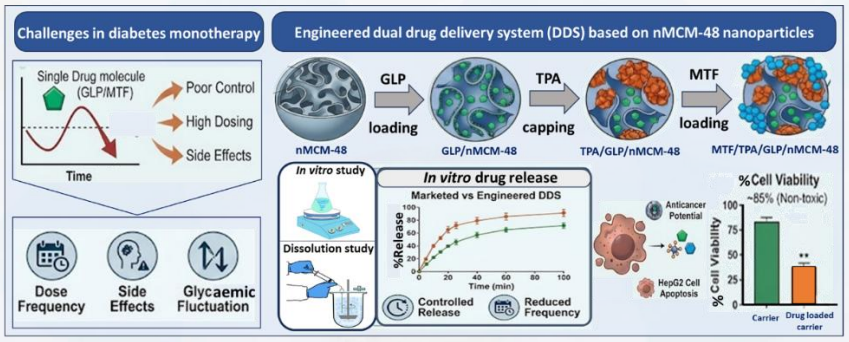
Diabetes mellitus (Type 2) is a heterogeneous metabolic disorder necessitating complex therapeutic interventions. To manage this condition, Glipizide (GLP), a second-generation sulfonylurea, and Metformin Hydrochloride (MTF), a biguanide, are widely administered as frontline treatments. However, monotherapy with these drugs frequently fail to achieve optimal glycaemic control due to short biological half-lives and dose-dependent side effects like hypoglycaemia. Consequently, clinical management has shifted towards dual drug therapy to leverage synergistic effects and improve patient compliance. In this direction, designing a nano drug delivery system (DDS) demonstrates potential advantages in enhancing drug solubility, controlling release and overcoming physiological barriers [1-3].



In the present work, a dual DDS based on 12-tungstophosphoric acid (TPA) and MCM-48 nanoparticles (nMCM-48) was engineered as well as characterized for the co-delivery of GLP and MTF. *In vitro* release studies were conducted at pH 1.2 and pH 7.4 at 37 °C, supported by dissolution studies using a USP Type II apparatus. The results were compared with marketed formulations, including Glynase, Glycomet and Glirum-MF, demonstrating that the DDS exhibits a more controlled release profile. Furthermore, considering the anticancer potential of these drugs, MTT assay against HepG2 cells indicated that the carrier is non-toxic while the drug loaded nanocarrier exhibits significant apoptotic activity. This study highlights a promising hybrid dual DDS that addresses the limitations of monotherapy while providing secondary therapeutic benefits in oncology.

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IL-7

Mechanistic Insight into the Electroreduction Pathway of Nitrate to Ammonia on Metal Oxides

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Selective conversion of nitrate, a well-recognized nitrogen contaminant, into a value-added product like ammonia, through an electrochemical approach, offers various advantages over chemical methods as it requires nominal energy, doesn't require reducing agents, leaves no hazardous by-products, and achieves high selectivity under mild conditions. Moreover, a better aqueous solubility of $[NO_3]^-$, "N=O" bond dissociation energy of only 204 kJ mol^{-1}, and positive electrochemical potential ($E^0_{[NO3]^-/NH3}$: 0.88 V vs SHE) make the electrochemical nitrate reduction reaction (eNO_3RR) a thermodynamically more favourable pathway of NH_3 production than the conventional Haber-Bosch or electrochemical N_2 reduction. Production of NH_3 through NO_3RR proceeds through multistep ($8e^-/9H^+$) process forming various active intermediates (*NO_2, *NO, and *NH_2OH; *: active site). However, the design of an NH_3 selective electrocatalyst for NO_3RR study and understanding the reaction pathway remains a fundamental challenge. Recently, our group has worked on various metal oxide-based cathode materials for the selective reduction of nitrate to ammonia. In-depth electro-kinetics, in-situ spectroscopy and labelling studies were performed to establish the eNO_3RR pathway. In my talk, I will be delivering an overview of our current findings.

IL-8

Tuning the functional properties of flavin entity for biological applications

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Abstract:

Naturally occurring flavin derivative encompassing a tricyclic core is known to play a significant role in diverse biochemical process.[1] Nature utilizes the apoprotein matrix to regulate the inherent properties of the flavin entity for its desired application. Interestingly many of its these properties failed to exhibit themselves in absence of protein matrix. Considerable efforts were made to design and develop synthetic models built around the flavin core especially toward harnessing its catalytic behaviour.[2] However, efforts to harness its intrinsic properties for biological application are limited, plausible due to solubility related issues with the synthetic design for cellular studies and or, loss of functional behavior within the cellular system. Our interest in creating subtle chemical modification to tune to functional properties of the flavin core, has led us to design and development of synthetic model around the flavin core with enhanced cellular internalization, while retaining its emissive nature. The present talk will focus on some of the recent finding with focus on developing flavin analogues for biological applications.[3-5]

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IL-9

Natural Products as Dual-Target Agents: Bridging UPR and Redox Signaling

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The pathogenesis of Parkinson's disease (PD) is increasingly recognized as a multifaceted failure of cellular homeostatic mechanisms, primarily driven by the reciprocal relationship between the Unfolded Protein Response (UPR) and redox imbalance. The accumulation of misfolded proteins, specifically α-synuclein, within the endoplasmic reticulum triggers UPR signaling, which in turn exacerbates oxidative stress. Conversely, a compromised redox status further impairs protein folding, creating a self-perpetuating cycle of neurodegeneration. While Levodopa remains the clinical prime treatment for PD, it primarily provides symptomatic relief without halting disease progression, underlining the urgent need for neuroprotective agents suitable for chronic administration. Utilizing experimental models of PD, we demonstrate that bioactive natural scaffolds can simultaneously attenuate ER stress-induced signaling and neuronal apoptosis. Our findings reveal that these compounds do not merely function as passive scavengers of reactive oxygen species, but rather as sophisticated modulators of the UPR-redox axis—recalibrating key markers such as GRP78 and GADD153 while restoring mitochondrial integrity. By bridging these two pivotal signaling pathways, natural products offer a poly-pharmacological advantage over conventional mono-targeted therapies, supporting their potential as holistic neuroprotective strategies in the management of Parkinson's disease.

IL-10

Drug Discovery Approaches through Structure, Computation and Chemistry: A Case Study on Anti-CoVID Molecule Development

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Abstract

The structure of the molecule or biological target is the key, which tells where to work and how. Computation and algorithm, including AI/ML, animate and analyze the facts to understand complex phenomena and provide the means for that might work. Overall structure, computation, and biological studies guide medicinal chemists, ultimately leading to cures.

COVID-19 has impacted the world and underscored the need for preparedness in our scientific efforts to address genuine societal demand to protect human health in adverse situations. The FDA approved antivirals remdesivir and molnupiravir, which target non-structural proteins essential for viral replication. However, issues such as drug side effects, mutations and other drug-like limitations drive new-molecule discovery. Molnupiravir contains a hydroxylamine (NH-OH) moiety, a key pharmacophore that inhibits RdRp by being incorporated into the primer strand. Herein, we report a new non-nucleoside inhibitor containing a 2-pyridone-3-carboxylic acid scaffold with an NH-OH group, demonstrating improved efficacy, reduced toxicity and potent activity against SARS-CoV-2 replication in vitro. The SAR study shows that substituting the NH-OH group for NH-R reduces activity. This finding demonstrated the pharmacophoric role of the amino hydroxyl group in the scaffold's activity. One identified compound demonstrated significant activity comparable to the existing anti-SARS-CoV-2 drug nirmatrelvir. The identified compound does not inhibit the SARS-CoV-2 RdRp or 3CL protease, suggesting that the lead candidate acts through a novel antiviral mechanism.

References: Japanese Patent Filed Followed by PCT Filing by our research group, in collaboration with Kagoshima University, Japan, for the development of an Anti-CoVID molecule: JP2025-504258527, 29/12/2025

IL-11

Cooperative Catalysis in Electrochemical Ammonia Oxidation

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Ammonia (NH_3) is a promising carbon-free energy carrier due to its high energy density and hydrogen storage capacity. Its utilization in energy systems relies on the ammonia oxidation reaction (AOR), which is critical for direct ammonia fuel cells (DAFCs) and hydrogen production. Herein, we will discuss two distinct mechanisms for ammonia activation using homogeneous molecular catalysts: i) a robust and inexpensive Ferrocene-based molecular electrochemical mediator, *N*-pyridylferrocenecarboxamide (Fcpy), for AOR. The Fcpy- mediated AOR exhibits the N_2 Faradaic efficiency (FE) of 94.7 %, along with the concomitant production of H_2 (FE = 87.3 %). Mechanistic studies reveal the crucial role of H-bonding through the pyridyl moiety of Fcpy in facilitating N–H bond activation.[1] ii) a cooperative effect of tris(4-methoxyphenyl)amine as a redox mediator in homogeneous Cu-catalyzed AOR. We show that the mediator's lower redox potential, higher diffusion coefficient, and faster heterogeneous electron-transfer kinetics lead to dramatic rate enhancements at a lower potential relative to direct $Cu^{III/II}$ cycling, which suffers from higher redox potentials, slower mass transport, and sluggish electrode kinetics. This mediator-assisted pathway not only circumvents the high N-H BDFE of the Cu(II)-NH_3 precursor but also facilitates the key bimolecular hydrazine-forming step, thereby lowering kinetic barriers and enhancing overall catalytic turnover.

Together, these findings establish a mediator-enabled design paradigm for molecular AOR catalysis and highlight how rational redox-cooperative strategies can unlock challenging N-H bond activation.

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IL-12

Computation-Driven Rational Design of Peptides as Inhibitors of Human Islet Amyloid Polypeptide Fibrillation in Type 2 Diabetes

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Abstract: The fibrillation of the neuropancreatic hormone human islet amyloid polypeptide (hIAPP) to β-sheet-rich cytotoxic aggregates has been implicated in the pathogenesis of T2D (type 2 diabetes).[1] Scrocchi et al. unveiled a fragment peptide SNNFGA (residue 20-25) of hIAPP as a potential inhibitor of hIAPP fibrillation.[2] Continuing with our efforts to illuminate the inhibitory mechanism of various inhibitors against protein aggregation-derived diseases,[3] a library of 863 hexapeptides based on amyloidogenic fragment peptide SNNFGA has been computationally designed and evaluated against hIAPP fibrillation in this work.[4] The MM-PBSA analysis depicted peptides TNNWPL, TQNWAP, and TQNWVP bind to hIAPP with higher affinity than SNNFGA. Notably, TQNWVP displays a more pronounced inhibition effect than other peptides due to its ability to block the conformational transformation of hIAPP from a random coil to aggregation-competent β-sheet conformation. TQNWVP exhibited the highest inhibitory activity (Inhibition=75%, IC_{50}=6.19 ± 0.31 μM) against hIAPP fibrillation, consistent with the computational results. Importantly, DLS analysis confirmed that TQNWVP reduces the size of hIAPP aggregates. Peptides exhibited a satisfactory safety-efficacy profile and efficiently alleviated the hIAPP aggregates-induced cytotoxicity in rat insulinoma (INS-1) and human embryonic kidney HEK293 cells. The *in silico* and *in vitro* studies in this work highlight a new peptide, TQNWVP, designed by the modifications in the amyloidogenic core region sequence of hIAPP as a promising inhibitor of hIAPP aggregation. Furthermore, the synergistic effect of three key mutations (N→Q, F→Y, and A→P) in the amyloidogenic fragment of hIAPP (NFGAILSS) in yielding a new potent inhibitor (QYGPILSS) of hIAPP fibrillation will also be discussed (Fig. 1).[5]

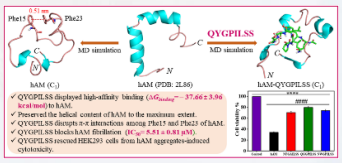

Fig. 1: Combined *in silico* and *in vitro* techniques highlight a new peptide, QYGPILSS, derived from the amyloidogenic core sequence (NFGAILSS) of hIAPP by key mutations as a promising inhibitor of hIAPP fibrillation.

Keywords: Type 2 diabetes; peptides, hIAPP fibrillation; molecular dynamics; thioflavin T assay

Acknowledgements: B.G. acknowledges the CSIR, India [02(0451)/21/EMR-II] and ANRF, India (CRG/2023/000088 and CRG/2022/008244) for the financial support. D.R. thanks CSIR, India [02(0451)/21/EMR-II] for the JRF.

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IL-13

Metal Free Porous Carbon Materials Based Electrocatalyst for Sustainable Hydrogen Fuel Production

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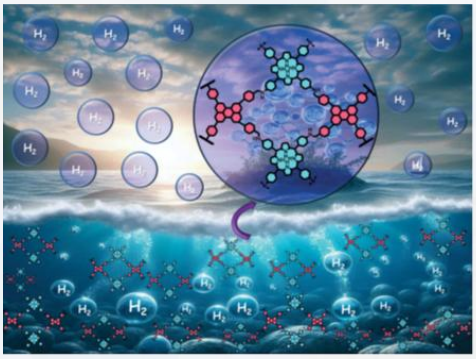
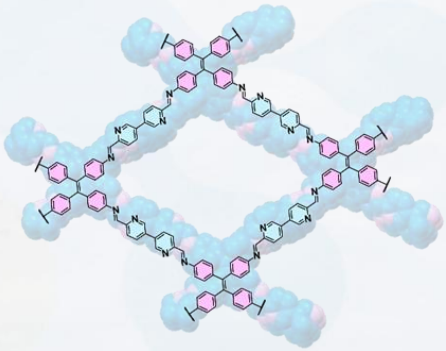
Due to the rise of global warming and climate change, people have started moving away from fossil fuels and leaning towards green, renewable solar and wind energy. Hydrogen, as a renewable and clean energy resource, is a promising future fuel. Hydrogen production through metal-free electrocatalyst water splitting is crucial for obtaining sustainable and clean fuel. Plentiful, economically viable, and easily processed materials are commercially important for green hydrogen production.[1-7] Herein, we are devoted to developing greener energy through the integration of chemistry and materials, optimal utilisation of carbon resources, chemical energy storage and conversion, and commercially viable low-cost carbon material preparation for energy production and storage applications.





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

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IL-14

Application of cellulose-based nanomaterials in the sensing of pesticides

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Abstract:

Materials based on cellulose and nanocellulose have shown great promise as pesticide-sensing platforms due to their unique properties, including high surface area, tunable surface chemistry, biodegradability, and superior mechanical properties. Numerous hydroxyl groups on the surface of nanocellulose can be readily functionalized with recognition elements, such as conducting polymers, enzymes, or antibodies, enabling specific detection of pesticide residues. These materials act as a supporting matrix for the active sensing component and are widely used in the fabrication of electrochemical, optical, and colorimetric sensors. Nanocellulose can enhance electron transfer in electrochemical sensors and serve as a scaffold for immobilizing enzymes such as acetylcholinesterase to detect various pesticides, including organophosphates and carbamates. Additionally, cellulose-based sensors offer low-cost, portable, and disposable solutions for on-site monitoring, particularly in environmental and agricultural applications. Herein, we report the synthesis of various cellulose- and nanocellulose-based materials for the efficient sensing of organophosphate and carbamate pesticides using different approaches, such as colorimetric and potentiometric methods. The developed sensor exhibits excellent sensitivity, selectivity, and detection limits. Overall, cellulose- and nanocellulose-based sensing platforms represent sustainable, efficient alternatives for rapid, sensitive, and eco-friendly pesticide detection.

IL-15

Abha Mishra

Professor, School of Biochemical Engineering, IIT BHU

Abstract Awaited

IL-16

Atropisomerism in the Realm of Pharmaceutically Relevant Compounds

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Since the collisions in the steric bulk of adjacent big substituents limit the atropisomers' rotation around a single bond, they are not superimposable stereoisomers.[1] Biaryl atropisomers are archetypical axially chiral compounds having a single stereogenic axis. Conversely, protocols for the simultaneous installation of multiple stereogenic axes onto different substrate sites have not been widely reported because of the difficulties in managing the sterically impacted multiple stereogenic axes diastereoselectively and enantioselectively.[2] An efficient cross-dehydrogenative coupling of electronically rich and sterically congested benzofulvene with bi-(hetero)aryl moieties to construct an axially chiral benzofulvene core with good reactivity and excellent enantioselectivity has been realized.[3]

Atropisomeric pyrazoles are widely found in natural products, pharmaceuticals, ligands and catalysts owing to their featured biological and catalytic activities.[4] However, facile and de novo construction of these motif remains largely underexplored. Herein, we report silver phosphate catalyzed direct 5-endo-dig nucleophilic cyclization of alkynyl naphthalene substituted hydrazides under mild conditions, affording various C−C axially chiral pyrazoles in excellent yields and enantioselectivities.[5]

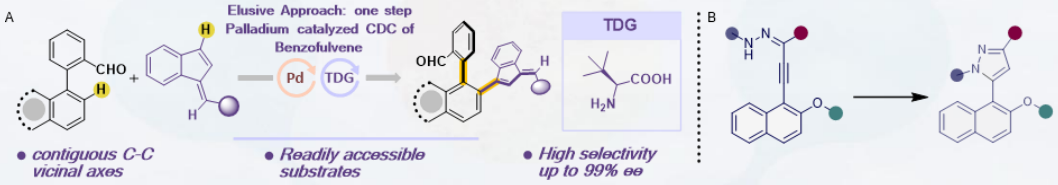

Figure 1. Atropselective synthesis: [A]. Chiral 1,2- diaxial biaryls, [B]. Axially chiral aryl pyrazoles

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IL-17

Transition Metal-Catalyzed Annulation Platforms for Pharmacologically Relevant Tetralone and Chromanol Frameworks

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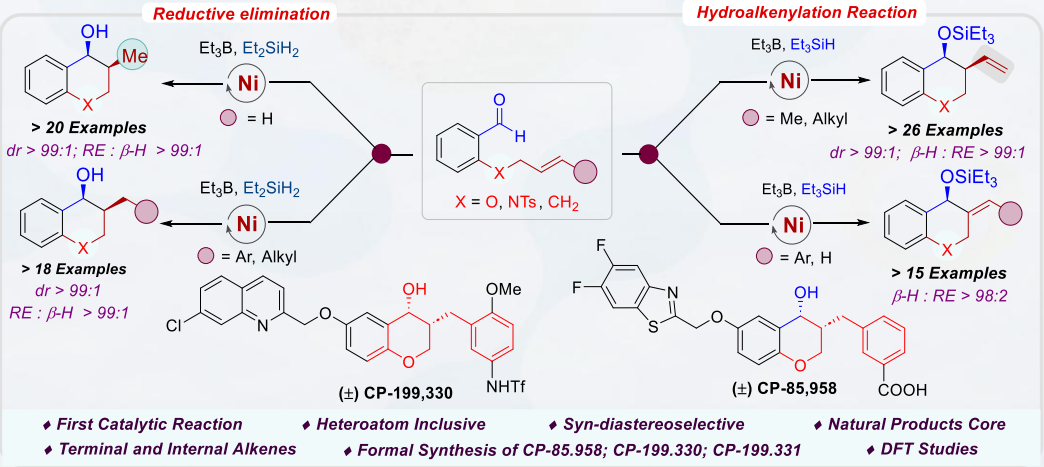
Transition-metal-catalyzed approaches that rapidly assemble complex, heterocycle-rich scaffolds from simple precursors are central to bridging synthetic chemistry with modern chemical biology and drug discovery. In this context, our group has developed a unified annulation platform using palladium(0) and nickel(0) catalysis to access tetralone, chromanone, and chromanol motifs that recur in bioactive natural products and clinical candidates. A Pd(0)-catalyzed [3+2] cycloaddition between vinylcyclopropanes and activated coumarins delivers cyclopenta[c]chromanones bearing up to four contiguous stereocenters with high diastereocontrol. Complementarily, a Pd(0)-catalyzed (3+3) annulation of donor-acceptor vinylcyclopropanes with 2-formyl phenylboronic acid derivatives furnishes vinyltetralones under mild conditions via a π-allyl–palladium zwitterionic intermediate, providing versatile tetralone frameworks for downstream functionalization. Orthogonally, a Ni-catalyzed diastereoconvergent intramolecular alkene-aldehyde reductive coupling of *O*-allyl/*O*-cinnamyl salicylaldehydes affords *syn*-chromanols from both terminal and internal alkenes, enabling formal syntheses of leukotriene D4 antagonist chromanols CP-199.330, CP-199.331, and CP-85.958. The same reaction manifold, in the presence of Et_3B/Et_3SiH as reducing agent, promoted regioselective *β*-hydride elimination, delivering *syn*-selective vinylchromanols. The biological evaluation of these compounds revealed that the cyclopenta[c]chromanones possess interesting anti-cancer activity.



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IL-18

Rational Design of Phenol–Triazole Derivatives as Modulator of Aβ/ Cu^{2+}–Aβ Aggregation and Cytotoxicity

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Alzheimer's disease (AD) is a neurological disorder characterized by a spectrum of symptoms such as memory loss and cognitive decline. AD is a multifaceted disease and designing multipotent ligands is an effective stratagem for AD treatment [i]. In this regard, the pharmacophore moiety of clioquinol (CQ, metal chelator) was employed to design the multifunctional phenol–triazole derivatives **4(a–p)**. In particular, **4k** with an *o*-I group on the phenyl ring was as efficient as curcumin in inhibiting $A\beta_{42}$ aggregation (inhibition efficiency **4k**= 90.5%, IC_{50}= 6.51 ± 0.01 μM) (Fig. 1). Furthermore, **4k** significantly disassembled the preformed $A\beta_{42}$ fibrils (Aβf, 92.5%), chelate Cu^{2+} ions, and inhibit Cu^{2+}–mediated $A\beta_{42}$ aggregation. Compound **4k** ceases the production of reactive oxygen species (ROS) as it acts as an antioxidant due to the presence of a phenolic hydroxyl group. Compound **4k** has a sufficient safety–efficacy profile and alleviates the cytotoxicity by $A\beta_{42}$ aggregates in SH–SY5Y cells. In addition, to study the modulation in the fibrillary architecture, hydrodynamic size, and structural transition of $A\beta_{42}$ in the presence of **4k** we resorted to transmission electron microscopy (TEM), dynamic light scattering (DLS), and circular dichroism (CD), respectively. The molecular dynamics (MD) simulations depicted a notable reduction in the conformational transformations in $A\beta_{42}$ monomer (Aβm) and Aβf on the incorporation of **4k**. Compound **4k** modulates $A\beta_{42}$ fibrillation by maintaining helix conformation and simultaneously reduces the sampling of β–sheet structures in Aβm, consistent with the CD results. The MM-PBSA analysis depicted a favorable binding of **4k** to Aβm (–42.12 ± 7.14 kcal/mol) and Aβf (–74.42 ± 4.98 kcal/mol) with a significant contribution of van der Waals interactions to the binding free energy. The deformation in Aβf chains in the presence of **4k** as visualized in the conformational snapshots depicts the destabilization potential of **4k** against Aβf. Finally, our results uncovered the potential of phenol−triazole derivatives as a promiscuous ligand for targeting multifaceted Aβ toxicity.

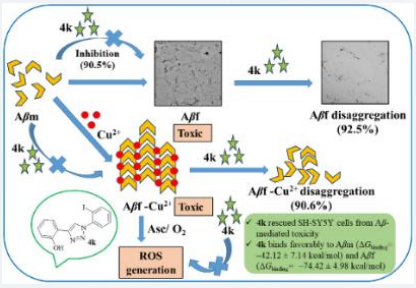

Figure 1: Combined experimental and computational studies in this work unveiled phenol–triazole derivative **4k** as a promising multifunctional inhibitor of AD targeting $A\beta_{42}$ and Cu^{2+}-induced $A\beta_{42}$ fibrillation as well as inhibiting the formation of ROS.

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IL-19

Synergistic Effect of $CoFe_2O_4$-85S Nano Bio-glass Composites for Hyperthermia

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Cancer, a devastating disease is a significant cause of mortality in recent times, continues to pose a formidable challenge in terms of finding effective treatments. In light of this challenge, we present a pioneering approach that combines bone tissue regeneration, hyperthermia and controlled drug delivery along with antimicrobial properties. This innovative strategy utilizes nanocomposites of 85S ($85SiO_2$-$10CaO$-$5P_2O_5$ (mol%)) bio-glass and cobalt ferrite ($CoFe_2O_4$) nanoparticles, synthesized using Stober's method and a modified microwave reflux method, respectively exhibit exceptional bioactivity and stability in simulated body fluid (SBF). A critical 7.5 wt% of cobalt ferrite based composite demonstrating the highest bioactivity substantiated by the formation of a hydroxyapatite layer upon immersion in SBF, indicates its potential for facilitating bone tissue regeneration. Significantly, CFO_7.5 stands out among the various nanocomposites due to its remarkable antimicrobial activity against both E. coli and S. aureus cells. Moreover, these nanocomposites demonstrate superparamagnetic behaviour at room temperature, making them amenable to hyperthermia applications, validated through magnetic measurements. The synergistic effects of hyperthermia and control drug delivery in treating cancer including *In-vitro* experiments is thoroughly discussed.

IL-20

Access to Functionalized N-Heterocycles via Electrochemical Synthesis and Annulation Reactions

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Benzazepines, dibenzoxazepines, benzoxazines, benzosultams, acridines, and tetrahydroisoquinolines constitute important heterocyclic frameworks frequently encountered in natural products and pharmaceutically relevant molecules. Owing to their broad biological significance, the development of efficient and sustainable synthetic methodologies for their construction and diversification remains highly desirable. In this presentation, recent advances from our group will be highlighted, focusing on the development of selective C–H functionalization strategies for these heterocycles. Our approach integrates electrochemical activation, transition metal catalysis, and spiro-annulation techniques to achieve structurally diverse and densely functionalized architectures under mild conditions. These methodologies provide streamlined access to complex heterocyclic scaffolds with potential biological relevance. [1-11]

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IL-21

Environmental sustainability approaches: Indian Pharmacopoeia Perspective

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Indian Pharmacopoeia Commission (IPC), Ghaziabad, a standard setting organisation is dedicated to upholding the highest standards of pharmaceutical quality and safety in India by regularly publishing Indian Pharmacopoeia (IP). IP quality standards are authoritative in nature and legally enforceable by law. In addition to contributing towards quality and safety, IP standards are supporting environmentally sustainable efforts by adopting modern analytical methods and technologies, more-ecofriendly alternatives for quality testing of drugs and pharmaceuticals. Key achievement includes transition from Thin layer chromatography (TLC) to High-Performance Liquid Chromatography (HPLC) and Gas chromatography (GC), decreased use of hazardous substances including carbon tetra chloride, chloroform and fluorinated solvents in testing. Moreover, IP is continuously moving towards reducing reliance on animal testing, supporting 3 R's (Replacement, reduction, refinement) initiatives by replacing *in vivo* rabbit pyrogen tests with *in vitro* bacterial endotoxin tests (BET), inclusion of general chapter on Monocyte activation test (MAT). In this way, IP is supporting environmental sustainability while maintaining high quality, safer product and regulatory compliance. Moving forward, IP is continuously collaborating with stakeholders to explore how changes in IP quality standard can promote environmental sustainability approaches.

IL-22

AI-Driven *Camellia sinensis* Inhibitors of P-Glycoprotein: From Nature to Market

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Abstract

Cancer is an ongoing public health concern due to its severe complications and high mortality rate. The available therapeutics are limited, and the ongoing resistance makes them ineffective. Concerning this P-Glycoprotein, a transporter and multidrug resistance protein belonging to the adenosine triphosphate (ATP)-binding cassette (ABC) family (ABC1), it plays a major role in drug resistance. Also, studies have found that green tea (Camellia sinensis) has anticancer properties. The process of discovering new drugs is being further enhanced by computational research aided by artificial intelligence. Therefore, this study aims to identify potent compounds in *Camellia sinensis*, which are further enhanced through AI-guided steps to improve their activity, followed by docking and dynamics analyses. The compounds of *Camellia sinensis* were collected from databases and used for high-throughput virtual screening using SP and XP modules, and docking analysis was performed. The docking analysis identified quercetin as a potent compound compared to others. Furthermore, the quercetin derivatives were designed using WADDAICA, an AI-based server, and subsequently redocked against P-gp, yielding Q5 as an enhanced, optimized compound. Subsequently, the simulation and post-simulation were performed, demonstrating the stability of the docked complex. The ADME analysis exhibits the drug-like properties of Q5. Collectively, the study suggests that the AI-assisted ligand could be a promising strategy for identifying compounds from *Camellia sinensis*. However, the result needs to be validated through an experimental approach to ensure the findings.

Keywords: Artificial Intelligence, Camellia sinensis, Docking, Dynamics, and quercetin

IL-23

Advancing Therapeutic Strategies for Microbial Resistance Through Multitargeting Hybrid Molecules

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ABSTRACT

The rising prevalence of multidrug-resistant (MDR) infections poses a substantial threat to global health and requires the development of innovative, comprehensive treatment strategies. The excessive and inappropriate use of antibiotics has facilitated the emergence of MDR bacterial strains [1]. Global estimates show that bacterial resistance caused about 1.27 million deaths in 2019 and contributed to nearly 4.95 million deaths worldwide [2]. Traditional 'one molecule–one target' drugs often become less effective due to resistance. In contrast, multitarget drugs offer greater efficacy with fewer side effects and reduced resistance. As a result, drug development is moving toward a 'one molecule–multi-target' strategy using hybrid molecule design [3].

In a study, a library of 52 virtual 1,4-naphthoquinone (NQ) hybrids incorporating natural moieties was screened using molecular docking and ADMET filters to identify multitargeting leads. Selected leads were synthesized and evaluated for antibacterial, antifungal, and anticancer activities. NQ hybrids with Menthol, thymol, and uracil demonstrated potent antibacterial activity (MICs of 4–12 μg/mL) against both Gram-positive and Gram-negative bacterial, as well as fungal strains. Derivatives showed anticancer activity against MCF-7, A549, MDA-MB-231, and SK-BR-3 cell lines presenting option for the treatment of cancer and associated microbial infections [4]. In several of our continued studies, NQ and coumarin-1,2,3-triazole hybrids have shown potential antimicrobial activity, as evidenced by promising results from both *in silico* analyses and subsequent experimental validation [5,6]. Overall, hybrid molecules offer opportunities to develop cost-effective, safer, broad-spectrum, less toxic, and multitargeting drug candidates for advancing therapeutic strategies for microbial resistance.

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IL-24

Preparation and Structural Characterization of Organometallic Complexes with Potential Biological Applications

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Abstract:

Organometallic chemistry has attracted considerable attention due to the diverse structural features and potential biological applications of metal-carbon bonded compounds [1-7]. In the present work, the design, synthesis, and structural characterization of novel organometallic complexes have been carried out using organic ligands containing nitrogen and oxygen donor atoms capable of coordinating effectively with metal centers.

wields and recrystallised The plexes were synthesized through controlled reactions of the selected ligands with appropriate metal precursors under optimized conditions. The resulting compounds were obtained in gr using standard methods. Their structural and bonding characteristics were investigated using various physicochemical and spectroscopic techniques, including elemental analysis, IR spectroscopy, and NMR spectroscopy. These studies provided important information regarding the coordination behavior of the ligands and the geometry around the metal centers. In addition, the crystal structures of selected complexes were determined by X-ray crystallography, confirming their molecular structures and coordination modes.

The analytical and spectral data indicate the formation of stable organometallic complexes with well-defined coordination environments. The results suggest that the geometry around the metal centers depends on the nature of the ligand and the metal ion involved.

These complexes are of particular interest because organometallic compounds have shown promising biological activities, including antimicrobial and anticancer properties.

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IL-25

Sustainable Design, Synthesis and Biological Evaluation of Novel Ferrocene Derivatives as Pyruvate Kinase M2 Modulators for Oral Cancer Therapy

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Abstract:

Metal-based compounds have emerged as promising therapeutic agents in cancer chemotherapy, particularly as current treatment regimens are limited by systemic toxicity and chemoresistance associated with cisplatin and other platinum-based drugs. Among organometallic scaffolds, metallocenes such as ferrocifens and related derivatives have shown notable anticancer potential in recent years. Pyruvate Kinase M2 (PKM2), a key glycolytic isoform responsible for catalyzing the conversion of phosphoenolpyruvate to pyruvate in the final step of glycolysis, plays a central role in sustaining the Warburg effect and is significantly overexpressed in oral squamous cell carcinoma. In this study, we report the sustainable design and synthesis of twenty novel ferrocenyl-pyrazoloquinolinone hybrids inspired by podophyllotoxin scaffolds, prepared through an efficient multicomponent synthetic strategy. Biological evaluation identified compound **4b** as the most potent analogue, exhibiting an IC_{50} value of **27.04 ± 3.91 µM** against the cisplatin-resistant oral cancer cell line **CAL27**. Mechanistic studies revealed that compound 4b induced early apoptosis and caused **S-phase cell cycle arrest**, indicating disruption of DNA replication processes. Furthermore, treatment with compound 4b resulted in a significant reduction in PKM2 expression, supporting its role as a PKM2-targeted anticancer agent. Electrochemical investigations demonstrated a favorable redox profile for 4b, highlighting the importance of the ferrocene moiety in mediating biological activity. Overall, these findings establish ferrocenyl hybrids as promising next-generation candidates for oral cancer therapy, capable of selectively targeting malignant cells while preserving normal cell viability.

IL-26

Organophotoredox-mediated Sustainable Chemical Synthesis

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Abstract:

The sustainable organic synthesis using clean, green and sustainable source of energy i.e. sunlight is the need of the hour. The use of visible light for carrying out chemical transformations has helped achieving this goal to a great extent. In last decade, the field of visible light-mediated organic synthesis has seen unprecedented refinement, innovation, and application. However, the use of metal-based photocatalysts i.e. polypyridyl complexes of iridium and ruthenium is not only against the principles of green chemistry, the high cost of these photocatalysts also render them unfavourable for industrial use. The discovery and successful application of several highly oxidizing as well as highly reducing organo-photocatalysts lately has helped developing more sustainable visible light photoredox-mediated chemistry.

In this context, we explored the reactivity of selected strong photoreductants (Hantzsch ester and Rh-6G)[1-3] as well as strong photooxidants (acridinium salts and pyrylium salts)[4-5]. In this presentation, our group's results on visible light-mediated synthesis of several valuable heterocycles/carbocycles employing the abovementioned organo-photocatalysts will be discussed.

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IL-27

Designing greener energy conversion system for a sustainable future

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Abstract

Global energy requirements are touching new meridians with the gradual advancement in the living standards and the day-by-day growing world population. This necessitates the exploration to seek for greener and sustainable energy reservoir systems which ought to be environmentally agreeable for such an intriguing purpose. Electrochemical energy conversion and storage devices offer some most alluring aptitudes for providing clean energy. To name a few of these include fuel cells, rechargeable metal-air/peroxide batteries and HCl/ H_2S electrolysis and likewise.[1,2] Oxygen being central to the processes in these devices, a lot of attention has been focused upon the study of oxygen chemistry in terms of oxygen reduction reaction (ORR) and also Hydrogen evolution reaction (HER) and thence to the melioration of the associated electrocatalysts. In the past decade research has depicted tremendous improvement towards the betterment of fuel cells/Zn based batteries/hydrogen production in its legions of shortcomings or corrigible features.[3,4] But still an infinite pursuit towards the exploration of effective, sturdy and energy efficient catalysts continues. The talk addresses,

- several strategies pursued to replace noble-metal free electrocatalysts for ORR/HER.
- Zn based battereis
- visualization of local electrocatalyic activity by SECM.

Keywords: ORR, HER, electrocatalyst, Zn based batteries, SECM

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Advancing Carbohydrate Chemistry through Aryl Diazonium-Mediated Transformations

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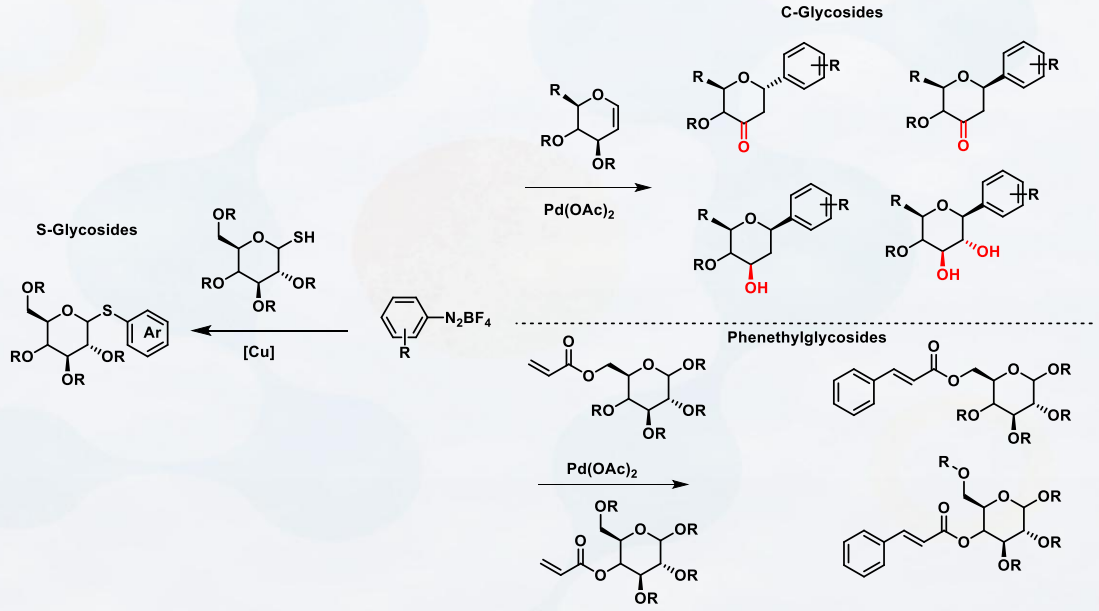
Aryl diazonium salts are highly versatile and reactive intermediates widely utilized in organic synthesis for the construction of C–C, C–O, C–N, and C–S bonds. Their unique reactivity makes them valuable tools for functionalizing carbohydrate scaffolds, offering new routes to aryl-substituted glycosides and related derivatives. In our studies, we have explored the application of aryl diazonium chemistry to carbohydrate frameworks, particularly the synthesis of C-glycosides and S-glycosides.[1-6] These transformations enable direct arylation at anomeric or other reactive centers of sugars, leading to structurally diverse and functionally rich carbohydrate derivatives. The developed methods highlight the synthetic utility of aryl diazonium salts for modifying carbohydrate scaffolds and open new possibilities for designing novel glycomimetics and biologically active molecules.



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IL-29

Introducing Sustainability in Allylic Cross-Animations

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Abstract:

Allylic amination is a key transformation in organic synthesis, yet it is traditionally dominated by precious-metal catalysis in organic solvents with limited attention to sustainability. In this talk, I will present a nanomicelle-enabled, additive-free 'in-water' nickel-catalyzed allylic amination of allylic alcohols operating under mild conditions. The method exhibits broad substrate scope, accommodating diverse amines, including electron-deficient N-heterocycles, with excellent chemo-, regio-, and stereoselectivity and high functional-group tolerance. Practical attributes such as gram-scale synthesis, recycling and reuse of aqueous micelles, low E-factor, and minimal residual nickel further enhance its sustainability profile.

Beyond reaction development, a comprehensive sustainability assessment of allylic amination is disclosed for the first time. Reactivity-utility profiling of 26 allylic precursors in water versus organic solvents, identification of competing side reactions, and evaluation of green metrics demonstrate that water is as versatile as organic solvents and that earth-abundant nickel is a viable, and in water superior, alternative to palladium. The utility of this approach is highlighted by an all-water synthesis of marketed drugs including flunarizine, cinnarizine, and naftifine. Collectively, this work establishes a practical framework for sustainable allylation chemistry in academia and industry.

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IL-30

Synthesis and Characterization of Complex Perovskite Oxides

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Abstract

$ACu_3Ti_4O_{12}$ (ACTO, where A = Ca, $Y_{2/3}$, $Bi_{2/3}$) type of ceramics were successfully synthesized by semi-wet route. The Single-phase formation of these ceramic was confirmed by powder X-ray diffraction studies. These ceramics were further characterized by dielectric and impedance studies. The dielectric constant (ε_r) was found very high for these ceramics at room temperature. The tangent loss (tan δ) value of these ceramics was found slightly high. Scientists have been working to reduce dielectric loss by doping or partial substitution of different elements at Cu and Ti sites independently or simultaneously by applying different synthesis route. The dielectric constant and tangent loss both decrease with increasing frequency in the lower frequency regions, while these are almost constant in the higher frequency regions. Impedance studies were used to see the contributions of grain and grain boundaries effect.

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IL-31

Design, synthesis and applications of Chemosensors for the Naked Eye Detection of metal ions, anions and amino acids

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Abstract

The development of colorimetric chemosensors capable of detecting a wide range of analytes with high selectivity and sensitivity has emerged as an important area of research due to their potential applications in environmental monitoring, analytical chemistry and biological systems. Among the various analytes of interest, **metal ions, anions and amino acids** play crucial roles in many chemical and biological processes. However, abnormal levels of these species may lead to serious environmental contamination and health-related problems. Consequently, the development of efficient sensing systems for their rapid and reliable detection has attracted considerable attention in recent years.

In this lecture, our recent work published and ongoing (communicated) on the design, synthesis and applications of heterocyclic chemosensors for the naked-eye detection of metal ions, anions and amino acids **will be presented.** The research focuses on the development of novel molecular probes based on heterocyclic scaffolds such as **1,4-dihydropyridines, triazoles, pyranopyrazoles, rhodamine derivatives and pyridine-dicarbohydrazide frameworks**. These compounds have been synthesized using efficient and environmentally friendly synthetic strategies including **multicomponent reactions and click chemistry**, which enable the preparation of structurally diverse molecules with desirable photophysical properties.

The synthesized probes exhibit remarkable **colorimetric and fluorometric sensing behaviour** toward a variety of analytes including **metal ions, anions and amino acids**. Several sensors developed in our laboratory have demonstrated selective recognition of important metal ions such as **Fe^{3+}, Cu^{2+}, Ni^{2+}, Cr^{3+} and Pb^{2+}**, along with biologically relevant species including **biothiols and amino acids**. In many cases, the interaction of the probe with the target analyte produces a distinct **visible colour change**, enabling rapid **naked-eye detection** without the need for sophisticated instrumentation.

Several of the developed probes have also demonstrated promising applications in **real sample analysis, molecular logic gate systems and cellular level detection**, highlighting their potential use in environmental and biological studies. Overall, these results demonstrate that carefully designed heterocyclic frameworks provide efficient platforms for the development of versatile optical chemosensors for the selective detection of **metal ions, anions and biologically important molecules**.

IL-32

What does ‘natural’ mean anyway…?

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The term “natural” is widely used in the flavor and fragrance (F&F) industry, though its scientific and regulatory definitions vary across global markets. This work explores how traditional natural materials, such as botanical extracts and essential oils, are being transformed into sustainable aroma ingredients through selective chemical modification of renewable feedstocks. A comparison of US and EU regulations highlights how differences in permitted processes, catalysts, and solvents influence innovation, cost, and commercial viability. The conversion of naturally derived alcohols into high-value esters with fruity and green sensory profiles is discussed for applications in food, beverages, personal care, and fine fragrance. Together, chemistry, sustainability, and regulation are shown to be key drivers shaping the future of F&F innovation.

IL-33

Green Corrosion Inhibitors: A Sustainable Journey from Fundamentals to Industrial Applications

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Abstract

Corrosion represents a persistent and costly challenge for global industries, with worldwide economic losses estimated at approximately 2.5 trillion USD annually—equivalent to 3.5% of the global gross domestic product. Among the most practical and cost-effective strategies for mitigating corrosion is the application of corrosion inhibitors. This lecture provides a comprehensive overview of **Green Corrosion Inhibitors**, addressing their fundamental principles and diverse industrial applications. Key topics include the phenomenology and mechanisms of inhibition, the use of modern electrochemical techniques for inhibitor characterization, the influence of molecular structure on performance, and the role of synergism in enhancing protective efficacy.

Driven by stringent environmental regulations, significant efforts have been directed toward developing environmentally benign inhibitors derived from renewable sources. However, challenges related to their stability and effectiveness remain. In response, this presentation highlights the synthesis of next-generation green inhibitors founded on the principles of green chemistry, aiming to overcome these limitations.

Finally, the discussion elaborates on the practical application of corrosion inhibitors across various industrial environments. The lecture covers over 35 years of dedicated research conducted at IIT BHU (India) and KFUPM (Saudi Arabia), offering both scientific insight and practical perspective on sustainable corrosion control.

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IL-34

Molecular Design Strategies for Selective and Sensitive Chemosensing of Ions, Environmental Pollutants, and Bioactive Compounds

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The rapid and reliable detection of chemical species remains a central challenge in modern analytical chemistry. Although advanced instrumental techniques are well established for the qualitative and quantitative detection of ions and environmental pollutants but their high operational cost, sophisticated instrumentation, and requirement for skilled personnel limit their widespread application in routine and on-site analysis.

Consequently, the development of small-molecule chemical sensors has attracted considerable attention as a simple, rapid, and cost-effective alternative for the detection of ions, environmental pollutants, and bioactive compounds.

In this presentation, three representative case studies are discussed to demonstrate diverse molecular design strategies in sensor chemistry and to highlight the conceptual distinction between sensitivity and selectivity in molecular sensing systems.
The first case study describes the development of a quinoxaline-based chemosensor capable of detecting nineteen different analytes in a DMSO–water (8:2, v/v) medium through multiple coordination interactions, exhibiting remarkable sensitivity toward a broad range of ionic species at ppb level.

The second case study reports a rhodamine-derived sensor that demonstrates exceptional selectivity toward HSO_4^- ions and provides a dual-mode detection response, involving both visible colorimetric change and fluorescence emission. Notably, the sensor also shows promising applicability for the recognition of pharmaceutical compounds containing the HSO_4^- functional group.

The third case study focuses on a series of ninhydrin-based sensors designed to systematically investigate the influence of structural substitutions on sensing performance under identical environmental conditions, thereby providing insights into the structure–sensing relationship in molecular chemosensors.

These studies collectively demonstrate how rational molecular design can be employed to tailor sensitivity, selectivity, and application scope in small-molecule chemosensors for the detection of diverse chemical targets.

IL-35

Design and Synthesis of Recoverable Chiral Catalysts for Asymmetric Organic Transformations

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The synthesis organic compound such as bulk chemicals, fine chemicals and pharmaceutical intermediates through catalysis makes methodology sustainable. Transition metals salts and complexes, oragnocatalysts and enzymes are mostly used in the organic reactions for generation of the variety of valuable chemicals.[1] Our research group are focused on development of recoverable organocatalyst by tagging (L)- prolinamides, (L)-prolinol with ionic liquids for asymmetric organic transformations. We have developed new chiral C1 symmetric salalen/salan-Mn(III) and Cu(II) complexes for asymmetric Henery and Strecker reaction. The Mn(III) salen complexes **1a-c** and **2a-c** tagged with imidazolium based ionic liquids[2] and their catalytic activities were evaluated in the oxidative kinetic resolution of (±)-1-phenylethanol with *N*-bromosuccinimide (NBS) as an oxidizer in biphasic solvent system [H_2O - organic solvent (2: 1, v/v)] at 0 °C. The organocatalysts tagged with ionic liquids show excellent catalytic activities and recoverabilties for asymmetric organic transformations.

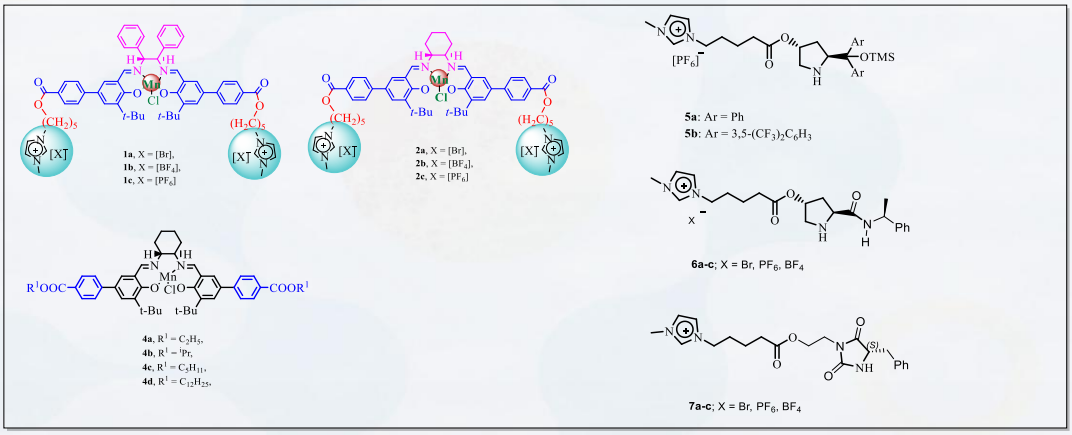

Figure: Chiral Mn (III) Salen and chiral organocatalyst tagged with ionic liquid for asymmetric organic transformations.

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Electro-catalyzed Functionalization of Indolizine Frameworks

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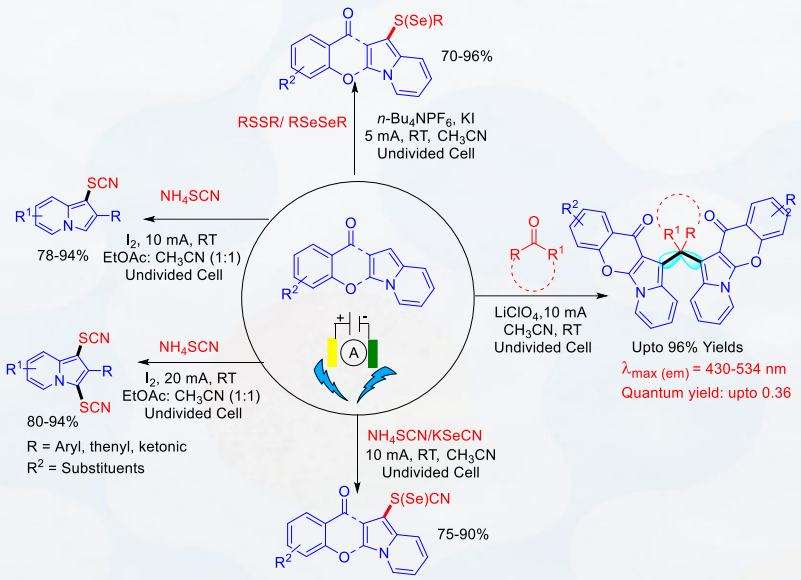
Electro-organic synthesis provides a sustainable approach that utilizes electrons as reagents for molecular transformations, thereby eliminating the need for excess reagents.[1] Our research group has recently developed various electrochemical approaches for the functionalization of indolizine moieties *via N*-centered radical translocation. During my presentation, I will provide a detailed discussion of these approaches.[2]



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IL-37

Pre-clinical evaluation of phytosterol-ionic liquid conjugated-derivatives shows enhanced anti-cancer activities in colon cancer cells

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ABSTRACT

Colorectal cancer (CRC) remains a leading cause of cancer-related mortality worldwide, and current treatments are limited by low efficacy, toxicity, and resistance [1]. To develop novel steroid-based agents with improved anticancer potential, we chemically modified β-sitosterol (BST), a naturally occurring phytosterol [2], through the conjugation with imidazolium-based ionic liquid [3] moieties for generating a series of β-sitosterol-ionic liquid derivatives (BST-ILs). The synthesized derivatives were characterized using spectroscopic techniques, and their physicochemical and pharmacokinetic properties were evaluated through *in silico* ADMET and density functional theory (DFT) analysis. Notably, the ionic liquid derivatives exhibited improved membrane permeability, enhanced anticancer activity in human colorectal cancer (HC-T116) cells, and stronger binding to target enzymes involved in cholesterol biosynthetic pathways, correlating with their anticancer properties in regulating lipid metabolic pathways. The results showed a concentration-dependent reduction in cell viability, with the ionic liquid conjugates exhibiting significantly greater cytotoxicity than the parent compound. Furthermore, the derivatives effectively inhibited cell migration and induced apoptosis, as confirmed by morphological and gene expression analyses of cell proliferation and apoptosis. Molecular docking and molecular dynamics simulations were performed to investigate interactions with key enzymes of the mevalonate pathways. Our findings highlight BST-ILs conjugates as promising phytosterol-based anticancer drug candidates with the potential to target sterol biosynthesis pathways in colorectal cancer.

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IL-38

Flaxseed Mucilage based composite material as a sustainable flocculant for treatment of mining and Industrial Effluents

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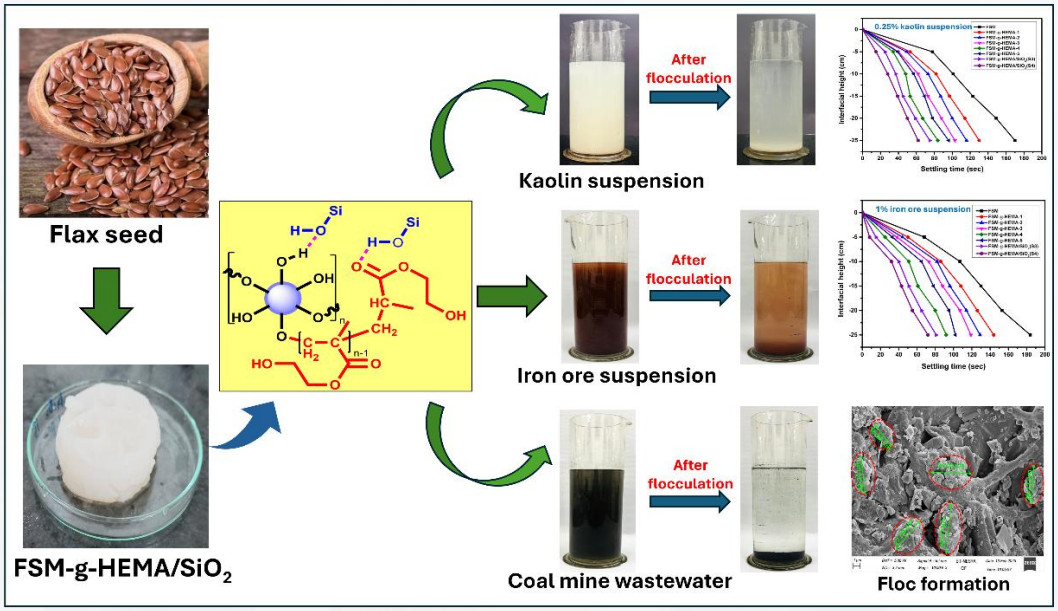

Bio-based flocculants are being explored for wastewater treatment, but their performance is often affected by low efficiency and poor stability under different conditions. To address this, a hybrid flocculant was prepared by grafting 2-hydroxyethyl methacrylate (HEMA) onto flaxseed mucilage (FSM) and adding silica nanoparticles to form FSM-g-HEMA/SiO_2. The material was characterized using FTIR, FESEM-EDX, XRD, and TGA. FTIR confirmed grafting and silica addition. FESEM-EDX showed a porous structure with silica particles distributed in the matrix. XRD and TGA indicated changes in structure and thermal behavior compared to FSM.

Flocculation performance of FSM, FSM-g-HEMA, and FSM-g-HEMA/SiO_2 was tested using turbidity removal, settling rate and floc size under different pH (2–10) and temperature (15–55 °C) conditions. The FSM-g-HEMA/SiO_2 composite showed higher efficiency, with removal of 82% for kaolin at pH 4 and 25 °C, 74.64% for iron ore at pH 4 and 35 °C and 70.02% for coal mine wastewater at pH 6.2. The results show that FSM-g-HEMA/SiO_2 can be used for the treatment of diverse industrial and mining wastewater systems.

Reference: Process Safety and Environmental Protection, 209, 2026, 108637, https://doi.org/10.1016/j.psep.2026.108637

IL-39

Formulation Innovation for Health: Triazine Dendrimers

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Abstract

Chemistry plays a vital role in addressing formulation challenges associated with poorly water- soluble drugs in pharmaceutical development. Dendrimers are nanoscale, highly branched macromolecules that have gained attention as functional excipients due to their ability to enhance drug solubility and stability. Their precisely controlled architecture and surface functionality enable efficient incorporation of bioactive pharmaceutical ingredients (APIs), leading to improved dissolution behavior and bioavailability. In the present work, triazine- based dendritic macromolecules of generations G1, G2, and G3 were developed and evaluated as novel solubility enhancers in pharmaceutical formulations. APIs were formulated using an inclusion complex approach and characterized by spectroscopic techniques. In vitro dissolution and sustained release studies demonstrated a significant improvement in solubility and controlled release profiles compared to free APIs. Safety evaluation through hemolysis and cytotoxicity assays confirmed good biocompatibility of the synthesized dendrimers. Notably, the triazine-based dendritic macromolecules exhibited superior formulation performance and safety compared to commercially available poly(amidoamine) (PAMAM) dendrimers. These results highlight the potential of triazine-based dendrimers as effective solubility-enhancing excipients for clinically relevant pharmaceutical formulations.

IL-40

Harnessing Electricity and Enzymes for Sustainable Organic Synthesis

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Electro- and enzymatic catalysis have emerged as powerful and sustainable strategies in modern organic synthesis, effectively integrating green chemistry principles with high efficiency and selectivity.[1,2] Electrocatalysis utilizes electricity to drive redox transformations, thereby reducing reliance on hazardous chemical oxidants or reductants.[3] In parallel, enzymatic catalysis offers remarkable chemo-, regio-, and stereoselectivity under mild reaction conditions, leading to lower energy consumption and minimized waste generation.[4] The convergence of these approaches provides new opportunities for the development of environmentally benign and scalable synthetic methodologies, particularly for complex molecular architectures.[5]

In this context, we have developed an electrocatalytic oxidative coupling of arylamines for the selective synthesis of azo aromatics.[6] Additionally, a metal-free electrochemical protocol was established for the regioselective *N*-sulfonylation of in situ-generated indole-based hydrazones using readily available sodium sulfinates.[7] We have also demonstrated the homocoupling of diazo compounds, enabling switchable and selective access to tetrasubstituted alkenes and azines.

On the biocatalysis front, we reported an α-amylase-catalyzed Friedel–Crafts reaction of isatin to synthesize symmetrical and unsymmetrical 3,3′,3″-trisindoles.[8] Notably, we have successfully integrated electrochemical and enzymatic catalysis in a one-pot approach for the regioselective synthesis of C-3 alkylated oxindoles.[9] Furthermore, the merger of electrosynthesis and biocatalysis has enabled access to sulfur-based chiral α-fluorinated carboxylic acids in a single operation.[10] More recently, we developed a highly stereoselective synthesis of 3-hydroxy-2-oxindoles by combining electrosynthesis with enzyme catalysis.

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IL-41

DEVELOPMENT OF A MULTISPECIES BIOFILM BIOFILTER: MICROBIAL INTERACTIONS, COMMUNITY DYNAMICS, AND HEAVY-METAL REMOVAL EFFICIENCY

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Abstract

Mixed-species bacterial biofilms show great promise for heavy metals bioremediation due to synergistic mechanisms (adsorption, precipitation, reduction). We developed a stable four-species biofilm consisting of *Deinococcus radiodurans* (GFP-tagged), *Pseudomonas aeruginosa* (mCherry-tagged, designated PC), *Escherichia coli* (RFP-tagged), and a lasR mutant of *P. aeruginosa*. A lab-scale polymicrobial biofilm-based biofilter system was also developed using these four species on a multi-layered filter bed (glass beads, sand, charcoal). Interspecies interactions were observed: the *lasR* mutant and *E. coli* RFP inhibited *D. radiodurans*, and together they disrupted the swarming motility of *P. aeruginosa* (PC). Growth kinetics varied across combinations, with some mixed cultures outperforming single-species biofilms. Over 15 days, metagenomics results tracked community dynamics, revealing *P. aeruginosa* PC as most dominant and *D. radiodurans* as least abundant. At 10 ppm U(VI) (uranyl nitrate), the four-species biofilm removed 99.62% of U(VI), outperforming triple-species consortia lacking the *lasR* mutant (98.69% removal) or lacking *E. coli* (99.25%). This efficiency far exceeded the 75–88% removal achieved by individual strains. Even under acute U(VI) stress (50 ppm for 4 h), the polymicrobial biofilm remained stable (minimal dispersion, high CFU counts) and removed >96% of U(VI), as confirmed by ICP-AES. The biofilm-based biofilter system using these four species removed >95% U(VI) from 1 ppm feedwater and reduced nitrate, nitrite, ammonium, phosphate, TOC, and BOD, broadening its application beyond radionuclide remediation. It also showed exceptional lead (Pb) removal efficiency (~98% Pb removal from 1 mg/L) in effluent. Results highlight the polymicrobial biofilter's multiplexed potential for practical water purification applications.

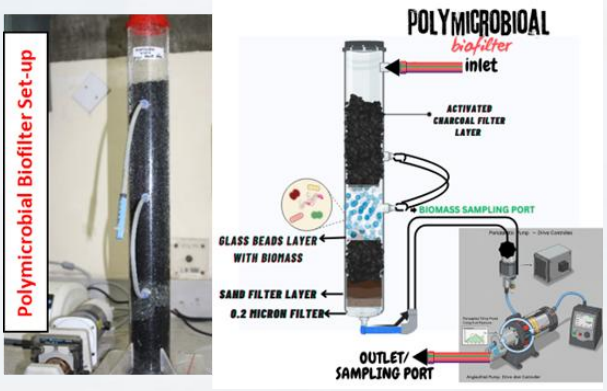

Figure 1: Polymicrobial biofilm-based biofilter set-up.

Keywords: Biofilms, Bioremediation, U(VI), Lead, Heavy Metals, *Deinococcus radiodurans, Pseudomonas aeruginosa*, *Escherichia coli*

IL-42

Tetrazole-Embedded Scaffold via Ugi Four-Component Reaction: Efficient Synthesis and Drug -Likeness Evaluation

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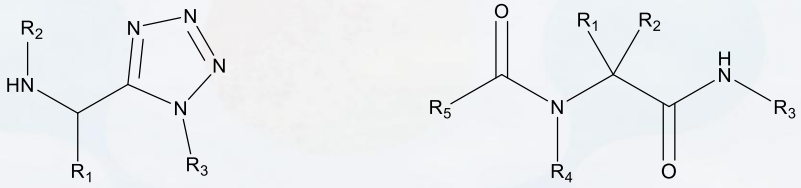
Abstract:

Heterocyclic compounds have long played a crucial role in medicinal chemistry. Among the most efficient strategies for generating novel heterocyclic derivatives are multicomponent reactions.[1,2] In this work, both conventional and non-conventional Ugi four-component (UGI-4CR) reactions, including microwave-assisted methods, are discussed. The Ugi-Azide reaction combine an aldehyde, primary amine, isocyanide, and azide in a single step to produce tetrazole derivatives through sequential intermediate formation and cyclization.[3] This one-pot method is efficient, simple and enables rapid generation of diverse compounds for drug discovery. Ugi-derived tetrazole compounds exhibit diverse biological activities, including antimicrobial, anti-inflammatory, anticancer antiviral etc. ADME Studies show good absorption, balanced distribution and enhanced metabolic stability. The integration of Ugi multicomponent reactions with tetrazole framework provide effective strategy for designing biological active compounds with promising drug like properties suitable for modern medicinal research. All synthesized compounds were characterized using spectroscopic techniques and evaluated for their anticancer activity against a panel of nine cancer cell lines.



Keywords: Ugi multicomponent reaction, heterocyclic compounds, anti-cancer activities, Medicinal chemistry

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IL-43

Transition metal Complexes as Molecular Electrocatalysts for OER, HER and CO2RR

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Mimicking the WOC in search of renewable energy in artificial system is extremely popular methodology. Transition metal complexes are the perfect candidate to explore the multi electrons redox reactions with their variable oxidation states and ability to adopt different structures. Starting with Ruthenium, 1st row transition metals e.g., Mn, Fe, Co, Ni and Cu with redox non innocent Pyridyl, imidazole and amide ligands have been utilized for both homogeneous and heterogeneous catalysis. Cu complexes of bis-amide tetradentate ligands show efficient electrocatalytic water oxidation with a TOF of 1462 s^{-1} at overpotential~700 mV takes place through WNA mechanism via ligand centered oxidation [1]. Another water soluble binuclear aquo Cu(II) amide complex [2] shows ternary role as an electrocatalyst for the OER, HER and CO2RR. HER TOF = 1679 s^{-1}, TON = 586 and F.E. = 83%; CO2RR (F.E.- 92%) shows percentage selectivity of ~99.99% conversion of CO_2 to $(COOH)_2$. A series of terpyridine and bis benzimidazolyl complexes have been explored for the HER [3] and OER [4] study in solution that displays high degree of stability as confirmed by different surface characterization techniques e.g. FESEM, TEM etc. (for electrodes) and DLS (for solution). An attempt to immobilize a Cu terpyridyl complex on the GC electrode surface leads huge increment in the current density compared to the homogeneous medium. When the catalyst is mixed with Graphene oxide and immobilized on Glassy carbon electrode, ~70 times increase in current intensity at the catalytic wave is noticed at an overpotential of ~407 mV.

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4. Electrocatalytic Proton Reduction by Mononuclear Cobalt Complexes of bis (benzimidazolyl) pyridine Ligands: Experimental and Theoretical Study; Sahanwaj Khan, Swaraj Sengupta, Md. Adnan Khan, Narayan Ch. Jana, **Bidraha Bagh,** Subhendu Naskar; ***New Journal of Chemistry***, **2025,** 49, 16134

IL-44

Engineering Charge Transfer in AIE Systems: From Molecular Design to Targeted Theranostic Applications

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Aggregation-induced emission (AIE) has emerged as a powerful strategy to overcome aggregation caused quenching, enabling the development of highly emissive functional materials for biomedical applications [1, 2]. Herein a rational molecular design approach to engineer charge transfer (CT) processes in AIE-active systems has been presented, with a focus on symmetric and asymmetric donor–acceptor (D–A) architectures, to achieve optimized photophysical and photochemical performance for targeted theranostic applications. The tuning of intramolecular charge transfer (ICT) processes by structural variations facilitates enhanced intersystem crossing (ISC) and reactive oxygen species (ROS) generation, prerequisites for efficient photodynamic therapy (PDT). Further, incorporation of classic chromophoric scaffolds such as BODIPY derivatives into AIE frameworks enables improved light-harvesting ability, red-shifted absorption, and higher singlet oxygen quantum yields [3]. The present work also explores the possibility of more effective ROS generation through enhancing the triplet state population via spin-orbit coupling facilitated by integration of transition metal complexes, particularly Ru(II) and Ir(III)-based systems [4]. These metallated AIE systems exhibit superior photostability, tunable emission, and improved performance in biological environments. Special emphasis is placed on organelle-targeted delivery through strategic functionalization, enabling selective accumulation in mitochondria, lysosomes, or endoplasmic reticulum, thereby improving therapeutic efficacy and imaging precision. Collectively, the synergy between molecular engineering, charge transfer tuning, and AIE characteristics offers a versatile platform for next-generation theranostic agents.

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IL-45

Drug Design, Synthesis and Study of Novel Series of Bio-active analogues

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Abstract:

The development of novel therapeutic agents is a key focus in medicinal chemistry, and pyridone and coumarin derivatives have emerged as promising scaffolds due to their diverse pharmacological profiles. This study reports the design, synthesis, and biological evaluation of a new series of pyridone and coumarin analogues with the goal of identifying potent drug candidates with enhanced efficacy. A variety of analogues were synthesized through efficient synthetic routes, with structural modifications aimed at optimizing the pharmacokinetic and pharmacodynamic properties. The synthesized compounds were characterized using a combination of spectroscopic techniques, including NMR and mass spectrometry, and their purity was confirmed through HPLC analysis. Biological screening against several targets, including antimicrobial, anticancer, and anti-inflammatory assays, revealed promising activity in select compounds. Structure-activity relationships (SAR) were established, highlighting the influence of functional group modifications on biological potency. The results indicate that the pyridone and coumarin analogues represent a promising class of compounds for further development and optimization as potential therapeutic agents (Liu et al., 2019; Kumar et al., 2020; Kaur et al., 2021; Jiang et al., 2018; Patel et al., 2022).

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IL-46

Metal- and Reagent-Free Approaches for the Synthesis of Bioactive Molecules

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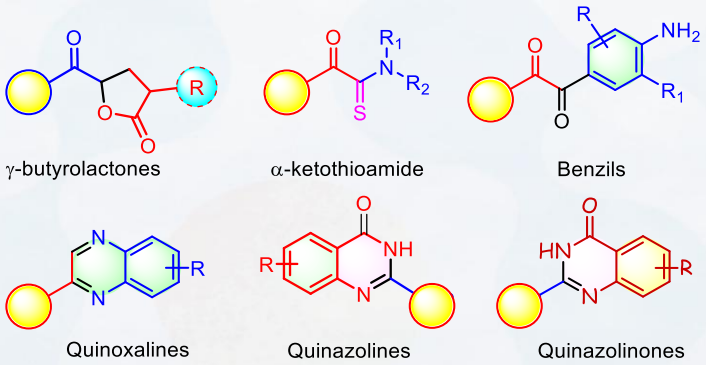
Metal-catalyzed transformations of sulfoxonium ylides have become valuable tools for constructing heterocyclic frameworks such as pyrroles, indoles, furans, pyrimidines, and quinolones. Despite this progress, their potential in metal-free synthesis remains relatively underexplored. In our work, we have shown that sulfoxonium ylides can serve as effective precursors for accessing a wide range of bioactive molecules. These studies have enabled the mild, metal-free synthesis of γ-butyrolactones, α-ketothioamides, α-ketoamides, benzils, quinoxalines, quinazolines, quinazolinones, and related scaffolds. The talk will highlight recent advances in sulfoxonium ylide chemistry with an emphasis on metal- and reagent-free strategies for the synthesis of bioactive molecules and other valuable compounds.



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IL-47

Redox-active Interlocked Molecules for Energy Storage Applications

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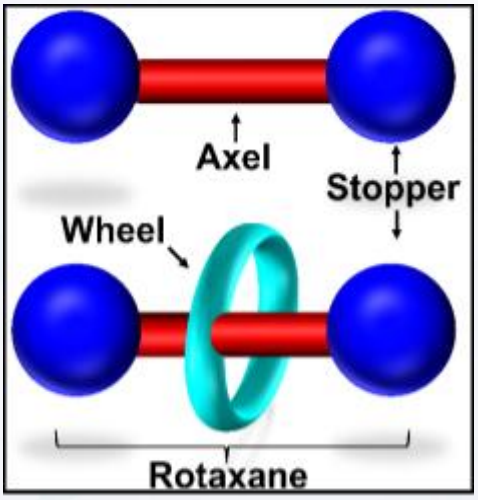
ABSTRACT

Dynamic Stereochemistry of Interlocked molecules is of fundamental interest as it inspires the design of artificial systems of definitive functions/ motions.[1] This led to Nobel Prize-winning discoveries of molecular rotors, shafts, and machines that depicted controllable movements and relative motions of molecular components that impact the properties of robust architectures.[2] These inter-connected molecular assemblies exert a symphony of *non-covalent interactions,* triggering the molecular motion from the sub-nanometre level to the macroscopic scale. Among the various classes of interlocked molecules, our prime interest is **Rotaxane**,[3-5] which consists of two components: i) a rod-shaped molecule with bulky stopper units termed **Axel** (dumbbell shape) and ii) a **wheel**-shaped macrocycle that is mechanically interlocked (Figure 1) through non-covalent interactions like halogen bonding[3, 5-7], π - π interaction,[3] electrostatic interactions, etc.[8, 9] In this work, we demonstrate a *self-assembled* rotaxane embedded with a redox-active ligand/ Lindqvist polyoxovanadates as the terminal to induce the redox properties. Electrostatic repulsion around the terminals forces the wheel inside the interlocked scaffold. Furthermore, the presence of the electron donor centers at the terminal enables it to get anchored on the oxygen atom-deficient surface of the Lindqvist polyoxovanadates, which have never been used as *stoppers,* and these can leverage the redox activity/ stability on the stopper itself. The size and shape of the POVs match well with the conventional stoppers, satisfying their key aspect (not to allow de-threading), but strongly differ from the architecture of the redox-inactive bulky stopper ends.



Keywords: Mechanically interlocked molecules, Rotaxane, Redox, Energy storage.

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IL-48

Carbohydrates and Copper for Sustainable Catalysis, Health Care and Environment

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Research Area: Sustainable Organic Synthesis Applications to Health care and Societal Applications.

ABSTRACT:

Recently, humankind has utilized more harmful chemical compounds and generated toxic waste in the environment. The anthropogenic activities have prompted our quest for a substitute chemical process that complies with sustainable and green chemistry principles. Carbohydrate-based ionic liquids are now the most intriguing alternatives due to their intrinsic properties, which encompass low cost, significant abundance, non-toxicity, high biodegradability, and elevated water solubility. The applications of carbohydrate-derived ionic liquids in asymmetric synthesis and the development of cascade reactions have garnered little attention, despite the prospective use of carbohydrate-based chiral auxiliaries, catalysts, and reagents in this domain. Consequently, our group is endeavouring to discover and synthesize a unique class of sugar ionic liquids derived from natural sugars. In this context, nature-derived sugars and abundant copper-based enzymes are an alternative to conventional organic synthesis for use in sustainable catalysis, health care, and the environment.

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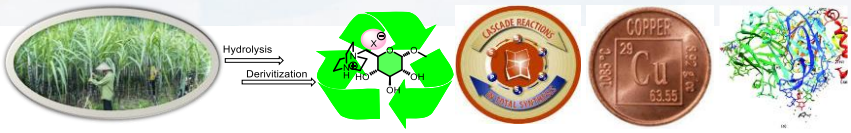

Scheme 1: Flow of my presentation

Keywords: Sustainable Organic Synthesis. Carbohydrates, Health care, Catalysis, and Copper-Sugar-Biocatalysis, Cascade reactions

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IL-49

Computational Exploration of Ligand-Directed C–H Activation in Bio-Inspired Metal–Oxo Complexes

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Synthetic metal–oxo complexes are increasingly important in C–H bond activation chemistry. However, rationalizing their reactivity patterns (eq. 1) remains highly challenging due to the complex interplay of kinetic and thermodynamic factors.

$$LM^{n}=O + H\text{-}R \rightarrow LM^{n-1}O\text{-}H + R\bullet \quad \text{(M, a Metal system e.g., Fe, Mn etc; L, a ligand system)} \quad (1)$$

Reactivity is governed by multiple parameters, including the identity of the central metal, its electrophilicity, spin and oxidation states, metal–oxo/peroxo character, and metal–oxygen bond strength. In addition, the ligand environment plays a critical role, encompassing axial and equatorial coordination, overall ligand architecture, acceptor orbital energies, the radical nature of the abstracting species, and quantum mechanical tunnelling effects.
In this presentation, an effort is made to rationalize how these factors collectively contribute to a coherent understanding of reactivity through several representative studies. These comparative analyses provide valuable mechanistic insights into how subtle electronic and structural variations influence catalytic efficiency and selectivity in C–H bond activation processes.

Keyword: **Metal**-oxo, C-H activation, Bio-inspired, computational study, reaction mechanism, DFT

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IL-50

Epigenetic modulation through nucleobase inspired scaffolds; Discovery of anti-cancer compounds targeting LSD1

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Lysine-specific demethylase 1 (LSD1/KDM1A) is a nuclear flavin-dependent enzyme that regulates chromatin dynamics and gene transcription, and its dysregulation is closely associated with cancer progression and conventional chemotherapeutic resistance. In our present study, a series of purine-based small-molecule derivatives were rationally designed and synthesized for LSD1 inhibition.

Structure–activity relationship considerations were applied to enhance biological efficacy in oral cancer cells. Hit molecule was identified based on its potent cytotoxicity against CAL27 oral cancer cells. This compound rewired the key cell death pathways in oral cancer cells via LSD1-modulated transcriptional reprogramming. Lead compound exhibited pronounced lysosomal dysfunction, including lysosomal membrane destabilization and enhanced acidification in CAL27 cells. It has induced lysosomal acidification in CAL27 cells and was identified as an early initiating event to activate the pyroptotic cell death pathway, marked by inflammasome-associated caspase-1 activation, cleavage of gasdermin D (GSDMD) and membrane pore formation. Concurrent activation of caspase-3/7 and apoptosis in CAL27 cells indicated a functional crosstalk between apoptotic and pyroptotic signaling downstream of epigenetic modulation, supported by transcriptome analysis. LD_{50} of compound 8a was determined to be greater than 2000 mg/kg in Sprague–Dawley rats following oral dosing and histopathological studies on major organs showed no identifiable morphological or structural abnormalities, strongly suggesting a favorable *in vivo* safety profile and low acute oral toxicity. These findings suggest that a rational epigenetic strategy to enforce transcriptional modulation of multiple and non-redundant cell death pathways can represent a promising approach to overcome chemoresistance in oral cancer.

IL-51

Rhodamine Based Cu(II) Complexes: Application as PDT Agent

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ABSTRACT

This work investigates the antiproliferative efficacy of rhodamine-based Cu(II) complexes (**CuL1** and **CuL2)** in breast cancer cell lines. The complexes, together with ligands (L1 and L2), exhibit exceptional solubility in DMSO and DMF, moderate solubility in ACN and $CHCl_3$, and are less soluble in water. The complexes exhibit two notable peaks: a sharp band corresponding to the $\pi \rightarrow \pi^*$ transitions at 310-320 nm and a broad band associated with the LMCT at 540-560 nm, accompanied by a moderate Stokes shift. The stability and photostability of the complexes were assessed in several media, including GSH, CYS, and water. Complexes exhibit remarkable stability in the aforementioned solvents. Viscosity and binding experiments with CT-DNA and EtBr confirm that complexes interact with CT-DNA through electrostatic interactions.Investigations on reactive oxygen species (ROS) indicate that complexes can progress via both Type I and Type II photodynamic therapy (PDT) pathways. *In vitro* cytotoxicity was assessed in HeLa and L929 cell lines under both light and dark conditions, revealing that the complexes exhibit minimal cytotoxicity in the respective cell lines.

Keywords: Rhodamine, Cu complex, PDT, ROS, DFT

IL-52

Current Approaches for the Search of New Bioactive Leads from Medicinal Plants

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Modern medicine and pharmacy rely on the knowledge of traditional medicine as nearly a quarter of new drugs are derived from natural sources. In the last decades, the improvement of the pharmaceutical industry has guided the rapid evolution of different methods for the extraction and separation of bioactive constituents from medicinal plans. Bioactive compounds from biological resources are expected to play a vital role for providing the new therapeutic agents which are biocompatible and generally considered safe as compared to synthetic therapeutic agents [1] of diverse activities. Even in recent times, natural products play a significant role in search of new therapeutic agents, with 6 of 53 new products approved by the FDA in 2023 has been derived from traditional medicinal plants and quickly attracting increasing attention among scientists. Keeping in view the importance of medicinal plants in the discovery new drugs and our continuous work and effort to search the new leads in parasitic area, recently, in our laboratory we have isolated and identified the many bioactive lead molecules viz. anthraquinones, spirostan saponins and triterpenoids from medicinal plants by using various separations and spectral techniques [2-4]. Current approaches for the search of new bioactive leads from medicinal plants will be discussed in detail during the presentation.

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IL-53

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Abstract Awaited

IL-54

Versatility of heteroallenes: 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-55

Replisome-Targeted Antimicrobials: Harnessing Indole Chemistry to Combat Drug Resistance

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ABSTRACT:

The escalating threat of antimicrobial resistance (AMR) demands innovative strategies for developing next-generation therapeutics. Indole, a privileged heterocyclic scaffold, exhibits exceptional structural versatility and biological relevance, making it a promising framework for antimicrobial drug development. Leveraging this potential, our research focuses on the rational design and synthesis of indole-based analogues that target essential components of the microbial DNA replication machinery, specifically DNA primase (DnaG) and DNA gyrase. These enzymes are indispensable for bacterial viability and differ significantly from their human counterparts, enabling selective therapeutic intervention.

Using fragment-based virtual screening and rational medicinal chemistry, dual-acting small molecules were designed to inhibit both enzymes by interacting with the conserved TOPRIM fold, leading to effective suppression of mycobacterial growth [1]. To enhance intracellular delivery and therapeutic efficacy, these inhibitors were conjugated with cell-penetrating peptides, significantly improving antimycobacterial potency and inhibiting biofilm formation in *Mycobacterium smegmatis*, a model organism for *Mycobacterium tuberculosis* [2]. Expanding this sustainable strategy, novel indole–chalcone and 4,5-dihydroisoxazole hybrids were synthesized, demonstrating potent activity against multidrug-resistant ESKAPE pathogens. Mechanistic studies, including molecular docking and DNA supercoiling assays, confirmed DNA gyrase inhibition, while additional membrane-disruptive effects suggested a synergistic dual mechanism of action [3].

Overall, these findings highlight indole-based chemotypes as sustainable and versatile candidates for combating persistent microbial infections. By integrating rational design, efficient synthetic methodologies, and multifunctional mechanisms, this work advances environmentally conscious and effective antimicrobial drug discovery.

KEYWORDS: Indole, Antimicrobial Resistance, Dual-Acting Inhibitors, Replisome Targeting, ESKAPE Pathogens

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IL-56

IPR for Natural Products – Scope & Boundaries

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Abstract

Natural products remain a vital source for drug discovery, nutraceuticals, agrochemicals, and traditional healthcare systems. With growing commercial interest in biological resources, Intellectual Property Rights (IPR) play a crucial role in promoting innovation while ensuring responsible and ethical utilization. However, the application of IPR to natural products is constrained by legal, scientific, and socio-ethical boundaries. The scope of IPR encompasses human- driven innovations such as novel extraction and isolation processes, structural modification of natural compounds, standardized formulations, synergistic compositions, and biotechnologically derived products. In contrast, naturally occurring substances, mere discoveries, traditional medicinal uses, and methods of treatment fall outside the patentable domain under national and international legal frameworks. Further highlights mechanisms such as traditional knowledge databases, geographical indications, plant variety protection, and access-and- benefit-sharing provisions under the Convention on Biological Diversity.

Keywords: Natural products, Intellectual Property Rights, Patents, Traditional Knowledge, Biodiversity

"Not every plant yields fruit, but one seed can."

IL-57

V. Ramanathan

Associate Professor, Chemistry, IIT (BHU)

Abstract Awaited

IL-58

Dr. Amita Sinha

Full Time on Contract Professor, Department of Architecture, Planning and Design, IIT (BHU)

Abstract Awaited

IL-59

Chandan Upadhyay

Professor and Coordinator of the School of Materials Science, IIT BHU, Varanasi, India

Abstract Awaited

Efficient Synthesis of 2-Deoxy Sugars: A Route to Substituted Chiral Quinoline-based Glycohybrids and Indole-C-glycosides

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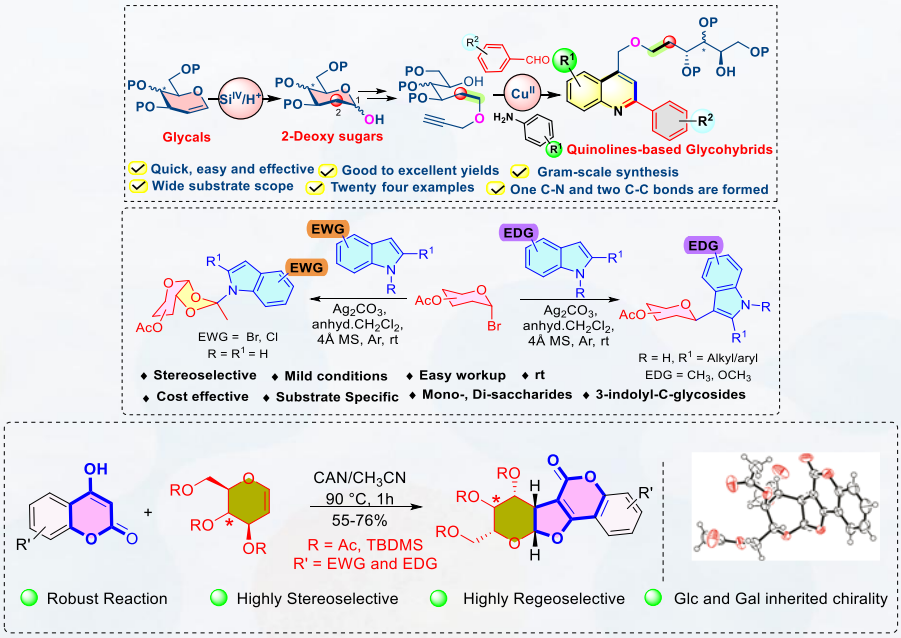

Abstract:

A mild and effective TMSCl-mediated method for the synthesis of diverse 2-deoxy sugars in excellent yields up to 98% within 1 h from diverse protected glycals has been developed. We utilized these 2-deoxy sugars to synthesize stereochemically pure and diverse 2,4-substituted quinoline-based glycohybrids through a Cu(II)-catalyzed, multicomponent one-pot cycloaddition reaction forming one new C-N and two C-C bonds. These 2,4-substituted chirally pure quinoline-based glycohybrids may have promising applications in medicinal chemistry.[1,2] Further a simple, environmentally benign and Ag(I) driven method for the stereoselective synthesis of indole C-glycosides and N-orthoester type glycohybrids has been successfully developed.[3] This process involves coupling of easily accessible various glycosyl bromides, including monosaccharides and disaccharides, with a diverse indole derivatives forming new Csp^3-Csp^2 bond. Quantum mechanical (QM) calculations revealed interesting findings towards product distribution. A key feature of this method are mild reaction conditions, easy workup along with the use of a non-toxic and biocompatible activator.[4]

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IL-61

Late-Stage C–H Activation–Functionalization of Heterocyclic Drug Candidates: An Annulative Pathway

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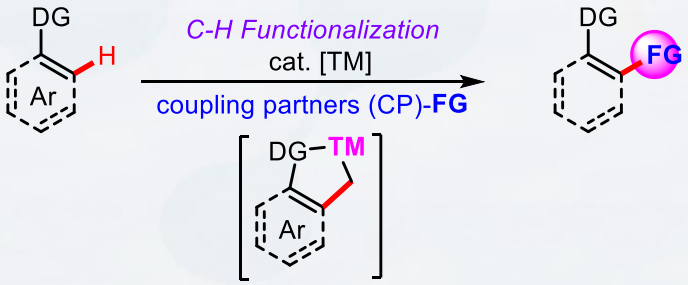
Late-stage C–H activation–functionalization has emerged as a powerful methodology for the construction of complex heterocyclic drug candidates over traditional approaches. C–H functionalization allows researcher to directly introduce the new functionality onto a pre-existing drug scaffolds/candidate. Late-stage modification of drug candidates and bioactive compounds have garnered significant interest due to its ability to introduce diverse elements into pharmaceutically important molecules promptly. In this context, from last few decades, great efforts have been shaped towards the modification and the construction of late-stage drug candidates via transition-metal-catalyzed and transition-metal free C–H bonds functionalization of various hetero(arenes) as well as a range of drug candidates with various types coupling partner. Particularly, the direct breaking and addition of C–H bonds to π-unsaturates C–X multiple bonds (r coupling partner) represent a valuable pursuit with profound synthetic potentials for the introduction of N, S, O, and halogens based functional groups into the molecules. A range of groups such as amide, amine, aldehydes, ester, ketone, azo, acids, imines, and etc. not only represent key structural motif found in various natural products, pharmaceuticals, and biological systems, but they also find application as crucial species for the preparation of various useful compounds and efficiently play the role of directing groups (DG), which coupled with various π-unsaturates to generate the related late-stage drug candidates.

Herein, I will present a brief summary of my research work targeted to the transition-metal-catalyzed and transition-metal free C–H bonds functionalization and annulation of various hetero(arenes) to afford the corresponding late-stage drug candidates. Ultimately, I hope my research work would serve as a valuable resource, facilitating the application of late-stage modification in the construction of novel molecules and inspiring innovative concepts for designing and building of new drugs to the pharmaceutical industries and academia.



IL-62

Intricate Interaction of Microbiome and its Reflection in Metabolome of ALS patients by NMR

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Amyotrophic lateral sclerosis (ALS) is a progressive and fatal neurodegenerative disease that affects motor neurons. Despite ongoing research, its exact causes are still not fully understood, and treatment options remain limited. Recent studies suggest that changes in the gut microbiome, and metabolic disturbances may play an important role in the disease. In addition, saliva is emerging as a promising, non-invasive biofluid for studying disease-related changes. We conducted a multi-omics case-control study combining shotgun metagenomics and ^{1}H NMR-based metabolomics. Samples of stool, serum, and saliva were collected from ALS patients and healthy household controls who shared similar diets and environments. This approach allowed us to examine microbial and metabolic changes across different body systems, with a particular focus on saliva as an easily accessible diagnostic fluid. We observed clear differences in the gut microbiome of ALS patients compared to controls. Beneficial genera such as *Bifidobacterium, Lactobacillus*, and *Enterococcus* were increased in ALS, while *Lactiplantibacillus* and *Klebsiella* were more abundant in controls. Metabolomic analysis identified 15 significantly altered metabolites, including six in stool and nine in serum. These included important compounds such as short-chain fatty acids (butyrate and propionate), branched-chain amino acids (isoleucine and leucine), and energy metabolism intermediates. Importantly, similar metabolic patterns were also detected in saliva, indicating that salivary metabolites reflect metabolic biochemical changes in ALS. Important metabolites such as isoleucine (AUC = 0.83), butyrate (AUC = 0.798), and citrate (AUC = 0.719) showed good diagnostic potential. Also, pathway analysis showed disruptions in energy and nitrogen metabolism, including the glucose-alanine cycle, urea cycle, ammonia recycling, and the Warburg effect, suggesting mitochondrial dysfunction and increased neuroinflammation in ALS. This study demonstrates a link between gut microbiome changes and metabolic disturbances in ALS. The presence of these biomarkers in emphasizes its usefulness as a non-invasive tool for disease detection and monitoring.

IL-63

A Fast, Sensitive, and Validated Analytical Method for Quantitation of Imidacloprid Pesticide Residual in *Mangifera indica* Matrix by LC-Tandem Mass Spectrometry (LC-ESI-MS/MS)

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Abstract

The Alphonso mango is often called the "king of fruits," but even kings sometimes attract unwanted guests. One such guest is imidacloprid, a widely used neonicotinoid pesticide applied to protect crops from insect pests, but that can leave trace residues in edible fruits. Although these pesticides play an important role in modern agriculture by improving crop yield and quality, their residual presence in food products raises concerns regarding consumer safety and regulatory compliance. Therefore, sensitive and reliable analytical techniques are required to monitor pesticide residues at very low concentration levels in food matrices. In this study, a rapid and highly sensitive analytical method was developed to detect and quantify imidacloprid residues in *Mangifera indica* (Alphonso mango). The analytical procedure was based on the QuEChERS extraction technique (quick, easy, inexpensive, effective, robust, and safe), which provides an efficient sample preparation strategy for pesticide residue analysis. Following extraction and clean-up, the analyte was quantified by ultra-performance liquid chromatography coupled with electrospray ionisation tandem mass spectrometry (UPLC-ESI-MS/MS), providing high selectivity and sensitivity for the target compound. The developed method demonstrated excellent linearity over the concentration range of 0.025 - 1.640 µg/L, with a correlation coefficient greater than 0.99. The detection and quantification were determined to be 0.010 µg/kg and 0.50 µg/kg, respectively, highlighting the high sensitivity. Precision and accuracy were evaluated through recovery experiments, which showed recovery values ranging from 70 to 120% with relative standard deviations below 20%, confirming acceptable analytical performance.

Furthermore, the matrix effect was minimal (9.90%), indicating reliable quantification within the mango matrix without significant suppression or enhancement. In general, the method proved fast, sensitive, and robust in detecting trace levels of imidacloprid in mango samples. In short, while insects may try to hide their chemical footprints in the "king of fruits," modern analytical chemistry ensures that no residue escapes detection.

Keywords: Imidacloprid, *Mangifera indica*, UPLC-ESI-MS/MS, Matrix-matched calibration, and Residual plot

SIL-1

Mucin-Inspired Filamentous Amphiphilic Copolymers Effectively Inhibit Human Respiratory Syncytial Virus (hRSV) Infectivity

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Mode of presentation: Podium

Abstract:

Human respiratory syncytial virus (hRSV) is a leading cause of acute lower respiratory tract infections in infants, as well as in elderly individuals and high-risk adults with chronic lung conditions. Preventing hRSV infection at its early stages represents an effective strategy to inhibit viral progression. The interaction between negatively charged heparan sulfate proteoglycans (HSPGs) and the positively charged heparin-binding domain (HBD) of hRSV glycoproteins is a common and critical feature of hRSV-mediated infection, making it an attractive target for the development of negatively charged antiviral agents. In this regard, mucin-inspired biomaterials have been developed, demonstrating excellent inhibitory activity against a range of pathogens owing to their unique characteristics, including high molecular weight, filamentous structure, and strong electronegative charge.[1]

Here, we designed mucin-inspired amphiphilic copolymers (MIACPs) composed of ~70% dendronized sulfated groups and ~30% C11 hydrophobic units. The sulfated groups are intended to inhibit viral binding via electrostatic interactions with positively charged regions on viral surface proteins, while the hydrophobic C11 domains are expected to provide virucidal activity by disrupting the viral membrane. These biocompatible MIACPs exhibit strong, sulfate-dependent inhibition of hRSV, with exceptionally low IC_{50} values (~0.25 μg/mL).[2] Virucidal activity was also assessed, confirming that MIACPs demonstrate potent virucidal effects, indicating a very strong binding affinity of the polymers to hRSV.

The synthesis and characterization of MIACPs using cryo-electron tomography (Cryo-ET) and small-angle neutron scattering (SANS), along with the assessment of their biocompatibility and evaluation of their antiviral and virucidal efficacy against hRSV, will be discussed in the presentation.

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ORAL

O-1

Biosynthesis of Rutinose from Broccoli flower head pulp using F. monilliforme MTCC-2015

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Abstract

Rutinose is a high valuable compound of potential, medicinal and cosmetic values due to the presence of rhamnosyl unit in it. Existing methods of its preparations depend on purified rutinoside substrates and isolated enzyme catalysts. Methods of its preparations using natural rutinoside sources are not available in the literature and need to be developed. This communication reports a preparation of rutinose directly from a natural rutin source, broccoli flower head pulp, using a fungal strain *Fusarium moniliforme* MTCC-2015. The process involves growing the fungal strain in its growth medium containing the pulp, removing the mycelial mat, filtering the culture broth, denaturing the remaining enzyme, recovering rutinose from the aqueous medium by mild evaporation. Relatively pure rutinose in quantitative yield is achieved. This method is cost effective.

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O-2

Sensitive electrochemical detection of ciprofloxacin using a GO/LDH composite-modified screen-printed electrodes

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Abstract:

The widespread use of antibiotics in medical, agricultural, and livestock practices has led to their persistent presence in aquatic environments, raising concerns regarding public health, ecological stability, and the emergence of antibiotic-resistant microorganisms. Although conventional analytical techniques offer high sensitivity and reliability, their application is limited by high cost, operational complexity, and the requirement for sophisticated laboratory infrastructure. Consequently, there is a growing demand for portable and efficient point-of-care (POC) sensing systems for on-site detection of antibiotic residues. In this regard, electrochemical nanosensors based on two-dimensional nanomaterials have attracted significant attention due to their large surface area, excellent electrical conductivity, and tunable surface properties, enabling sensitive and selective detection. In the present study, graphene oxide (GO) and NiAl layered double hydroxide (LDH) composite had been synthesized and subsequently coated onto a screen-printed carbon electrode (SPCE) to fabricate a sensitive electrochemical sensing platform for ciprofloxacin (CIP) detection. Electrochemical characterization technique, including cyclic voltammetry (CV) had also been carried out to investigate the resistance to charge transfer (Rct) and interfacial properties of the modified electrode. The synergistic interaction between GO and NiAl LDH had enhanced the electroactive surface area, facilitated rapid electron transfer, and improved the overall sensing performance. The fabricated sensor had exhibited a wide linear detection range of 0.01 µg/L-0.5 µg/L, and a low limit of detection (LOD) of 0.11 µg/L, demonstrating its capability for trace-level analysis. Furthermore, the sensor had shown good selectivity in the presence of potential interfering substances, along with satisfactory stability and reproducibility.

O-3

Expanding Optochemical Ligation Chemistry through Cation–Cation Photosensitization

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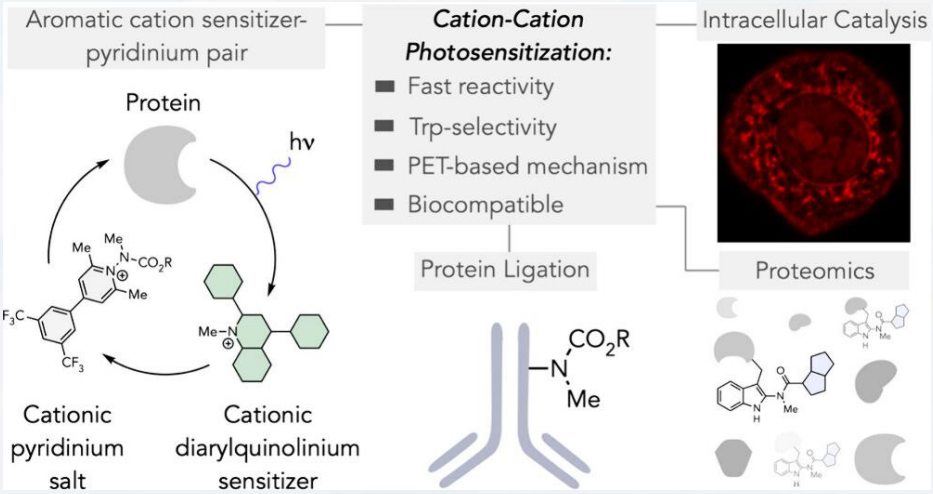
We report a photosensitized strategy [1] for rapid and selective protein labeling based on the activation of N-substituted pyridinium salts using a 2,4-diaryl-*N*-methyl quinolinium scaffold. Systematic structure–reactivity studies enabled optimization of the sensitizer, yielding a platform that achieves efficient protein labeling within minutes at micromolar reagent concentrations. Mechanistic investigations support a photoinduced electron transfer (PET)-driven sensitization pathway.

The mild and tunable nature of this system allows its application across diverse biological environments. We demonstrate efficient labeling of purified biomolecules, complex proteomes, and both lysate- and live-cell systems, highlighting its broad biocompatibility. Fluorescence imaging of photolabeled HeLa cells reveals catalytic activity distributed across multiple intracellular compartments.

Chemical proteomic analysis [2] at the lysate level enabled enrichment of 319 proteins with 93% selectivity for tryptophan residues, while live-cell labeling identified 101 enriched proteins, predominantly localized to the nucleus. Together, this work establishes cation-based photosensitization as a versatile optochemical platform for protein ligation and intracellular catalysis with high spatial and residue-level selectivity.



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Visible-Light-Mediated S-C Bond Cleavage for the Synthesis of Amides

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A green and metal-free photocatalytic method for amide synthesis has been developed using Eosin Y as an organic photocatalyst under ambient conditions. This strategy avoids the use of metal catalysts and proceeds efficiently at room temperature, offering high selectivity and reactivity. Further, this method provides broad substrate scope and functional group tolerance, highlighting its potential applicability in sustainable organic synthesis and pharmaceutical development [1-3]. It represents a green, cost-effective, and efficient alternative for amide bond formation.

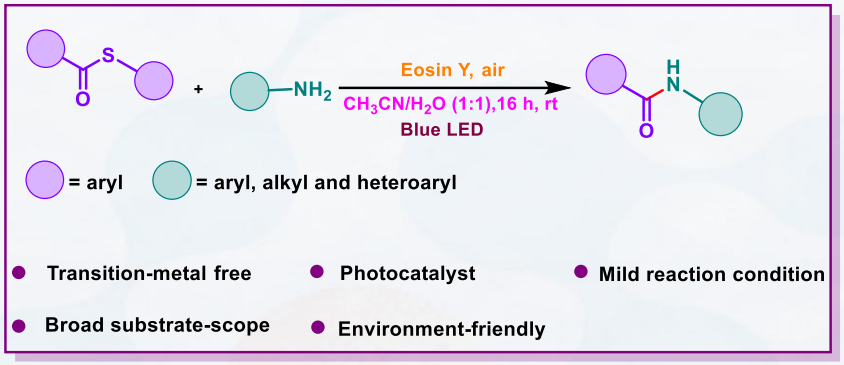

Figure 1. Synthesis of Amides from thioesters and aniline under visible light

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O-5

Horseradish Peroxidase immobilized GO-SWCNT Hybrid Biocatalytic Platform for Efficient Degradation of Bisphenol A

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Abstract

BPA contamination, primarily from plastic waste and industrial discharge, poses significant risks to human health by interfering with hormonal systems; therefore, its immediate removal from wastewater is essential. While bio-catalytic enzyme-based methods are highly efficient for BPA degradation, their practical application is often limited by non-reusability, low storage stability, and sensitivity to environmental conditions. To address these challenges, horseradish peroxidase (HRP) was immobilized onto a graphene oxide–single-walled carbon nanotube (GO–SWCNT) hybrid nanocomposite to enhance both catalytic performance and stability. The GO–SWCNT support provides a high surface area, abundant functional groups, and excellent storage and thermal stability, enabling effective enzyme loading and improved storage. The immobilization process, achieved via EDC/NHS-mediated covalent bonding, resulted in a high 98% immobilization efficiency. Structural and morphological characterization using FTIR, SEM, XRD, and Raman spectroscopy confirmed the successful synthesis of the composite and preservation of its graphitic framework after enzyme immobilization. Enzyme kinetic of prepared GO–SWCNT/HRP composite was analyzed using Lineweaver–Burk plot revealing a lower Km indicating higher affinity toward BPA. Optimal degradation conditions achieved up to 96% BPA removal within 3 hours at pH 6. Additionally, the immobilized biocatalytic platform showed improved resistance to environmental variations (pH and temperature) and retained significant activity after prolonged storage (up to 30 days). Overall, the GO–SWCNT/HRP composite presents a promising, stable, and reusable platform for efficient BPA remediation in wastewater treatment applications.

O-6

Visible-light-driven photocatalytic esterification of thioesters involving radical pathway via sigma bond cleavage

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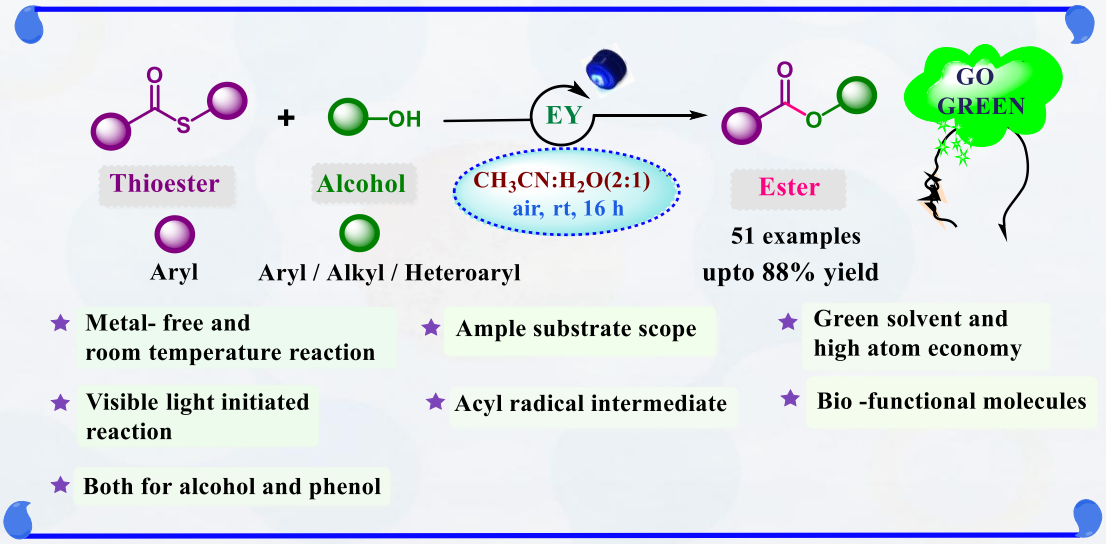
Esters constitute a significant class of compounds in organic chemistry, owing to their synthetic versatility and widespread utility in industries such as food flavouring, perfumery, cosmetics, and agrochemicals. A metal-free esterification strategy has been developed utilising Eosin Y as an organo-photocatalyst under mild reaction conditions. This protocol provides a sustainable and environmentally benign route for ester synthesis, while underscoring the catalytic efficiency of Eosin Y in visible-light-mediated transformations. Upon irradiation with visible light, Eosin Y is photoexcited, facilitating the esterification of a variety of thioesters. The methodology exhibits broad substrate scope, demonstrating compatibility with diverse alcohols and enabling the efficient synthesis of structurally varied ester derivatives with potential relevance in pharmaceutical chemistry.



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O-7

Synthesis of Imidazo[1,2-a]pyridine via Sustainable Photocatalytic C (sp)3–H Functionalization of Ethylarenes and Their Luminescence Investigations

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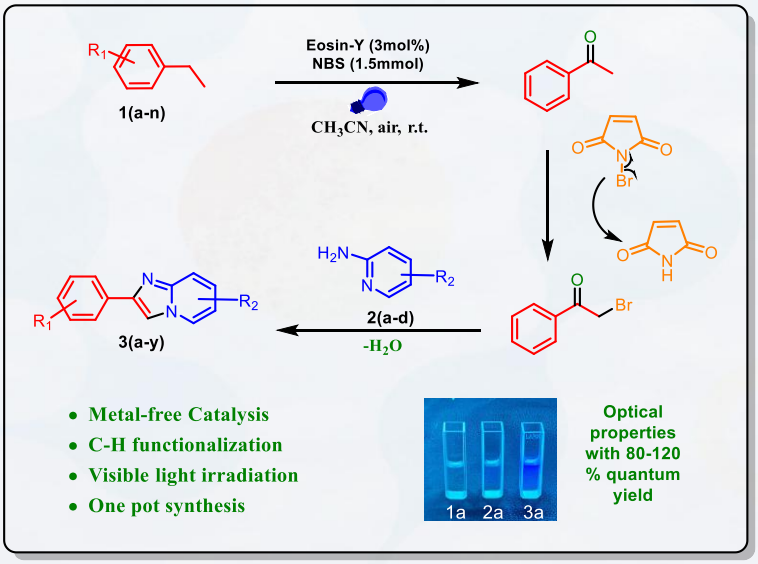
This work describes a one-pot, metal-free, visible light-induced photocatalytic synthesis of imidazopyridines employing ethylarene, 2-aminopyridine, NBS, and Eosin-Y as a photocatalyst. Here, ethylarene's C–H bond is activated and oxidized by Eosin-Y. This is followed by bromination in the presence of NBS, which uses catalytic quantities of the halogenating agent to generate the C–N bond via coupling with aminopyridine. This approach effectively transforms ethylbenzene and aminopyridine into desirable products with a yield of 70-87 % that show the biological activities along with photophysical properties, having a quantum yield ranging from 80-120 %. This approach is suitable for biologically active compounds with luminescence properties as it highlights sustainability with its high atom efficiency, metal-free, environmental friendliness, and use of visible light as a renewable energy source.



O-8

Synthesis of cyclic carbonates from CO_2 and epoxides under ambient conditions

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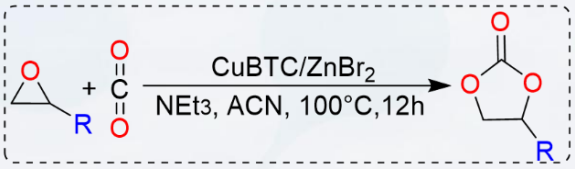
Abstract

The present study describes a green and mild thermocatalytic method for the synthesis of cyclic carbonates, offering a phosgene-free route that is relevant for both academic research and industrial applications. Cyclic carbonates possess significant industrial value, finding wide applications in pharmaceuticals, agrochemicals, and polymeric materials, particularly as key building blocks for polycarbonate (PC) and polyhydroxyurethane (PHU) production[1]. Carbon dioxide (CO_2), a major greenhouse gas, can be utilized as a sustainable C_1 source for the production of fuels and value-added chemicals[2].The incorporation of CO_2 into epoxide rings provides an alternate atom economical synthesis of cyclic carbonates via cycloaddition route. So far, a number of metal based and metal free catalytic systems involving ionic liquids (ILs), bifunctional and multifunctional metal-ligated complexes, metal–organic frameworks (MOFs), and supported metal catalysts for the synthesis of cyclic carbonates from CO_2. However, most of the reported methods require higher temperature, expensive catalytic systems, co-catalyst TBAB and higher CO_2 pressure.[3]

Herein, we demonstrate that dual-functional catalysis using Cu-BTC/$ZnBr_2$ in the presence of triethylamine (TEA) enables the direct incorporation of CO_2 into epoxides under mild thermocatalytic conditions, affording cyclic carbonates in high yields and selectivity. Notably, the methodology avoids the use of tetrabutylammonium bromide (TBAB) while operating at atmospheric CO_2 pressure. This approach provides a simple, greener, and efficient strategy for cyclic carbonate synthesis from CO_2, contributing to the development of a sustainable carbon circular economy.



Scheme 1: Cyclic carbonate synthesis from cycloaddition of CO_2 and epoxides

Keywords: -CO_2 utilization, Cyclic Carbonates, Dual functional catalysis, C_1 Chemistry, Sustainable Carbon economy

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O-9

Small organic metabolites produced by *Lactobacillus rhamnosus* with anti-biofilm properties against *Streptococcus mutans* biofilms

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Abstract

Oral microbiome is the second largest microbial community in the human body. Oral cavity harbours more than 700 bacterial species and is a complex and dynamic microbial community. Dysbiosis of these microbial communities known to cause periodontal diseases such as periodontitis and dental caries. Dental caries is caused primarily due to growth of cariogenic Streptococci such as *Streptococcus mutans*. *S. mutans* form robust biofilms and is recalcitrant to antibiotics treatments. Lactobacillus species are prominent probiotics and are generally considered safe for humans. Many Lactobacilli are also members of the human microbiome and provide beneficial effects by immune modulation and antimicrobial actions. Apart from producing organic acids, Lactobacillus also produces bacteriocins and other small effector molecules that inhibit the outgrowth of pathogenic bacteria. Thus, Lactobacillus species can serve as a potential source for new metabolites with anti-microbial properties. In this study we have isolated and characterized small organic molecules from *Lactobacillus rhamnosus* and *Lactobacillus plantarum* and evaluated their anti-biofilm activities on *S. mutans*. Cell free supernatant *L. rhamnosus* was able to inhibit *S. aureus* biofilm. The cell free supernatant was further fractionated into aqueous and organic fractions and the organic fraction was fractionated using flash chromatography. Mass spectrometry and NMR analysis identified the active compound to Cyclo (-L-Leu-L-Pro) and the pure compound was able to abolish *S. mutans* biofilms. These bioactives decreased expressions of genes involved in major pathways, including two component systems, quorum sensing and EPS formation, in *S. mutans*. Thus small metabolite produced by *Lactobacillus* are effective in attenuation of biofilm of *S. mutans* and can serve as a potential anti-biofilm agent.

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Keywords: Lactobacillus, S. mutans, dental caries, cyclic dipeptide, small metabolites

O-10

Development of Sodium Alginate-Based Microcapsules for Controlled Release of Coenzyme Q_{10}

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Abstract

Coenzyme Q_{10} (CoQ_{10}) is a crucial antioxidant involved in ATP production and protection against oxidative stress. CoQ_{10} deficiency is linked with several health disorders, including neurological degeneration, ageing, and cardiovascular diseases. Given its critical roles, it is necessary to supplement CoQ_{10} with a nutraceutical formulation. However, a major challenge in utilising CoQ_{10} is its high molecular weight (863 Da), extreme lipophilicity (log P ≈ 21), and poor water solubility, which limit its oral bioavailability. To overcome these limitations, CoQ_{10}-loaded microcapsules were developed using sodium alginate (SA), sodium alginate–starch (SA+ST), chitosan-coated sodium alginate (CH-coated SA), and chitosan-coated sodium alginate–starch (CH-coated SA+ST) systems. Microcapsules were formulated via ionotropic gelation and further modified with a chitosan coating to enhance structural stability and release behaviour. The formulations were characterised using scanning electron microscopy (SEM) and FTIR spectroscopy. SEM analysis revealed wrinkled and collapsed microcapsules with a compact internal structure, indicating effective crosslinking. FTIR analysis revealed characteristic peak shifts and functional group interactions, confirming the successful incorporation of CoQ_{10} into the polymeric matrix. Further studies included encapsulation efficiency, in vitro release, and antioxidant activity. Among the formulations, the chitosan-coated sodium alginate–starch (CH-coated SA+ST) system demonstrated improved encapsulation efficiency (93.7% ± 0.50), sustained release (70.5% ± 0.12) over 36 hours at pH 8, and DPPH scavenging activity (51.98% ± 0.47). Overall, the study highlights the potential of chitosan-coated alginate-based microcapsules as promising carriers for improving the stability and oral delivery of CoQ_{10}.

Keywords: Coenzyme Q_{10} (CoQ_{10}); biopolymers; Chitosan; sodium alginate; starch; encapsulation.

O-11

"IN VITRO ANTI-INFLAMMATORY AND ANTI-CANCER ACTIVITY OF FERMENTED FRUIT EXTRACT IN LIPOPOLYSACCHARIDE-STIMULATED RAW 264.7 MACROPHAGES AND $CaCO_2$ CELLS"

Rashmi D[1*], Prerana Bhat[1], Preethi Jinesh[1], Subbalakshmi[2], Harsha K M[2], Kalpana R[2]

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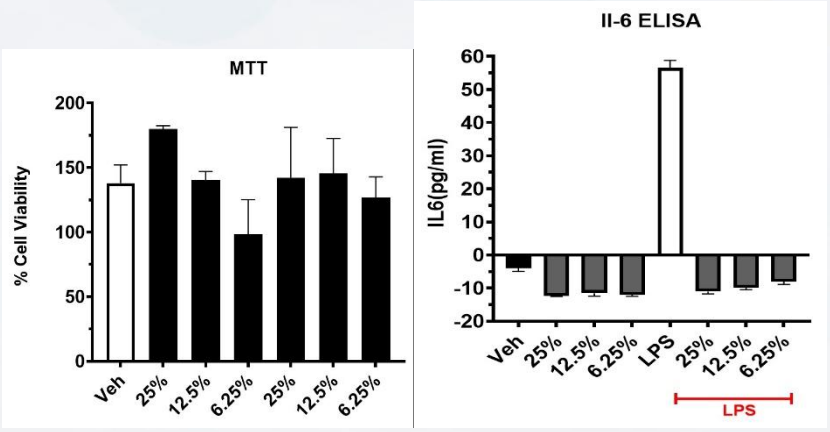
ABSTRACT

Regular administration of Probiotics would help in improving the gut microflora that has gained importance as bacteriotherapy which prevents the gastro-intestinal disease caused by pathogenic microorganisms. The fermented Plant-derived extracts confer for diverse bioactive components, the postbiotics exerts safe pleiotropic effects such as immunomodulatory, anti-inflammatory, anti-microbial and antioxidant effects. The present study was carried out to know the benefits of fermented product using the kefir grains that had active lactic acid bacteria to initiate the fermentation of fruit extracts that produced bioactive molecules including organic acids, flavonoids, polyphenols, SCFA's and vitamins that were analysed through LC-HRMS. This study evaluated the anti-inflammatory potential of a fruit extract using an in vitro macrophage model. LPS (Lipopolysaccharide) stimulation in vehicle-treated cells induced IL-6 production to approximately 60 pg/mL. In contrast, IL-6 (Interleukin-6) levels in all extract-treated groups were below the limit of detection of the assay, demonstrating near-complete inhibition of LPS-induced IL-6 secretion even at the lowest concentration (6.25%). Antiproliferative potential of fermented sample was tested on $CaCo_2$ colon cancer cells exposed to the fermented samples that showed dose and time dependent increase in the potent antiproliferative activity at 48h compared to 24h. The fruit extract exhibits potent anti-inflammatory activity by strongly suppressing LPS-induced IL-6 production in RAW 264.7 macrophages without compromising cell viability. These findings suggest that the extract may modulate key inflammatory signaling pathways and support its potential as a natural therapeutic candidate for chronic inflammation-related conditions.

Keywords: Probiotics, LC-HRMS, LPS, Macrophages, Cancer cells, Interleukin-6



O-12

Polarity-Tunable Curcumin-Derived Carbon Quantum Dots for Multifunctional Liposomal Theranostics

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Abstract.

Carbon quantum dots (CQDs) are promising nanomaterials for bioimaging, drug delivery, and theranostics due to their excellent biocompatibility, tunable photoluminescence, and adaptable surface chemistry.[1–3] Herein, we present a curcumin-derived, single-precursor strategy to engineer hydrophobic CQD (Hb-CQD) and hydrophilic CQD (Hp-CQD) via solvothermal synthesis (with/without 3-APTMS), enabling their spatially controlled integration within biomimetic liposomal architectures. Surface polarity dictated their preferential localization: Hb-CQDs were embedded within the lipid bilayer (L-Hb-CQD), while Hp-CQDs were confined to the aqueous core (L-Hp-CQD), including hierarchical liposome-in-liposome structures.[4] Encapsulation conditions were optimized to achieve uniform dispersion, enhanced colloidal stability, and improved fluorescence. Structural integrity, encapsulation efficiency, and nanoscale positioning were confirmed by fluorescence spectroscopy, TEM, and confocal microscopy. Flow cytometric analysis revealed distinct scatter and fluorescence signatures for liposomes, L-Hb-CQD, and L-Hp-CQD systems. Upon mixing, redistribution of CQDs and shifts in fluorescence populations were observed, indicating dynamic inter-vesicular interactions and polarity-driven re-partitioning rather than simple co-existence.

Biological evaluation in MDA-MB-231 cells demonstrated efficient uptake of Hp-CQDs, which was significantly enhanced after liposomal encapsulation. Encapsulated Hp-CQDs exhibited improved cellular penetration and enhanced cytotoxicity in compare to free Hp-CQDs, highlighting the role of membrane mimicry and nano-confinement in therapeutic modulation. Beyond bioimaging and drug delivery, Hp-CQDs also demonstrated sensitive picric acid detection (LOD = 88 nM) capability, notable antioxidant activity, and semiconducting behavior, broadening their functional scope. Overall, this unified precursor-driven polarity engineering strategy provides a rational framework for directing CQD localization within membrane-mimetic systems and designing multifunctional nano-hybrids for sensing, bioimaging, targeted therapy, and advanced theranostic applications.

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O-13

Lewis Acid-Controlled Divergent Transformations of Glycals: Stereoselective Access to Fused Pyran Frameworks, C-Glycosides, and Glycoconjugates

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Abstract:

The stereo- and regioselective functionalization of glycals presents a powerful strategy in the synthesis of structurally diverse and biologically relevant glycosides. We report a unified approach for the selective transformation of glycal dienes, enabling access to a broad range of glycosylated products and branched sugars with high regio- and stereocontrol. Utilizing Lewis acid catalysis, we achieved chiral azidation of C2-substituted glycals under mild and scalable conditions, introducing azido groups at the C3-position with excellent selectivity. Mechanistic studies reveal the pivotal role of the C2 electron-withdrawing group in directing regioselectivity. Expanding on this framework, we developed a novel domino annulation sequence employing substituted glycals and β-naphthols to synthesize annulated 1,2-C- glycosides. This reaction proceeds via glycosylated intermediates that undergo [3+2] or [3+3] cycloadditions, forming fused pyran systems with broad substrate compatibility and mild reaction conditions. The annulation pathway is substrate-dependent, and detailed DFT studies provide mechanistic insight into the regio- and stereochemical outcomes of both azidation and annulation processes. This methodology represents a versatile platform for constructing complex glycosidic architectures, offering practical access to novel carbohydrate-based scaffolds with potential applications in drug discovery and materials science.[1-3]

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O-14

Sustainable Synthesis of Silver nanoparticles (AgNPs) using *Kanchanara guggulu* extract: Antioxidant, and Cytotoxic Potential.

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ABSTRACT

Kanchnara Guggulu is a compound Ayurvedic formulation used in the Green-synthesised silver nanoparticles (AgNPs). The present study investigates their antioxidant and cytotoxic potential. This study addresses the synthesis and characterization of silver nanoparticles (AgNPs) based on polyherbal formulated Kanchanara Guggulu extract, as well as their antioxidant and cytotoxic potential. The information of homogeneous, spherical shaped AgNPs with an average size of 89 nm was confirmed by XRD, SEM, EDAX, TEM, UV-Vis spectroscopy, and FTIR analysis. The cytotoxicity of the aqueous extract of Kanchnara guggulu having a potent antiproliferative effect, may be due to the presence of flavonoids and phenolics. These findings imply that the environmentally friendly production method and potent antioxidant, antibacterial and cytotoxic potential of the biosynthesized AgNPs hold promise for upcoming biomedical applications. Kanchnara guggulu exhibited a cytotoxic effect by inhibiting cell division (antimitotic) and reducing cell proliferation. These results substantiate its potential for the treatment of cancer and support its traditional use in the treatment of cancer.

Keywords: Kanchanara guggulu (Ayurvedic formulation); Green synthesis; Silver Nanoparticles, Antioxidants; Cytotoxic activity.

O-15

Quercetin induces BMAL1 and targets METTL3/m⁶A–SND1–Mediated Epitranscriptomic novel Axis to Attenuate Hepatocellular Carcinoma under Circadian Disruption

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Abstract:

Hepatocellular carcinoma (HCC) is a leading cause of cancer-related mortality and is associated with alcohol consumption, Hepatitis B virus (HBV) infection, and circadian rhythm disruption, all of which contribute to hepatocarcinogenesis. The International Agency for Research on Cancer classifies circadian disruption due to shift work as a Group 2A probable carcinogen. Circadian disruption downregulates the core clock gene BMAL1, impairing hepatic metabolic homeostasis and upregulating pro-inflammatory cytokines and oncogenic regulators such as METTL3 and SND1. It also contributes to cognitive impairment through altered neuroinflammatory balance and synaptic dysfunction**. In the present study, we aimed to elucidate the novel molecular mechanism by which Quercetin, a flavonoid with anti-inflammatory and antioxidant properties, regulates the BMAL1-METTL3/m⁶A–SND1 axis under circadian disruption in HCC and evaluate its tumor-suppressive effects.**

In this study HCC cell lines (HepG2 and Huh7) were treated with Quercetin (10, 20, 50 µM), and cell viability was assessed using the Trypan Blue exclusion assay. Gene expression analysis revealed upregulation of BMAL1 along with reduction in METTL3, SND1, and pro-inflammatory cytokines. In vivo, male C57BL/6 mice were subjected to circadian disruption (18 h light/6 h dark for 33 days) followed by Quercetin administration (100 mg/kg). Circadian disruption reduced BMAL1 expression and enhanced inflammatory and oncogenic signaling**. Here we explored the novel mechanism by which Quercetin induces BMAL1 and targets METTL3/SND1-mediated m⁶A modified mRNA stability and decreases FASN and SREBP activity, lipid metabolism and this resulted in restoration of circadian synchronization, improved lipid homeostasis, and tumor suppression.**

O-16

Cytotoxic and Genotoxic Effects of Aluminum Oxide (Al_2O_3) Nanoparticles on Human Haematocytes: An In Vitro Study

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Abstract

Nanotechnology has emerged as a rapidly advancing field with extensive biomedical and industrial applications. Among various nanomaterials, aluminum oxide (Al_2O_3) nanoparticles (AL NPs) are widely used; however, concerns regarding their potential cytotoxic and genotoxic effects remain. The present study aimed to evaluate the impact of AL NPs on haematocytes through particle characterization and in vitro toxicological assessments. Transmission Electron Microscopy (TEM) analysis revealed that the nanoparticles ranged between 250–300 nm in size, with evidence of agglomeration in suspension. Cell viability was assessed using trypan blue exclusion and MTT assays following 48-hour exposure to varying concentrations of AL NPs. Results demonstrated that overall cell viability remained above 95%, even at the highest tested concentration (300 µg), although mild morphological alterations and dose-dependent mitochondrial dysfunction were observed. Apoptotic changes were confirmed through Hoechst 33342 staining, which revealed chromatin condensation at higher concentrations, indicating induction of apoptosis. Genotoxic potential was evaluated using the comet assay, which showed a significant increase in DNA strand breaks in treated cells compared to controls. However, no chromosomal aberrations were detected in lymphocytes at the tested concentrations, suggesting that AL NPs induced DNA-level damage without affecting overall chromosomal structure. In conclusion, AL NPs at the studied doses exhibited mild cytotoxic effects and measurable genotoxicity at the DNA level in haematocytes. These findings highlight the importance of further investigations using different nanoparticle sizes, higher concentrations, and diverse cell types to better understand the potential health risks associated with aluminum oxide nanoparticles.

Keywords: Nanotechnology; Aluminum oxide nanoparticles (Al_2O_3 NPs); Haematocytes; Cytotoxicity; Genotoxicity; Comet assay

O-17

Bioprospecting of *Endophytic Aspergillus niger* Associated with *Withania somnifera* for Pharmacologically Active Metabolites

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Date of Birth of the Presenting Author: 27/09/2001

Abstract

Medicinal plants have long served as nature's pharmacy, harbouring an extraordinary wealth of bioactive compounds. However, their escalating global demand has triggered alarming overexploitation, threatening both biodiversity and sustainable supply chains. In the search for alternative BioSource's, endophytic fungi have emerged as silent yet prolific biochemical factories residing within plant tissues. Motivated by their potential, the present study ventured into the rich botanical landscape of Amreli district, Gujarat, India, to explore endophytic fungal diversity from medicinal plant samples. Distinct 5 fungi were successfully isolated from various plant parts, purified via successive sub-culturing, and established as stable pure cultures. Among the isolates, *Aspergillus niger* was selected and identified through detailed morphological and microscopic examination. Cultivation parameters—including temperature, pH, agitation speed, carbon source and incubation period—were strategically optimized to maximize metabolite yield and enhance production efficiency. Ethyl acetate–based liquid–liquid extraction effectively isolated secondary metabolites, exhibiting well-defined and promising banding profiles on Thin-Layer Chromatography (TLC) Miller et al. [1]; Octaverina et al. [2]. Further, Gas Chromatography–Mass Spectrometry (GC–MS) analysis Emanuela et al. [3]; Reinstadler et al. [4]8 revealed a diverse and compelling chemical repertoire, including Cyclo (L-prolyl-L-valine), Pyrrolo [1,2-a] pyrazine-1,4-dione and d-Altronic acid—compounds with each one carrying notable pharmacological significance. Collectively, these findings highlight *Aspergillus niger* isolated from Ashwagandha as a potent and sustainable BioSource, offering a promising alternative to direct plant extraction.

Keywords: Endophytic Fungi, *Withania somnifera*, GC-MS, Secondary Metabolites, Sustainable Biotechnology, Bioprospecting, Gujarat.

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O-18

Green Biologics and Mechanistic Toxicology: Advancing Sustainable Pharmaceutical Development

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Abstract:

Biologics represent one of the fastest-growing sectors of the pharmaceutical industry, largely driven by monoclonal antibody therapies. This diverse class including peptides, proteins, antibodies, and selected vaccines is primarily manufactured using living systems and was historically regarded as environmentally benign. However, biologics research, development, and large-scale production demand substantial quantities of water, energy, single-use plastics, filtration systems, and caustic reagents, generating significant environmental burdens. These challenges underscore the need to integrate sustainability principles early in biologics development.

Green chemistry provides a strategic framework for environmentally responsible innovation, particularly through the concept of **atom economy**, which emphasizes "100% input → 100% output," ensuring that all materials used in a process are incorporated into the final product with minimal waste generation. Adapting green strategies and atom-economical design to biologics manufacturing requires optimization of bioprocess efficiency, solvent reduction, renewable feedstocks, waste valorisation, and energy-efficient downstream processing.

Simultaneously, twenty-first century medicinal toxicology has shifted from classical dose–response assessment to mechanistic, pathway-based evaluation. Advances in computational chemistry, in silico toxicology, quantitative structure–activity relationship (QSAR) modelling, physiologically based pharmacokinetic (PBPK) modelling, and artificial intelligence enable predictive identification of adverse outcome pathways (AOPs) and molecular initiating events (MIEs). Integration with mechanistic in vitro systems such as organ-on-chip platforms and high-content screening supports safer-by-design biologics while reducing reliance on animal testing.

Innovation in green pharmaceutical chemistry must also align with intellectual property frameworks. Under United States patent law, inventions must satisfy criteria of novelty, non-obviousness, and utility, necessitating strategic patent planning for sustainable biologics technologies.

The convergence of green strategy, atom economy, systems toxicology, and regulatory science establishes a comprehensive model for sustainable biologics development, ensuring therapeutic efficacy, human safety, and minimized environmental impact within a circular bioeconomy paradigm.

Keywords: Green chemistry; Atom economy (100% input–100% output); Medicinal toxicology; Monoclonal antibodies; Sustainable manufacturing; In silico toxicology; Adverse outcome pathways; Patent strategy; Circular bioeconomy.

O-19

Design, Synthesis and Antiviral Activity of Pyrazole-linked Fused Curcumin Glycoconjugates against Influenza A Virus (H3N2)

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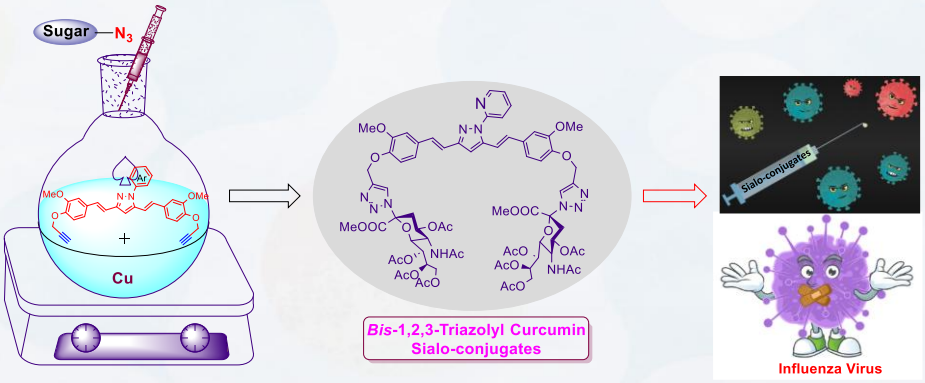
Influenza is a highly pathogenic disease caused by the influenza virus, an acute respiratory disease that is highly contagious.[1-2] Novel anti-influenza drugs must be developed immediately due to the ongoing growth of drug-resistant virus strains. Building on these findings, we have synthesized a series of pyrazole-linked fused curcumin 1,2,3-triazolyl glycoconjugates, incorporating heteroatom substituents, using a click protocol with excellent yield, thereby making them more important in medicinal chemistry. By using structural diversification, this strategy is targeted to increase antiviral potency.[3] Of the resultant our developed pyridine sialo-glycoconjugate, showed a low 50% cytotoxic concentration and superior antiviral efficacy against the Influenza A Virus (H3N2).



Scheme 1. Synthesis of 1,2,3-Triazolyl Curcumin-based Glycoconjugates *via* click Chemistry

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O-20

Microalgal consortia-derived biogenic fluorescent carbon dots exhibiting multispectral emission

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Abstract:

Fluorescent nanoparticles (FNPs), defined as discrete materials with dimensions between 1 to 100 nm, exhibit unique photoluminescence, high photostability, and modifiable surfaces, making them indispensable for advanced bioimaging and sensing. Traditional "laboratory" synthesis of FNPs often relies on non-renewable, hazardous chemical precursors, necessitating a transition toward sustainable "green" methodologies. This study investigates the biogenic synthesis of carbon dots (CDs) utilizing microalgal biomass as a renewable, nitrogen-rich carbon source. Algae are uniquely advantageous due to their natural enrichment of nitrogen and sulfur, which facilitates "self-doping" for enhanced fluorescence, and their ability to act as efficient carbon sinks via CO_2 sequestration. In the present study multi-spectral CDs emitting in blue, green, and red wavelengths were successfully synthesized using microalgal consortia (containing chlorella, spirulina) through hydrothermal-assisted carbonization at 130°C–160°C. Blue carbon dots (BCDs) were derived directly from microalgal biomass suspended in deionized water, while green carbon dots (GCDs) were synthesized with citric acid and H_2O_2 as co-precursors, and red carbon dots (RCDs) were obtained using 95% ethanol as co-solvent. Structural characterization via XRD confirmed stable graphitic cores, whereas, DLS verified uniform hydrodynamic size distribution. Finally, FTIR confirmed the presence of oxygen containing and nitrogen containing groups indicating the successful synthesis of CDs. The synthesized CDs can be applied as high-sensitivity fluorometric probes for the detection of biomedical analytes, food contaminants, and environmental pollutants. Ultimately, this research supports a "zero-waste" algal biorefining model, transforming low-value biomass into high-value nanomaterials for advanced environmental and theranostic applications.

O-21

Evaluation of single and combined effects of Dimethyl phthalate and Bis (2-ethyl hexyl) phthalate on Reproductive and Neural health in Sprague Dawley rats.

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Abstract

Phthalates such as Dimethyl phthalate (DMP) and Bis(2-ethylhexyl) phthalate (DEHP) are widely used plasticisers with known endocrine-disrupting properties. This study evaluated their systemic toxicity using an Extended One-Generation Reproductive Toxicity Study (EOGRTS) in Sprague Dawley rats. F_0 parental animals were randomly assigned to five groups: control (corn oil), DMP-High (1000 mg/kg/day), DEHP-High (1000 mg/kg/day), combined low dose (DMP + DEHP, 300 + 300 mg/kg/day), and combined high dose (1000 + 1000 mg/kg/day). All treatments were administered orally on a daily basis.

Reproductive outcomes in the F_0 generation and reproductive and neurobehavioral parameters in the F_1 generation were assessed. High-dose DEHP and combined high-dose exposure produced the most pronounced toxicity, characterised by significant reproductive impairment and marked histopathological degeneration in testicular tissues. In contrast, DMP alone and the combined low-dose group showed comparatively minimal adverse effects.

In F_1 offspring, developmental exposure resulted in notable neurobehavioral alterations along with histopathological changes in both brain and testicular tissues. Alterations observed in neurohistopathological sections indicate disruption of normal neural architecture, highlighting the susceptibility of the developing nervous system to phthalate exposure.
Mechanistically, these findings are consistent with endocrine disruption, potentially mediated through anti-androgenic activity and related molecular pathways. Overall, the combined reproductive and neurological impairments underscore the potential health risks associated with high-dose and multigenerational phthalate exposure, emphasising the need for continued regulatory oversight and long-term toxicological evaluation.

Keywords: Phthalates (DMP, DEHP), Endocrine disruption, Reproductive toxicity, Neurobehavioral alterations, Histopathology, Multigenerational exposure.

O-22

Beyond Bulk Measurements: Decoding Nanoscale Electrocatalysis with Scanning Electrochemical Microscopy

Koushik Barman

ABSTRACT

The performance of electrocatalysts is fundamentally governed by local atomic structures, where defects, edges, and corners often serve as the primary active sites. While bulk measurements provide average performance data, they obscure the critical influences of morphology, dimensions, and surface attachment on catalytic activity. This talk explores the advancement of nano-electrochemical tools specifically Scanning Electrochemical Microscopy (SECM), designed to bridge this gap through high-resolution, in situ reactivity mapping.

We first introduce a novel SECM approach utilizing chemically modified nanoelectrodes. By immobilizing redox mediators like $Ru(bpy)_3$ or ferrocene on carbon and platinum nanotips (dia. ~50-100 nm), we overcome the common challenge of surface fouling and passivation during inner-sphere reactions. This technique enables stable, high-resolution mapping of critical processes, including hydrogen evolution (HER), oxygen evolution (OER), and oxygen reduction (ORR).

Furthermore, we discuss the operando observation of overall water splitting (OWS) at the single-particle level. Using photo-SECM with through-tip illumination, we quantitatively resolve simultaneous hydrogen and oxygen evolution fluxes on individual microcrystals of Al-doped $SrTiO_3$ and P-doped $BiVO_4$. These measurements reveal significant kinetic heterogeneity, demonstrating how photogenerated carriers selectively accumulate on specific crystal facets. Collectively, these methodologies provide a powerful framework for assessing the intrinsic kinetics of photo(electro)catalyst particles, and 2D materials at the nanometer scale.

O-23

Unravelling the Novel Mechanism of Anti-Tumor Role of Sodium Butyrate: SND1-mediated Telomerase and miR-155 Pathway Suppression in HCC.

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Abstract

Hepatocellular carcinoma (HCC) is a major global health challenge arising from complex interactions among chronic inflammation, metabolic dysregulation, altered gene expression, and lifestyle factors. Among post-transcriptional regulators, the RNA-induced silencing complex (RISC) and its key component SND1 play critical oncogenic roles in hepatocarcinogenesis. MicroRNAs, particularly miR-155, function as oncogenic regulators by promoting inflammation, proliferation, and metabolic reprogramming in cancer. PPARγ and PPARα are nuclear receptors essential for hepatic lipid metabolism, anti-inflammatory signaling, and cell survival, exhibiting tumor-suppressive functions. Dysregulation of miR-155 may suppress PPARγ/α expression, thereby contributing to HCC progression. However, the precise mechanism remains unclear. Short-chain fatty acid (SCFA)-Sodium Butyrate (NaBu) are gut microbiota-derived metabolites that maintain cellular homeostasis and modulate liver physiology through the gut–liver axis by influencing metabolic, inflammatory, and epigenetic pathways. **Our current study aims to elucidate the molecular mechanism of SCFA-NaBu in regulating SND1-mediated signalling in telomerase expression in HCC and evaluate its anti-tumor effects using in-vitro models.** HCC cell lines (Huh7&HepG2) were treated with NaBu, and IC_{50} was determined using a WST-1 assay. Cells were transfected with miR-155-5p mimic and SND1-siRNA, followed by NaBu treatment. Gene and protein expression analyses were performed using qPCR and Western blotting. Functional assays including CAM assay, angiogenesis array, and cytokine profiling were conducted. NaBu treatment significantly downregulated SND1 and telomerase expression, angiogenic markers, and pro-inflammatory cytokines, indicating its potential to modulate oncogenic pathways. These findings reveal a novel NaBu anti-tumor mechanism in HCC by suppressing telomerase and miR-155 via SND1-mediated.

O-24

Fostering Environmental Responsibility at secondary school level through NCERT Chemistry Kits

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Introduction: Environmentally benign and sustainable chemistry, often referred to as green chemistry, focuses on the design of chemical products and processes that minimize or eliminate the use and generation of hazardous substances. With increasing environmental challenges such as pollution, resource depletion, and climate change, the need for sustainable chemical practices has become more critical.

Methodology: Environmentally benign and sustainable chemistry can be effectively introduced at the secondary school level through the use of standardized chemistry kits provided by the National Council of Educational Research and Training (NCERT). These kits are designed to promote safe, resource-efficient, and eco-friendly laboratory practices among students. By incorporating the principles of green chemistry such as minimizing chemical waste, using less hazardous substances, and optimizing the use of small-scale experiments, NCERT chemistry kits provide a practical framework for sustainable learning. Use of these kits was started in GGIC Lucknow. It sparked not only interest among students but also fostered a sense of responsibility and ownership for environment. The experiments done with these kits emphasized microscale techniques, which significantly reduce the consumption of reagents and the generation of toxic by-products. This approach not only safeguards students' health but also instills environmental awareness and responsibility at an early stage of scientific education.

Conclusion: The integration of environmentally benign chemistry within NCERT secondary school laboratory kits plays a crucial role in nurturing a generation of environmentally conscious learners.

O-25

An integrative approach combining computational simulation and spectroscopic analysis elucidates the stability of L-asparaginase on the nanocomposite surface

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Abstract

The synthesis of nanomaterials and their functionalization through enzyme immobilization play a pivotal role in the development of next-generation biosensing systems [1, 2]. In this study, L-asparaginase (asnB) was covalently immobilized onto a novel nanocomposite using glutaraldehyde as a crosslinking agent. The nanocomposite was synthesized and subsequently characterized using X-ray diffraction (XRD), Fourier-transform infrared spectroscopy (FTIR), and circular dichroism (CD) spectroscopy, which collectively confirmed successful material formation and effective enzyme immobilization.

To gain molecular-level insights, all-atom molecular dynamics simulations were conducted. The results demonstrated that immobilization significantly reduces the global conformational flexibility of the enzyme while promoting localized structural compaction. This behaviour is evidenced by a decrease in solvent-accessible surface area from approximately 26,400 Å² in the free enzyme to 23,300–25,400 Å² in the immobilized state. Furthermore, orientation analysis indicated that the enzyme adopts a stable binding configuration on the nanocomposite surface. Importantly, secondary structure analysis revealed that key α-helical and β-sheet elements remain largely preserved upon immobilization.

Overall, the integration of spectroscopic characterization with computational modelling provides comprehensive mechanistic insights into enzyme–nanomaterial interactions [3]. This combined approach offers a robust framework for the rational design of stable, activity-retaining enzyme–nanocomposite interfaces for biosensing and biocatalytic applications.

Keywords: L-asparaginase; nanocomposite; immobilization; simulation

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O-26

DESIGN OF A BATCH BIOREACTOR UTILIZING A DEVELOPED MICROBIAL-NANOCOMPOSITE BEAD SYSTEM FOR SCALE-UP OF HEAVY METAL REMEDIATION PROCESS FROM AQUEOUS SYSTEMS

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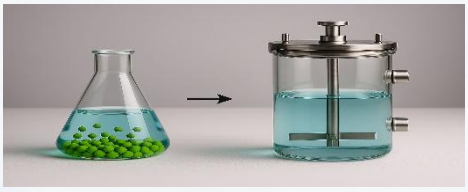
ABSTRACT: Heavy metal contamination in industrial wastewater remains a critical global challenge, demanding scalable and sustainable treatment solutions beyond conventional laboratory studies. This work presents a novel integration of engineered microbial-nanocomposite biosorbent system chemically immobilized onto glass beads with a custom designed batch bioreactor system. Thus, bridging the gap between material development and process scale application for heavy metal remediation. For this, a cylindrical PVC based bioreactor (5 L total volume, 3 L working volume) was designed with integrated bead retention architecture, optimized inlet-outlet hydraulics, and controlled mechanical agitation. The system was operated under optimized conditions (pH 6, 25°C, 150 rpm) in a sequential batch mode without aeration, enabling efficient solid-liquid interaction and process stability. The reactor design ensured uniform hydrodynamics with minimal dead zones, supported by internal configuration and freeboard optimization. The immobilized biosorbent beads, combining microbial surface functionality with nanoscale interactions, demonstrated efficient multi-metal removal and operational stability across repeated treatment cycles. The incorporation of a dedicated bead retention zone prevented material loss, enabling consistent re-usability and enhancing process feasibility. Unlike conventional biosorption studies limited to shake flask systems, this work establishes a scalable reactor platform suitable for real wastewater applications. The study highlights a significant advancement in process development by integrating biosorption materials into an engineered reactor system, emphasizing cost-effective fabrication, reproducibility, and scale-up potential. This approach provides a practical pathway toward sustainable heavy metal remediation and positions immobilized bio-nanocomposite systems as viable candidate for industrial wastewater treatment.



Keywords: Heavy metal contamination; Engineered microbial nanocomposite; Batch bioreactor; Biosorption.

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O-27

Ultrasensitive Electrochemical Sensor for Nitroaromatics Using C_3N_4-MoS_2-Au Nanocomposite with Pendimethalin as a Real Sample

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Choice of mode- oral

Abstract

This work presents a highly efficient electrochemical sensing platform for detecting nitroaromatics based on a glassy carbon electrode (GCE) modified by C_3N_4-MoS_2-Au nanocomposite. The Structural and morphological characterisation of the fabricated nanocomposites (C_3N_4, C_3N_4-MoS_2, C_3N_4-Au, and C_3N_4-MoS_2-Au) was accomplished using XRD, FT-IR, SEM, HRTEM, and XPS. The C_3N_4-MoS_2-Au/GCE demonstrated better electrochemical performance than other materials, with detection limits of 0.219 µM, 0.615 µM, and 0.479 µM for 4-nitrophenol (4-NP), dinitrophenol (DNP), and trinitrophenol (TNP), within linear ranges of 0-1000 µM, 0-500 µM, and 0-500 µM, respectively. The sensor showed remarkable sensitivity and selectivity, with 4-NP having the lowest detection limit. Optimised pH conditions further improved detection efficiency, confirmed by cyclic voltammetry (CV) and linear sweep voltammetry (LSV). The modified electrode also demonstrated good stability and reproducibility, with a relative standard deviation (RSD) of less than 5% and a recovery rate between 95.5-102.4%. Integrating MoS_2 and Au significantly enhanced electron transfer kinetics, establishing this nanocomposite as a novel and efficient platform for detecting nitroaromatic pollutants. Successful detection of Nitrophenols in real water samples and a commercial herbicide (pendimethalin) demonstrated excellent recovery, validating its efficacy for environmental monitoring of explosives and herbicides.

O-28

Visible-light-initiated *N*-arylation of hydrazones with diazonium tetrafluoroborate via EDA complex formation

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A particularly simple and efficient strategy for the synthesis of hydrazones involves *N*-arylation. Although considerable advances have been achieved in the construction of hydrazone frameworks, the use of diazonium tetrafluoroborates as aryl radical precursors remains underexplored. Herein, we report a catalyst-free and environmentally benign protocol for the *N*-arylation of hydrazones under visible-light irradiation via an electron donor–acceptor (EDA) complex, employing DMSO as the solvent. The method demonstrates a broad substrate scope and excellent functional group tolerance, accommodating a diverse range of aromatic and heteroaryl hydrazones. Given the central role of hydrazones as versatile intermediates that bridge fundamental organic synthesis with applications in medicinal chemistry, materials science, and coordination chemistry, this operationally simple and sustainable approach provides an efficient platform for the construction of valuable *N*-aryl hydrazone derivatives.

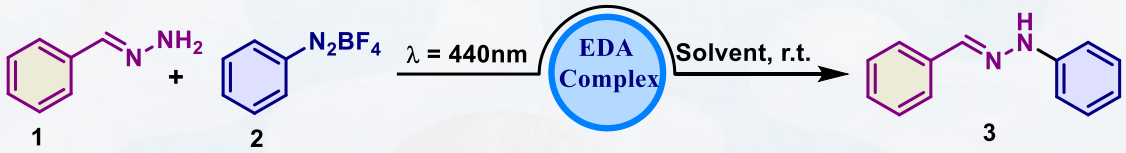

Figure 1. Visible light-mediated *N*-arylation of hydrazones.

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O-29

Synthesis of cinnamic esters and acids *via* palladium-catalyzed reactions of aryl diazonium salts and their biological evaluation

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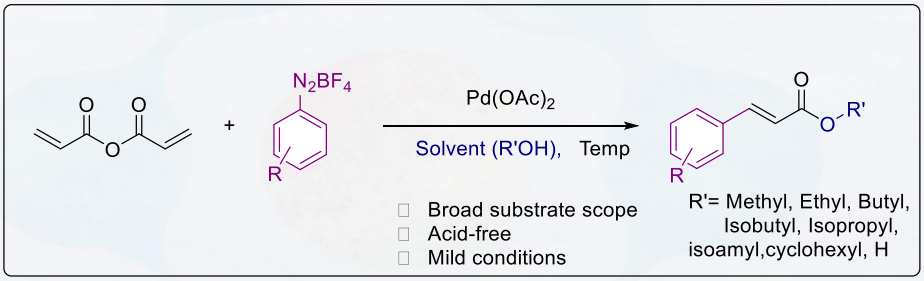
An efficient and practical method has been developed for the synthesis of cinnamic esters and cinnamic acids through the reaction of acrylic anhydride with aryl diazonium salts in various solvent systems. Cinnamic esters are formed smoothly at room temperature in the presence of palladium acetate, demonstrating mild and convenient reaction conditions. In contrast, cinnamic acids are obtained under basic conditions using potassium carbonate (K_2CO_3) at 80 °C in a DMF/H_2O mixture. This approach provides good yields and allows selective synthesis of both product types. The methodology is advantageous due to its operational simplicity, use of inexpensive and readily available starting materials, and relatively mild conditions. Additionally, the synthesized cinnamic esters were evaluated for their biological activity. Most compounds exhibited significant antioxidant potential, as determined by radical scavenging activity assays, while some derivatives showed moderate inhibitory effects on amyloid-β aggregation, suggesting their potential relevance in therapeutic applications.



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O-30

Bioprospecting of *Endophytic Aspergillus niger* Associated with *Withania somnifera* for Pharmacologically Active Metabolites

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Abstract

Medicinal plants have long served as nature's pharmacy, harbouring an extraordinary wealth of bioactive compounds. However, their escalating global demand has triggered alarming overexploitation, threatening both biodiversity and sustainable supply chains. In the search for alternative BioSource's, endophytic fungi have emerged as silent yet prolific biochemical factories residing within plant tissues. Motivated by their potential, the present study ventured into the rich botanical landscape of Amreli district, Gujarat, India, to explore endophytic fungal diversity from medicinal plant samples. Distinct 5 fungi were successfully isolated from various plant parts, purified via successive sub-culturing, and established as stable pure cultures. Among the isolates, *Aspergillus niger* was selected and identified through detailed morphological and microscopic examination. Cultivation parameters—including temperature, pH, agitation speed, carbon source and incubation period—were strategically optimized to maximize metabolite yield and enhance production efficiency. Ethyl acetate–based liquid–liquid extraction effectively isolated secondary metabolites, exhibiting well-defined and promising banding profiles on Thin-Layer Chromatography (TLC) Miller et al. [1]; Octaverina et al. [2]. Further, Gas Chromatography–Mass Spectrometry (GC–MS) analysis Emanuela et al. [3]; Reinstadler et al. [4]8 revealed a diverse and compelling chemical repertoire, including Cyclo (L-prolyl-L-valine), Pyrrolo [1,2-a] pyrazine-1,4-dione and d-Altronic acid—compounds with each one carrying notable pharmacological significance. Collectively, these findings highlight *Aspergillus niger* isolated from Ashwagandha as a potent and sustainable BioSource, offering a promising alternative to direct plant extraction.

Keywords: Endophytic Fungi, *Withania somnifera*, GC-MS, Secondary Metabolites, Sustainable Biotechnology, Bioprospecting, Gujarat.

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V^{IV}-TSC-based Metallodrugs: Solution Chemistry, Cytotoxicity, and Cellular Internalization

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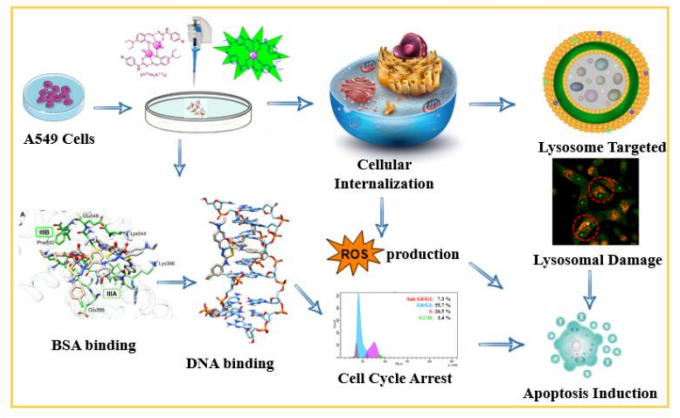
In recent years, vanadium compounds have been extensively studied for their biological, medicinal, and other therapeutic applications [1-4]. To date, only a limited number of non-oxido and dinuclear oxido V^{IV} complexes have been studied, mainly for their potential use in anticancer studies. So, exploring the toxicity potential of non-oxido compared to dinuclear oxido V^{IV} complexes could provide valuable insights into their solution-phase stability and biological effects. In this presentation, the synthesis, characterization, structure, DFT, and docking studies and solution behaviour of a series of mononuclear non-oxido and dinuclear oxido V^{IV} complexes will be highlighted in relation to their theranostic activity.



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O-32

"Targeting Breast Cancer Progression with Taurine: Inhibition of Proliferation, Metastasis, EMT, and RISC-Mediated Regulatory Pathways"

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Keywords: Breast cancer, RNA Induced Silencing Complex, Taurine, Epithelial-Mesenchymal Transition

Abstract:

Breast cancer is the most common cancer among women worldwide and remains a leading cause of cancer-related mortality, with disparities in outcomes due to differences in early detection and access to treatment. In India, it has emerged as the most prevalent cancer among women, often diagnosed at advanced stages due to limited awareness and screening. Socio-economic factors, healthcare accessibility, and lifestyle changes further contribute to the growing disease burden and poorer clinical outcomes. This challenge has intensified the search for safer and more effective therapeutic strategies, with increasing interest in naturally occurring bioactive compounds. Despite growing global attention to RNA-induced silencing complex (RISC) biology, studies integrating RISC machinery with natural compounds remain limited, with no systematic investigations from India. Taurine, a conditionally essential amino sulfonic acid with a strong safety profile, has emerged as a promising candidate in oncology. In this study, taurine exhibited significant anti-cancer activity against breast cancer cells by inhibiting proliferation, migration, and epithelial–mesenchymal transition (EMT). Dose-dependent assays demonstrated reduced cell viability, indicating cytostatic and cytotoxic effects, while migration assays confirmed its anti-metastatic potential. Mechanistically, taurine reversed EMT by downregulating mesenchymal markers such as N-cadherin and vimentin while restoring E-cadherin. Genomic analyses revealed suppression of key RISC proteins, suggesting disruption of tumor-associated microRNA regulation. Additionally, taurine modulated oncogenic pathways including TGF-β and NF-κB. These findings highlight taurine as a promising multi-targeted therapeutic candidate for breast cancer management.

O-33

Investigating the Emerging Neurotoxic Potential of Acetonitrile-d3 in a Zebrafish Model: Implications for Human Mental Health

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ABSTRACT

Acetonitrile-d3 is a commonly used solvent in the chemical and pharmaceutical industries. However, it has become a growing environmental pollutant with potential neurotoxic effects that are not well understood Ahmed et al [1]. The rise in industrial discharge containing acetonitrile-d3 raises concerns about its impact on aquatic ecosystems and vertebrate neurobiology. This is particularly concerning due to the compound's capacity to disrupt ionic balance and impair neurotransmitter function.

To address the knowledge gap regarding its adverse effects on neurobehavioral parameters, the current study used zebrafish (Danio rerio) as a model organism. Zebrafish share about 70% of their genetic makeup with humans and have similar genes linked to neurological disorders Howe et al [2]. In this study, adult zebrafish were exposed to acetonitrile-d3 at 150, 300, 500, and 700 ppm, alongside an unexposed control group and for each group, 3 zebrafish were used. The exposure period lasted for 96 hours. Next, a thorough set of behavioural tests was conducted, including the Novel Tank Diving Test (NTDT) to assess anxiety-related vertical exploration, the T-maze test to evaluate spatial memory and decision-making, and the Light-Dark Preference Test to measure anxiety, exploration, and depression-like states at 0, 3rd, and 7th days.

The behavioural analysis showed that exposure to acetonitrile-d3 caused dose-dependent changes in zebrafish. At the lowest concentration (150 ppm), the fish displayed subtle behavioural changes, including slight hypoactivity and more frequent freezing episodes. However, at moderate to high doses (300–700 ppm), the fish exhibited significant anxiety-like behaviours, memory problems, social withdrawal, and a marked decrease in exploratory activity. Heat map activity and track-plot patterns showed less spatial engagement and more bottom-dwelling behaviour at higher exposure levels. These findings represent the first *in vivo* evidence of acetonitrile-d3's neurotoxic potential in a vertebrate model. The study outcomes raise important environmental and public health concerns about the compound's risks in occupational settings and the ecosystem. Given the widespread industrial use of this compound and its presence in wastewater, the data highlight an urgent need for regulatory reviews, environmental monitoring, and risk assessments related to acetonitrile-d3 contamination. Future research should include molecular, biochemical, and long-term behavioural studies to clarify the mechanisms and lasting effects on brain function, as well as exploring effective countermeasures to neutralise the neurotoxicity. This research provides valuable baseline data for understanding how a proposed pollutant can cause neurobehavioral toxicity and reinforces the zebrafish as a useful model for environmental neurotoxicology. Zebrafish can serve as a reliable model for screening the industrial neurotoxicants that may have adverse neuropsychiatric effects in humans.

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O-34

EXPLORING MARINE DERIVED FUNGI FROM THE VISAKHAPATNAM COAST: AN ECO-FRIENDLY APPROACH TO MICROPLASTICS DEGRADATION

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Abstract:

The convenience of plastic has led to a significant increase in its usage worldwide. Besides their usage, plastics have become an important cause of environmental pollution (Khatua et al. [1]). Abiotic exposure, like UV and physical abrasion, causes fragmentation of plastic debris into microplastics (MP) of size 1µm – 5mm, which is difficult to degrade (Ikhimalo & Ugbenyen, [2]). These particles are then released into water bodies, which harm human health and marine life. Polythene makes up over 64% of the garbage generated by synthetic plastics in marine environments, and these microplastics are accumulated in all the tissues of marine specimens (Keerthika et al. [3]). Regular decomposition processes negatively influence the environment, and to mitigate this problem, different microbial species utilize a bioremediation process to break down the microplastics.

Mycoremediation, facilitated by filamentous fungi, has shown promising results for plastic biodegradation due to their saprophytic lifestyle, extensive hyphal networks facilitating substrate colonization, secretion of amphipathic hydrophobin proteins, and robust extracellular oxidative enzyme systems (Barrech, [4]). In the coastal regions of Visakhapatnam, there is a large amount of microplastic trash. In our current study, we aim to identify marine fungi capable of degrading MPs. This research work examines the degradation of High-Density Polyethylene (HDPE) (<100 microns) by marine-derived fungi isolated from the Visakhapatnam Coastal site. We have isolated a few fungal strains that can degrade MP more effectively when inoculated in MSM media and cultured for 30 days at 28°C. The degradation process was analysed using analytical tools such as FE-SEM with EDX, ATR-FTIR, and XRD. Further, the degraded end-products were characterized by GC-MS, and metabolomic profiling was performed by LC-MS/MS.

Keywords: Microplastics, Mycoremediation, Marine-derived fungi, Visakhapatnam coast, Analytical tools.

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O-35

Streptococcal Surfaceome-Host Interactions Drive Adhesion, Invasion, and Divergent Inflammatory-Apoptotic Signaling in Oral Cancer Cells

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ABSTRACT

The oral microbiome plays a critical role in modulating tumor behavior in oral squamous cell carcinoma (OSCC), yet the molecular mechanisms by which individual microbial species influence cancer cell fate remain poorly understood [1]. *Streptococcus* species dominate the oral microbiota and express diverse surface-associated proteins that interact with host immune and death receptors [2]. In this study, we combined structural modeling, molecular docking, molecular dynamics simulations, and *in vitro* validation to investigate how pathogenic and commensal streptococci differentially influence oral cancer progression. Surface proteins from *Streptococcus mutans* and *Streptococcus oralis* were modeled and docked with host receptors, revealing strong interactions between *S. mutans* Antigen I/II and TLR2 (-14.7 kcal/mol) and between *S. oralis* penicillin-binding protein 1a and CD95 (-12.6 kcal/mol), which were further validated by molecular dynamics simulations. Functional assays in CAL27 cells demonstrated that *S. mutans* significantly enhances bacterial adhesion and invasion, induces necrotic responses, and triggers a ~7-fold increase in IL-6 secretion ($p < 0.01$), indicating a pro-inflammatory phenotype. In contrast, *S. oralis* exhibited reduced invasiveness but promoted reactive oxygen species accumulation, apoptosis, cell cycle alterations, and delayed cell migration, along with modulation of TGF-β1 levels. These findings reveal a commensal-pathogen dichotomy in streptococcal surfaceome interactions that governs adhesion, invasion, and divergent inflammatory versus apoptotic signaling in oral cancer. This study highlights microbial-host receptor interfaces as potential targets for microbiome-informed and sustainable theranostic strategies in oral cancer.

Keywords: *Streptococcus*, Oral Cancer, Dysbiosis, Surfaceome Interactions.

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O-36

Alpha-Terpineol: From Human Exposure to Molecular Toxicity - Mechanistic Insights into Reproductive and Developmental Effects

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ABSTRACT

Alpha-terpineol (α-terpineol) is a widely distributed monoterpene alcohol present in essential oils and extensively used in fragrances, cosmetics, pharmaceuticals, food additives, and household products. Due to its broad industrial applications, human exposure occurs through inhalation of volatile emissions, dermal absorption from personal care products, and oral ingestion via food and medicinal formulations. Following exposure, α-terpineol readily penetrates biological membranes owing to its lipophilic nature and undergoes hepatic biotransformation, resulting in systemic distribution and elimination via urinary metabolites.

Emerging evidence suggests that α-terpineol exerts biological effects through oxidative stress induction, mitochondrial dysfunction, membrane destabilization, and endocrine disruption. Mechanistically, α-terpineol exposure has been associated with increased reactive oxygen species (ROS) generation, lipid peroxidation (MDA), reduced antioxidant defenses (SOD, CAT, GSH), and disruption of mitochondrial membrane potential, leading to apoptosis and cellular dysfunction. Additionally, interference with steroidogenic pathways and hypothalamic–pituitary–gonadal axis signaling has been proposed as a key mechanism underlying reproductive toxicity.

Recent studies from our laboratory demonstrated dose-dependent reproductive and developmental toxicity of α-terpineol in rodent models. Observed effects included decreased testosterone levels, impaired spermatogenesis, azoospermia, histopathological alterations in reproductive organs, and developmental abnormalities. These findings were accompanied by elevated oxidative stress markers and altered antioxidant enzyme activity, supporting oxidative stress-mediated toxicity. Furthermore, mitochondrial dysfunction and endocrine disruption appear to contribute to reproductive impairment and developmental defects.

Collectively, these findings suggest that α-terpineol-induced toxicity is mediated through interconnected pathways involving oxidative stress, mitochondrial dysfunction, apoptosis, and endocrine dysregulation, underscoring the need for comprehensive toxicological evaluation and risk assessment.

Keywords: Alpha-terpineol; ROS, Reproductive toxicity, Oxidative stress markers, Endocrine dysregulation

O-37

"Effect of Polyethylene terephthalate (PET) micro plastics on pre- and post-natal development, including maternal function in Wistar rats."

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ABSTRACT

Microplastics are widespread environmental pollutants formed by the breakdown of larger plastic debris or manufactured for industrial applications. Among them, polyethylene terephthalate (PET) is of particular concern due to its extensive use in consumer products such as beverage bottles, textiles, and packaging. This study evaluated the potential toxic effects of PET microplastics on prenatal and postnatal development, including maternal function, in Wistar rats.

PET microplastics were administered orally in graded doses of 0, 300, 700, and 1000 mg/kg to parental (F0) female rats from gestation day 7 through lactation until postnatal day 21. Maternal observations revealed dose-dependent impairments, including reduced feed intake, altered weight gain during gestation and lactation, and compromised maternal care such as delayed pup retrieval, reduced nursing behavior, and increased pup neglect in higher dose groups. A significant reduction in litter size and number of live pups at birth was observed in treated groups compared to controls. Increased incidences of stillbirths and reduced pup survival index during early lactation were also recorded.

F0 dams were sacrificed at weaning, and selected F1 offspring were monitored until sexual maturity without further exposure. Developmental assessments of F1 pups indicated delayed physical milestones and reduced body weight gain in higher dose groups. Furthermore, reproductive performance of F1 animals showed a decline in fertility indices, resulting in fewer F2 pups. F2 litters exhibited reduced viability, with decreased number of live pups and increased early postnatal mortality by lactation day 4. In conclusion, this study provides evidence of the prenatal and postnatal developmental toxicity of PET MPs in Wistar rats following subchronic exposure. The findings of this study have implications for human health risk assessment and highlight the need for further research on the potential health effects of microplastic pollution.

O-38

Sustainable production of biodiesel from waste frying oil using biowaste-derived CaO/K_2CO_3 nanocomposite catalyst: RSM optimization and E-metrics study

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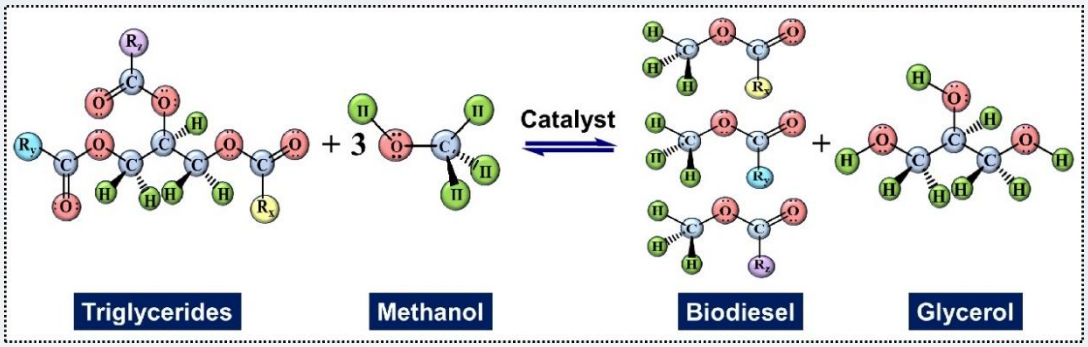
Abstract

Sustainable biodiesel production from waste-derived feedstock utilizing an efficient, eco-friendly catalyst offers dual benefits of waste mitigation and renewable energy generation. In this work, an environmentally benign heterogeneous nanocomposite catalyst was synthesized from biowastes, including *Unio pictorum* shells and *Musa acuminata* peels, for the production of biodiesel from waste frying oil (WFO). Physicochemical characterizations revealed that the synthesized catalyst was predominantly composed of CaO and K_2CO_3 as active constituents responsible for the methanolysis of triglycerides. Numerous transesterification process parameters were optimized using Response Surface Methodology (RSM) within the Box-Behnken Design (BBD) model to maximize biodiesel conversion while minimizing resource utilization. An excellent biodiesel conversion of 98.2% and a yield of 97.5% were achieved under optimal reaction conditions. Additionally, the proposed catalyst demonstrated exceptional reusability over 7 catalytic cycles with minimal activity loss, indicating high conversion efficiency and structural stability throughout the reaction. Transesterification kinetics confirm the pseudo-first-order model, while thermodynamic studies indicate the reaction is non-spontaneous and endothermic. Achieving high turnover frequency and lower values of green metrics suggests that the subsequent transesterification process is clean, efficient, and environmentally friendly. Furthermore, several fuel characteristics, including calorific value, cetane number, kinematic viscosity, cloud point, and pour point, comply with ASTM D-6751 standards, rendering it suitable for diesel engines. This research showcases a clean and sustainable approach to producing biodiesel using biowaste-derived catalysts, aligning with green chemistry principles and promoting the circular economy.



O-39

Mechanistic Insights into α-Terpineol-Induced Reproductive Toxicity in Male Rats: Evidence from Molecular, Genotoxic, and Ultrastructural Analyses

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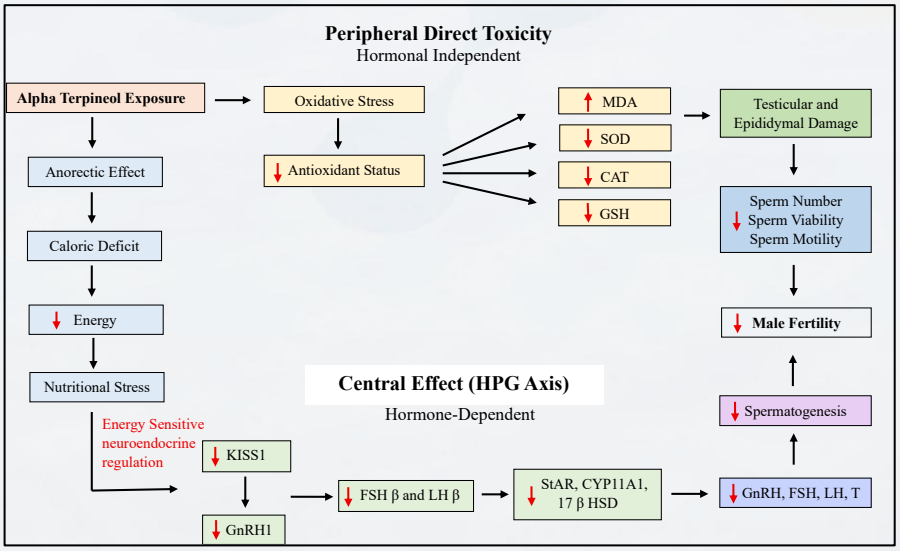
Abstract

Amid evolving lifestyle trends and expanding pharmaceutical and consumer product use, natural fragrance compounds such as α-terpineol ($C_{10}H_{18}O$) are increasingly utilized for their beneficial properties; however, comprehensive toxicological evaluation remains limited. Therefore, the present study aimed to investigate the sub-chronic effects of α-terpineol on the hypothalamic–pituitary–gonadal (HPG) axis in male Sprague–Dawley rats. Adult male rats were orally administered α-terpineol at doses of 0, 75, 150, and 300 mg/kg body weight for 28 days. Reproductive toxicity was assessed through evaluation of reproductive organ weights, testicular histomorphometry, oxidative stress biomarkers, comet assay, transmission electron microscopy (TEM), and quantitative real-time PCR analysis of HPG axis and steroidogenic genes. α-Terpineol exposure resulted in dose-dependent reductions in reproductive organ weights and significant histomorphometric alterations, including increased seminiferous tubule diameter and luminal area with reduced epithelial height, indicating impaired spermatogenesis. Biochemical analysis revealed elevated lipid peroxidation (MDA) and altered antioxidant enzyme activities (SOD, CAT, GSH), suggesting oxidative stress-mediated toxicity. Comet assay demonstrated significant DNA damage in testicular cells, while TEM revealed mitochondrial degeneration, hormonal analysis demonstrated significant reductions in GnRH, FSH, LH, and testosterone levels, indicating disruption of the hypothalamic–pituitary–gonadal axis. qRT-PCR analysis showed significant dysregulation of hypothalamic (GnRH1, KISS1), pituitary (LHβ, FSHβ), and testicular steroidogenic genes (StAR, CYP11A1, 17β-HSD). Collectively, these findings demonstrate that sub-chronic α-terpineol exposure induces reproductive toxicity via oxidative stress-mediated DNA damage and disruption of steroidogenic and spermatogenic pathways, highlighting potential toxicological risks associated with prolonged exposure.

Keywords: α-Terpineol; Reproductive toxicity; Hypothalamic–pituitary–gonadal axis; Oxidative stress; Genotoxicity, Comet assay



O-40

Ru(II)-Based Photoantibiotics: Light-Driven Eradication of Bacterial Biofilm and Rapid Healing of Infective Wounds in Wistar Rat

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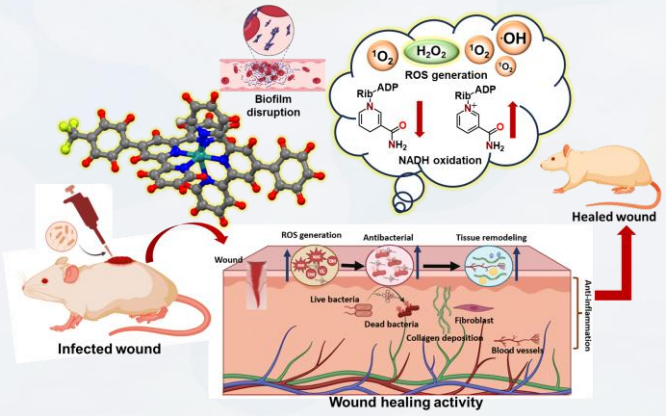
ABSTRACT

Wound healing is a natural skin repair process, but exposed wound tissue, size, diabetes, and poor care allow bacterial invasion, leading to chronic infections [1,2]. Multidrug-resistant pathogens (e.g., *S. aureus*, *E. coli*, *K. pneumoniae*) form biofilms and account for ~30% of surgical healthcare-associated infections and ~80% related mortality [3]. Escalating antibiotic resistance has driven interest in antibacterial photodynamic therapy (aPDT) as a non-invasive, light-activated alternative [3]. Herein, three novel Ru(II)-based photoantibiotics, *viz*., $[Ru(phtpy)(N,N,N)_2](PF_6)_2$, where N,N,N = 4′-phenyl-2,2′:6′,2″-terpyridine (phtpy, **Ru1**), 4-([2,2′:6′,2″-terpyridin]-4′-yl)-*N*,*N*-dimethylaniline (NMe_2tpy, **Ru2**), trifluoromethylphenyl)-2,2':6′,2″-terpyridine (CF_3tpy, **Ru3**) were developed with excellent photostability for visible light-activated antibacterial activities and infective wound healing. **Ru1-Ru3** exhibited an absorption in the 400–600 nm range, beneficial for aPDT application. Upon visible light exposure (400-700 nm), **Ru1-Ru3** inhibited bacterial growth of *Escherichia coli* (*E. coli*), *Staphylococcus aureus (S. aureus), and Bacillus subtilis (B. subtilis),* due to the effects of oxidative stress via ROS generation and photo-oxidation of NADH [4]. **Ru3** was identified as a lead photoantibiotic that further showed antibiofilm activities against *E. coli* under visible light exposure. **Ru3** was found to be biocompatible against rat red blood cells and human embryonic kidney cells. **Ru3+light** promoted rapid healing of infected wounds within 9 days, in an *E. coli*-induced rat model, highlighting its potential future use in healthcare [4].



Scheme 1. Schematic Presentation of Light-Triggered Antibacterial, Antibiofilm Properties, and Biocompatibility of Ru(II) Complexes.

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O-41

β-Cyclodextrin Xanthate-Acrylamide Hydrogel as a Sustainable Adsorbent for Cu^{2+} and Ni^{2+}: Adsorption and Biodegradability Assessment

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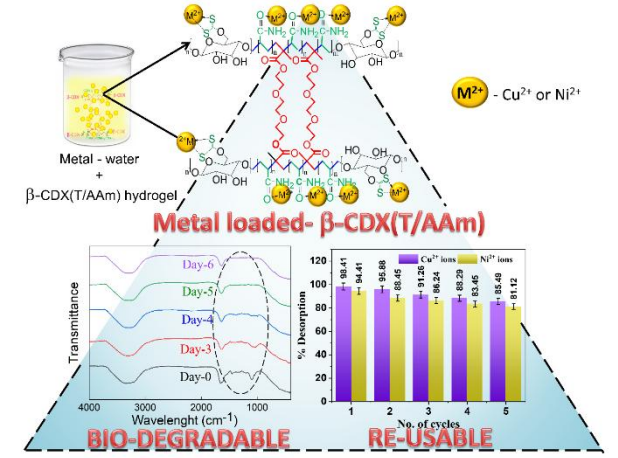
Abstract

In this study, β-cyclodextrin (β-CD) substrate was chemically modified into its xanthate, acrylamide (AAm) was used as the monomer, and triethylene glycol dimethacrylate (TEGDMA) as the crosslinker to develop a cross-linked hydrogel network denoted as β-CDX(T/AAm) via the free radical polymerization method. The uniqueness of the surface-modified β-CD lies in the synergistic effect of xanthate and amide groups, which significantly enhances its adsorption efficiency. Different grades of the cross-linked network (β-CDX(T/AAm)) were synthesized by varying the amounts of initiator (KPS), AAm, and TEGDMA. Thereafter, the best combination was optimized based on physicochemical characteristics such as swelling and Cu^{2+} and Ni^{2+} removal. The optimal conditions for Cu^{2+} and Ni^{2+} removal, including dose, pH, concentration, time, and temperature, were determined for the β-CDX(T/AAm) hydrogel as 2.5 g/L, pH 7, 1000 mg/L, 60 min, and 35ºC, respectively. Batch adsorption data suggest that the Langmuir isotherm model is best fits the data, with maximum adsorption capacities of 444.18 and 432.19 mg/g for Cu^{2+} and Ni^{2+}, respectively. The kinetic study follows the pseudo-second-order with rate constant of 4.62×10^{-4} and 4.38×10^{-4} g/(mg.min). In addition, the environmental compatibility of β-CDX(T/AAm) hydrogel has been confirmed through biodegradability tests. Further, the cost study suggests that β-CDX(T/AAm) hydrogel can be produced at a cost of 2.37 INR/g and shows successful reusability for up to 5 cycles. Overall, the synthesis, characterization, and applicability study of β-CDX(T/AAm) hydrogel confirm that it can be used as an efficient, economical and environment-friendly adsorbent for wastewater treatment.

Graphical abstract



O-42

Eco-Friendly Novel Gum Ghatti Xanthate-Based Hydrogel for Removal of Cu^{2+} and Co^{2+} Ions from Synthetic and Real Water

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Abstract

The purpose of this research was to synthesize a modified Gumghatti-xanthate based adsorbent for the adsorption of Cu^{2+} and Co^{2+} ions from water. GgXMD hydrogel were synthesized by using monomer (N, N dimethyl acrylamide) and Crosslinker (N, N methylenebisacrylamide) through the free radical polymerization technique using eco-friendly base material to enhance the swelling properties, adsorption capacity, seed germination and biodegradability. The resulting adsorbents were characterized using UV, FTIR, pH_{PZC}, TGA and SEM analysis, revealing changes in crystal structure and improvements in surface area after and before metal adsorption. The performance of the synthesized adsorbents was evaluated by batch adsorption of Cu^{2+} and Co^{2+} ions. The GgXMD-2 hydrogel showed high adsorption efficiency performance under suitable conditions. At 40 °C, pH 7 and 2.0 g of hydrogel adsorbed metal ions from a 500 $mg.L^{-1}$ solution with an adsorption capacity of 222.81 and 204.26 $mg.g^{-1}$ for Cu^{2+} and Co^{2+} ions. The adsorption of heavy metal ions followed the pseudo-second-order kinetic model and fitted well with the Langmuir isotherm, indicating monolayer adsorption. The process was found to be spontaneous and endothermic in nature. In addition, the hydrogel showed good reusability. After five adsorption cycles, the removal efficiency remained 85.87 % for Cu^{2+} and 84.42 % for Co^{2+} ions.

Keywords: Clean water and sanitation, adsorption efficiency, biodegradability, swelling, eco-friendly

O-43

Computational Investigation of Sulphur-Centred Hydrogen Bonds in Ethanedithiol-Solvent Clusters

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Keywords: Sulphur-centred hydrogen bonding (SCHB), Ethanedithiol (EDT), Atom in molecule (AIM), Vibrational spectroscopy, Cooperative Effect.

Abstract

Sulphur-centred hydrogen bonding (SCHB) is increasingly recognised as an important but still underexplored interaction in sulphur-containing systems. In this work, we examine how the nature of the hydrogen-bond donor and the size of the cluster influence the structure and stability of SCHBs in clusters of ethanedithiol (EDT) with small solvent molecules (HF, H_2O and NH_3).

The geometries of all clusters EDT-X_n (X= HF, H_2O, NH_3), (n = 1-3) were optimised at the MP2/aug-cc-pVTZ level and confirmed as true minima by vibrational frequency analysis. To obtain reliable energetics, interaction energies were calculated using DLPNO-CCSD(T)/aug-cc-pVQZ, with smaller systems benchmarked against canonical CCSD(T) calculations. Across all systems, the most stable structures tend to form cyclic or near-cyclic hydrogen-bonding arrangements, often involving dual interactions where the solvent both donates and accepts hydrogen bonds. We observe a clear trend in stability, with HF forming the strongest interactions, followed by H_2O and NH_3. As the number of solvent molecules increases, the interaction energies become more favourable, indicating cooperative effects. These trends are also reflected in the vibrational spectra, where noticeable red shifts, especially for the H-F stretching mode, point to strengthening hydrogen bonds. AIM analysis supports these findings, highlighting stronger electron density for F-H---S interactions.

O-44

Optimization of Acrylic Acid/Acrylonitrile functionalized Gg-based Hydrogel for Synthesis Eco-friendly, Cost-effective and Efficient Removal of Heavy Metal Ions

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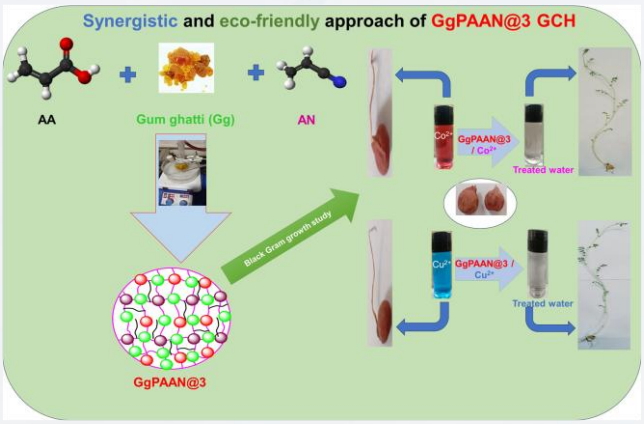
Abstract

This study includes the effective graft co-polymeric hydrogel (GCH) formation from gum ghatti (Gg), acrylic acid (AA), and acrylonitrile (AN), by optimizing the AA-to-AN ratio. Three hydrogel grades GgPAAN@1, GgPAAN@2 and GgPAAN@3 were fabricated and characterized through Fourier transform infrared spectroscopy, Thermogravimetric analysis, Point of zero charge, field emission scanning electron microscope and energy dispersive X-ray spectroscopy and X-ray photoelectron spectroscopy (XPS) analysis. Swelling, and water retention properties were studied. Among them, GgPAAN@3 exhibited superior swelling capacity (290.3 g/g) and % water retention ratio (66.11%) in distilled water. The adsorption performance of the hydrogels toward Cu^{2+} and Co^{2+} ions were systematically investigated under optimized conditions. Maximum adsorption capacities were obtained as 481, 495, and 529 mg/g for Cu^{2+} and 465, 486, and 499 mg/g for Co^{2+} with GgPAAN@1, GgPAAN@2, and GgPAAN@3, respectively. Adsorption data fitted well to the Langmuir isotherm, while kinetics follow the pseudo-second-order model with rate constants of 3.38×10^{-4} and 3.73×10^{-4} g/(mg.min) for Cu^{2+} and Co^{2+}. The GgPAAN GCH can maintain significant adsorption efficiency after three adsorption desorption cycles. Adsorption mechanism has been confirmed through XPS analysis. Additionally, seed germination experiments using black gram indicate improved root, shoot, and leaf growth with GCH treated water compared to untreated and tap water. Cost analysis and plant growth results suggest the eco-friendly and sustainable applicability of the synthesized GgPAAN GCH hydrogels.

Graphical abstract



O-45

From Synthesis to Simulation: Multicomponent-Derived Compounds Evaluated via Computer-Aided Drug Design, Molecular Docking, and ADME Profiling

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The development of structurally diverse and biologically relevant scaffolds through efficient synthetic strategies remains a key focus in modern medicinal chemistry. In the present study, a novel series of heterocyclic compounds was synthesized via a multicomponent reaction. This one-pot synthetic approach offers advantages such as operational simplicity, high atom economy, and the rapid generation of molecular complexity.

The synthesized compounds were structurally characterized using standard spectroscopic techniques, confirming the formation of the desired multicomponent-derived frameworks. To explore their potential as drug-like candidates, a comprehensive computer-aided drug design approach was employed. Preliminary biological activity prediction was carried out using PASS (Prediction of Activity Spectra for Substances), providing insight into possible pharmacological profiles. Furthermore, molecular docking studies were performed using AutoDock Vina to evaluate the binding affinity and interaction patterns of the synthesized compounds with selected biological targets.

In addition, pharmacokinetic properties, including absorption, distribution, metabolism, and excretion (ADME), were assessed using the SwissADME web tool to determine drug-likeness and oral bioavailability. The results suggest that several compounds exhibit favourable binding interactions and acceptable pharmacokinetic parameters, indicating their potential for further optimization.

Overall, this study demonstrates the effectiveness of integrating multicomponent synthesis with computational drug design strategies to identify promising molecular scaffolds for future drug discovery efforts.

O-46

Allyl Mannitol Crosslinked Pectin-Based Hydrogel for Efficient Adsorptive Removal of Cu^{2+} and Ni^{2+} Ions from Aqueous Solutions

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Abstract

A hydrogel developing by the allyl mannitol crosslinker was synthesized via the free radical polymerization procedure. In this preparation pectin assisted as the primary physical component, while acrylamide was working as the monomer, and allyl mannitol working as the crosslinking agent. The hydrogels go through general characterization using techniques such as thermogravimetric analysis (TGA), Fourier transform infrared spectroscopy (FTIR), scanning electron microscopy (SEM), and point of zero charge (pHpzc). These AMCL-PHs hydrogels were measured for their effectiveness in removing Cu^{2+} and Ni^{2+} ions from aqueous solutions, attaining prominent maximum removal efficiencies of 93.21% for Ni^{2+} and 95.44% for Cu^{2+} at an optimal pH of 6. The adsorption information closely conformed to the Langmuir isotherm model, representing monolayer adsorption. The maximum noted adsorption capacities were 245.57 (±9.787) $mg \cdot g^{-1}$ for Cu^{2+} and 234.57 (±9.614) $mg \cdot g^{-1}$ for Ni^{2+}. Kinetic studies shown that the adsorption procedure followed the pseudo-second-order model, with rate constants of 5.3×10^{-4} (±2.046) $g \cdot (mg \cdot min)^{-1}$ for Cu^{2+} and 5.2×10^{-4} (±2.057) $g \cdot (mg \cdot min)^{-1}$ for Ni^{2+}. Regeneration studies proved that the hydrogels kept high performance across various adsorption-desorption cycles, with only minor reductions in removal efficiency to 86.67% for Cu^{2+} and 84.66% for Ni^{2+}.

Keywords: Hydrogel, absorption, clean water, metal ion, reusability

O-47

Sunlight Mediated Yellow Fluorescence Detection of Mercury and Copper

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Abstract:

The development of efficient, selective, and sensitive chemical sensors for environmentally and biologically relevant analytes remains a critical challenge in analytical chemistry. In this study, two novel eosin Y-based fluorescent probes (HL1 and HL2) were successfully designed, synthesized, and evaluated for the detection of heavy metal ions in liquid media. Probe HL1 was developed via derivatization of eosin Y with 3,4,5-trimethoxybenzaldehyde, while probe HL2 was synthesized using salicylaldehyde as a modifying agent. Both probes exhibited remarkable dual-mode sensing behaviour upon interaction with Hg^{2+} and Cu^{2+} ions. In the visible region, HL1 showed a distinct colour transition from colourless to pink, whereas HL2 displayed a colourless to yellow transformation. Under fluorescence conditions, both probes demonstrated a "turn-on" response, producing bright yellow fluorescence from an initially non-fluorescent state. Notably, HL2 also exhibited selective recognition toward CO_3^{2-} anions, producing a similar yellow response in visible mode, thereby highlighting its multifunctional sensing capability. The developed probes demonstrated excellent sensitivity, with a detection limit as low as 1 ppm for the target analytes. Practical applicability was validated through successful detection of Hg^{2+} and Cu^{2+} in laboratory-prepared aqueous samples. Overall, this work introduces versatile eosin Y-derived fluorescent sensors with dual-mode detection, high sensitivity, and selective recognition properties, offering promising potential for environmental monitoring and analytical applications.

Keywords: Eosin Y, Sensor, Dual mode, Mercury, Copper, and Carbonate.

O-48

Colorimetric detection of cations and anions with eosin y-quinoxaline motif

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Abstract:

The design of colorimetric chemosensors capable of detecting both cationic and anionic species is of significant interest in modern analytical chemistry. In this work, a novel eosin Y-based fluorescent probe was developed through structural modification with a quinoxaline hydrazine motif. The synthesized probe exhibited excellent sensing performance in a DMSO: water (1:1, %v/v) medium, enabling the detection of both heavy metal ions and environmentally relevant anions. The probe demonstrated efficient colorimetric sensing behaviour toward Hg^{2+} and Cu^{2+} ions, as well as SO_3^{2-} anions. Upon interaction with the target analytes, the system showed distinct optical changes in visible, allowing for rapid and straightforward detection. The fluorescence response, coupled with noticeable colorimetric changes, highlights the probe's practical applicability for on-site and real-time monitoring. Importantly, the incorporation of the quinoxaline hydrazine moiety enhances the binding affinity and selectivity of the probe toward multiple analytes, enabling a single-platform detection strategy. The use of a mixed DMSO: water solvent system further supports its applicability in semi-aqueous environments. Overall, this study presents a versatile and efficient eosin Y-derived chemosensor with colorimetric detection capability for both cations (Hg^{2+} and Cu^{2+}) and anions (SO_3^{2-}), offering promising potential for environmental and analytical sensing applications.

Keywords: Eosin Y, Sensor, Colorimetric, Mercury, Copper, and Sulphite.

O-49

Studies on modified montmorillonite as catalyst to produce upgraded fuel oil from the pyrolysis of waste extended polystyrene

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Abstract

The escalating volume of waste expanded polystyrene (EPS) presents a critical environmental challenge owing to its persistent, non-biodegradable nature and limited conventional recycling efficiency [(Maafa, 2021), (Verma, Sharma and Pramanik, 2022), (Imani Moqadam *et al.*, 2015)]. This study explores the catalytic pyrolysis of waste EPS as a sustainable valorization route, focusing on the comparative performance of natural montmorillonite (MMT) and modified MMT (metal loaded and acid treated) as low-cost, eco-friendly catalysts. Pyrolysis experiments were performed in a semi-batch reactor under inert nitrogen atmosphere at 400–700 °C, with feed to catalyst ratios of 20:1 (w/w). Catalysts were characterized by X-ray diffraction (XRD), Scanning electron microscopy (SEM), N_2 adsorption–desorption (BET), Fourier-transform infrared spectroscopy (FTIR). Modification markedly enhanced the catalytic properties of MMT by increasing specific surface area, generating mesopores, and introducing stronger Brønsted and Lewis acid sites through partial delamination of the layered structure. The catalysts significantly lowered the decomposition temperature relative to non-catalytic pyrolysis and improved liquid oil yields while suppressing char formation. The modified MMT exhibited superior activity, achieving higher liquid yields (up to ~87 wt%) with enhanced selectivity toward valuable aromatic hydrocarbons, primarily styrene monomer, alongside reduced gas and residue fractions. Product distributions were analyzed by gas chromatography (GC), gas chromatography mass spectrometry (GC-MS) and FTIR, revealing a shift toward lighter aromatics and gasoline-range fractions under catalytic conditions. These results demonstrate that modified MMT is a highly effective, inexpensive catalyst for the conversion of waste EPS into high-value chemicals and fuels. The process offers a promising, scalable strategy for plastic waste upcycling, contributing to circular economic principles and reduced reliance on fossil resources.

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O-50

Development of Biocompatible Carbon Quantum Dots as Sustainable Alternatives to Traditional Sunscreen Ingredients

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Abstract

Conventional UV blockers like zinc oxide (ZnO), titanium dioxide (TiO_2), and oxybenzone provide broad-spectrum protection but pose significant risks: ZnO/TiO_2 nanoparticles induce cellular toxicity and environmental bioaccumulation, Smijs & Pavel [1]. In contrast, oxybenzone disrupts endocrine function and coral reefs, Downs et al. [2]. Carbon quantum dots (CQDs) offer a green, metal-free alternative with tunable UV absorption and antioxidant prowess. Herein, we report hydrophilic CQDs synthesized via a one-pot microwave-assisted method using citric acid and urea (1:3 molar ratio). FTIR spectroscopy confirmed the presence of oxygen-rich surface groups (hydroxyl, carboxyl), thereby boosting hydrophilicity for topical applications. Particles <10 nm exhibited intense blue fluorescence under UV and absorption maxima at ~350 nm, targeting UVB/UVA spectra. Antioxidant assays revealed phenolic content with up to 70% scavenging of superoxide and hydroxyl radicals, mimicking natural UV-protective polyphenols. Unlike prior CQDs biocompatibility studies limited to short-term cell lines or animal models, Havrdova et al. [3], leaving long-term human effects unknown, we employed multi-generational *Drosophila melanogaster* testing (10–100 mg kg^{-1} food across three generations). No abnormalities occurred in larval development, adult behaviour, or reproduction, demonstrating exceptional transgenerational safety and bridging critical gaps for chronic nanomaterial exposure. These CQDs thus emerge as a safe, multifunctional UV blocker, poised to replace problematic chemical filters in next-generation sunscreens.

Keywords: Carbon quantum dots, Drosophila biocompatibility, Hydrophilic nanoparticles, Sunscreen alternative

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O-51

Epitope-Level Insights for Immuno-Recognition of JEV NS1 via Gold Nanoflower-MXene Composite

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Abstract:

Early and accurate identification of Japanese encephalitis virus (JEV) is vital for effective outbreak control and surveillance in endemic regions. In the present study, we report the development of a highly sensitive electrochemical immunosensor for the identification of JEV non-structural protein 1 (NS1). The recombinant JEV NS1 antigen was expressed, purified, and subsequently refolded in vitro to recover soluble, functional protein. High-affinity mAbs were generated through hybridoma technology and characterized via indirect and competitive ELISA, western blotting, and biolayer interferometry (BLI). To gain molecular-level insights, antibody gene sequences were decoded using next-generation sequencing (NGS), and 3D structural models were constructed using Alpha fold3, and molecular docking analysis enabling epitope-paratope mapping. For the development of electrochemical immunosensor screen-printed carbon electrodes (SPCEs) were modified with the GNF-MXene nanocomposite, followed by immobilization of mAbs against JEV NS1. The GNF-MXene nanocomposite was thoroughly characterized by various physio-chemical analysis. Cyclic voltammetry (CV) and differential pulse voltammetry (DPV) were used to study the electrochemical reactions on the sensor surface and the fabricated immunosensor was thoroughly optimised and characterised for enhanced performance. The sensor exhibited a low detection limit of ~0.35 fM from a broad range concentration of JEV NS1 (1 fM-1 μM). The fabricated immunosensor was further evaluated with clinical samples and sensor showed high specificity (100%), sensitivity (95%), and accuracy (96.66%) with no cross-reactivity to other flavivirus NS1 antigens, and a rapid response time of 10 minutes. The developed electrochemical immunosensor can be used as a point-of-care, field-deployable diagnostic tool for the detection of JEV.

Keywords: Japanese encephalitis virus, gold nanoflower, voltammetry, monoclonal antibody, epitope, immunosensor

Visible light-induced C(sp2)-N bond-formation from diazonium tetrafluoroborates and secondary amines via Electron Donor−Acceptor Complex Formation

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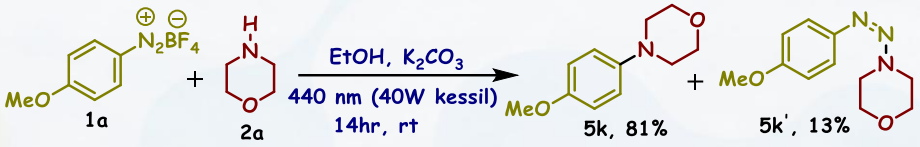
Recently, catalytic electron donor-acceptor (EDA) complexes have emerged as an effective and environmentally friendly alternative to metal-based (e.g., Ir, Ru) photoredox synthesis techniques. However, these complexes remain largely undiscovered and depend on properly designed acceptors that must be introduced beforehand. Here, we describe a novel EDA complex that utilises readily and inexpensively synthesised diazonium tetrafluoroborates as a catalytic acceptor for secondary amine arylation.



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Development of Neem-Mediated Phytonanoparticle-Based Nanocomposites for Enhanced Adsorption of Toxic Dyes from Wastewater

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Abstract

The rising discharge of toxic dyes from industrial effluents has arisen concern that demands attention and remediation technologies. Therefore, in this study, neem (*Azadirachta indica*) mediated phytonanoparticle was synthesized which was incorporated into an amylopectin-based biopolymer to fabricate a novel phytonanocomposite for the efficient removal of methylene blue and malachite green dyes through adsorption process. This phytonanocomposite has been characterized using various techniques like UV-Visible spectroscopy, FTIR Spectroscopy, XRD and SEM for its successful synthesis and structural integrity. The removal efficiencies have been evaluated through batch adsorption experiments under the different conditions of pH, adsorbent dosage, concentration, time and temperature. The highest removal efficiency for methylene blue and malachite green has been found to be 96.6 % and 94.8 % at pH 7. The maximum adsorption capacity has been calculated to be 179.239 mg/g and 174.501 mg/g for MB and MG dyes, aligning best with Langmuir isotherm model, indicating the adsorption to be monolayer. Kinetic studies were also performed resulting in the process to be pseudo-second order, validating chemisorption as the dominant mechanism. Also, thermodynamic studies have proven the process to be spontaneous and endothermic in nature. Reusability studies showed the phytonanocomposite to be reusable upto 4 distinctive cycles with maximum removal of 82.36 % and 80.67 % for MB and MG dyes. This approach serves as a pathway for high efficiency removal of toxic dyes utilizing the plant-derived compounds as reducing and stabilizing agents highlighting its potential to be environment friendly, cost-effective and sustainable material for wastewater treatment applications.

O-54

Newly found biological targets for the anti-helminthic drug niclosamide in cancer cells, highlighting its potential in cancer therapy

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Niclosamide, an anti-helminthic drug, exhibits anti-cancer effects. Its primary mode of action in killing tapeworm is functioning as a proton channel, thereby uncoupling mitochondrial oxidative phosphorylation. In cancer cells, it inhibits several signaling pathways (Wnt/beta-catenin, STAT3, mTORC1, Notch). We have recently discovered two additional biological processes relevant to cancer as targets for niclosamide. The drug blocks macropinocytosis and promotes ferroptosis, both actions pointing to its novel mechanisms in cancer therapy. Cancer cells exhibit increased demands for amino acids and hence upregulate selective amino acid transporters. Recently, we have identified SLC38A5 as a unique transporter that is upregulated in breast cancer and colon cancer. SLC38A5 does more than just transporting amino acids. Its transport mode involves amino acid-dependent sodium/proton exchange. Inhibition of this transporter causes intracellular acidification. Macropinocytosis is a novel mechanism by which cancer cells acquire amino acids by engulfing extracellular proteins. We have discovered that niclosamide is a potent inhibitor of SLC38A5 by direct interaction. It also suppresses SLC38A5 expression via suppression of specific signaling pathways. Blockade of expression/function of SLC38A5 not only prevents the transporter-mediated entry of amino acids into cancer cells but also blocks amino acid delivery via macropinocytosis. We also found niclosamide to inhibit the function and expression of another amino acid transporter, SLC7A11, which is obligatory for glutathione synthesis. In cancer cells, niclosamide decreases glutathione levels, increases lipid peroxidation, and induces ferroptotic cell death. In conclusion, our studies have identified two novel biological targets for niclosamide, highlighting its potential in cancer therapy.

ISCBC-2026

POSTER

P-1

In situ generated β-FeOOH nanoparticles Catalyzed Transfer Hydrogenation of Nitroarenes using Hydrazine Hydrate

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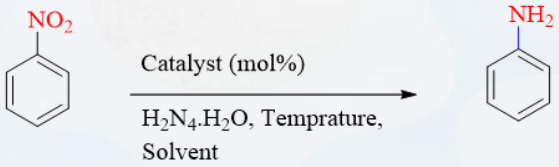
Abstract

This study reports the catalytic reduction of nitrobenzene derivatives using in situ generated β-FeOOH from $FeCl_2.4H_2O$ (1.25 mol%) as a catalyst and hydrazine hydrate as a transfer hydrogen reagent. The in situ generated β-FeOOH was characterized by powder XRD, Fe-SEM, EDX, FT-IR and XPS. The reaction conditions were optimized for the catalytic reduction of nitrobenzene, yielding aniline in >99% conversion after 90 minutes under reflux in methanol, with a turnover number (TON) of 80. Kinetic studies of the transfer hydrogenation of nitrobenzene revealed a first-order dependence with respect to both catalyst concentration and hydrazine hydrate concentration. The generality of this catalytic system was explored with various nitrobenzene derivatives, affording the corresponding anilines in 80-90% yields, with excellent tolerance toward nitrile and ester functional groups. Furthermore, the reduction of nitrophenones and nitrobenzaldehydes resulted in condensation with hydrazine along with simultaneous reduction of the nitro group to the corresponding aniline.

Table 1: Optimization of reaction conditions for the reduction of nitroarene



Keywords: Nitrobenzene, reduction, $FeCl_2.4H_2O$, hydrazine hydrate, transfer hydrogenation.

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P-2

Substitution-Driven Modulation of Crystal Packing and Turn-On Fluorescent Detection of Carbonate (CO_3^{2-}) and Hydrogen Sulphide (H_2S)

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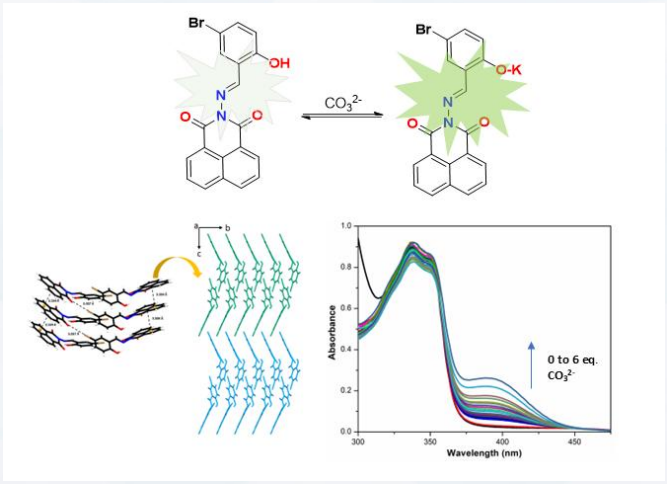
Four Schiff base derivatives of N-amino naphthalimide were synthesized and fully characterized by ^{1}H NMR, ^{13}C NMR, FT-IR, HRMS, and single-crystal X-ray diffraction. Solid-state structural analysis revealed the role of non-covalent interactions in governing crystal packing. The anion-sensing properties of these compounds were investigated using absorption and fluorescence techniques. Among them, NI-5B exhibited a selective turn-on fluorescence response toward H_2S and CO_3^{2-}. Binding constants were determined by Benesi–Hildebrand analysis, detection limits by the 3σ/k method, and Job's plot confirmed a 1:1 binding stoichiometry. Density functional theory calculations supported the experimental findings by elucidating the analyte-induced changes in electronic structure. Overall, NI-5B emerges as an efficient dual-responsive fluorescent sensor for H_2S and CO_3^{2-}.



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P-3

Fastest Catalytic Dearomatization of Arenols Employing an Unusual Arene-π-Tribromide Anion Complex

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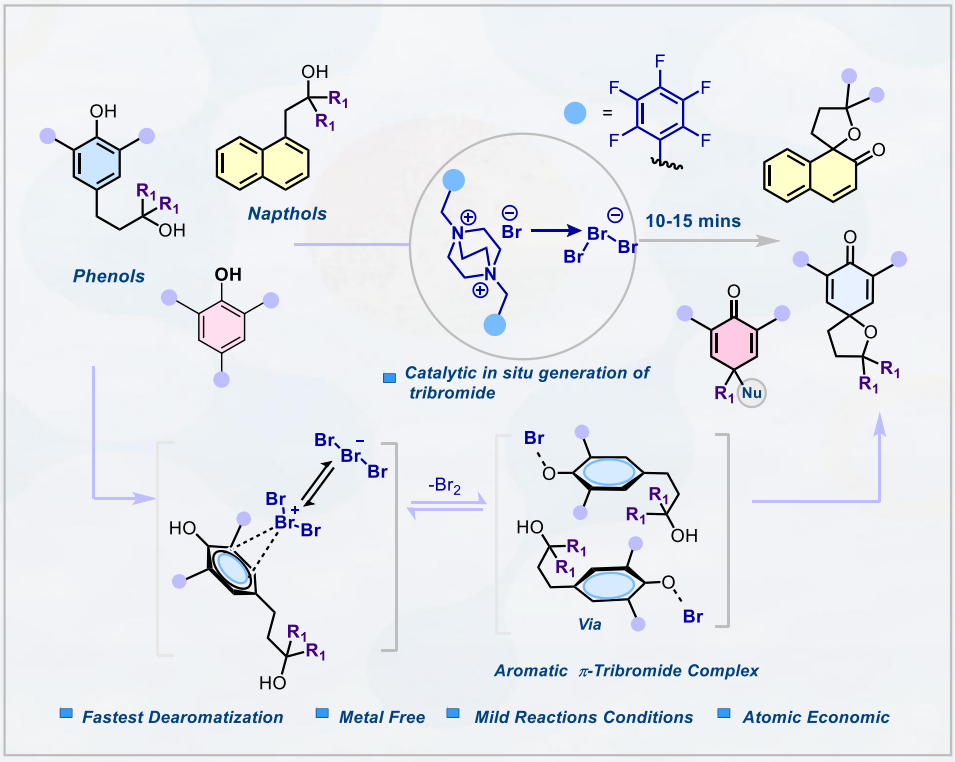
Abstract:

We introduce a novel Arene- π tribromide complex that enables the fastest Dearomatisation reactions in comparison to all available protocols reported till now. The highly electrophilic tribromide generated in situ from1,4-bis((perfluorophenyl)methyl)-1,4-diazabicyclo [2.2.2] octane-1,4-diium bromide (**C4**) in combination with Oxone as an oxidant. This system efficient converts arenols, including both **phenols and naphthols,** into a diverse array of **spirocyclic and etherified products** in **yields up to 95% within just 10–15 minutes** under mild, open-air conditions.

Figure/Scheme-1



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P-4

Sustainable Green Synthesis of TiO_2 NPs from *Prunus salicina* 'Santa Rosa' and Their Application in Dye-Sensitized Solar Cells

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ABSTRACT

This study presents a green and sustainable approach for synthesizing titanium dioxide (TiO_2) nanoparticles using *Prunus salicina* 'Santa Rosa' plum peel extract and explores their application in dye-sensitized solar cells (DSSCs). The bio-extract, enriched with phenolics, flavonoids, and organic acids, serves as an effective reducing and stabilizing agent, influencing nanoparticle formation, surface chemistry, and crystallinity.

The effect of varying extract concentrations on particle size, morphology, and photovoltaic performance was systematically investigated. TiO_2 nanoparticles were synthesized via a sol–gel reflux method and characterized using XRD, Raman, FTIR, UV–Vis spectroscopy, FESEM, TEM, BET surface analysis, and electrochemical impedance spectroscopy (EIS). The results reveal that extract concentration plays a crucial role in tuning the structural and optical properties of the nanoparticles, which directly impacts device efficiency.

Thin films were fabricated using controlled deposition techniques to optimize key parameters such as porosity, thickness, and surface area, enabling enhanced dye loading and improved electron transport. Overall, this eco-friendly synthesis strategy offers a viable alternative to conventional methods by reducing environmental impact while improving DSSC performance through better control over nanoparticle characteristics and photoelectrode design.

Keywords: TiO_2 Nanomaterials, DSSCs, Green synthesis, Thin films, Phytochemicals.

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P-5

MAX to MXene: Bridging Advanced Materials and Multifunctional Applications

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Two-dimensional (2D) materials have transformed materials science due to their exceptional physicochemical properties and wide-ranging applications. Among them, MXenes, a class of 2D transition metal carbides and nitrides, have gained significant attention owing to their excellent electrical conductivity, hydrophilicity, and tunable surface chemistry. These materials are derived from MAX phases, a family of layered nanolaminates that bridge the gap between metals and ceramics. MXenes are typically synthesized via selective etching of the A-layer using acid-based or molten salt methods, resulting in ultrathin, highly conductive structures (Alam et al., 2024).

Variations in synthesis conditions significantly influence structural features such as flake size, defect density, interlayer spacing, and surface terminations, thereby affecting their overall performance. Owing to these tunable properties, MXenes have been widely explored for applications in energy storage, water purification, sensing, electromagnetic shielding, and biomedical technologies (Downes et al., 2024). Their unique combination of properties and structural versatility positions MXenes as promising candidates for next-generation materials and advanced multifunctional applications.

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P-6

Ultrasound-assisted ring opening of epoxides in HFIP: THF: Synthesis, characterization, computational studies and molecular docking of novel 2-hydroxy dithiocarbamates

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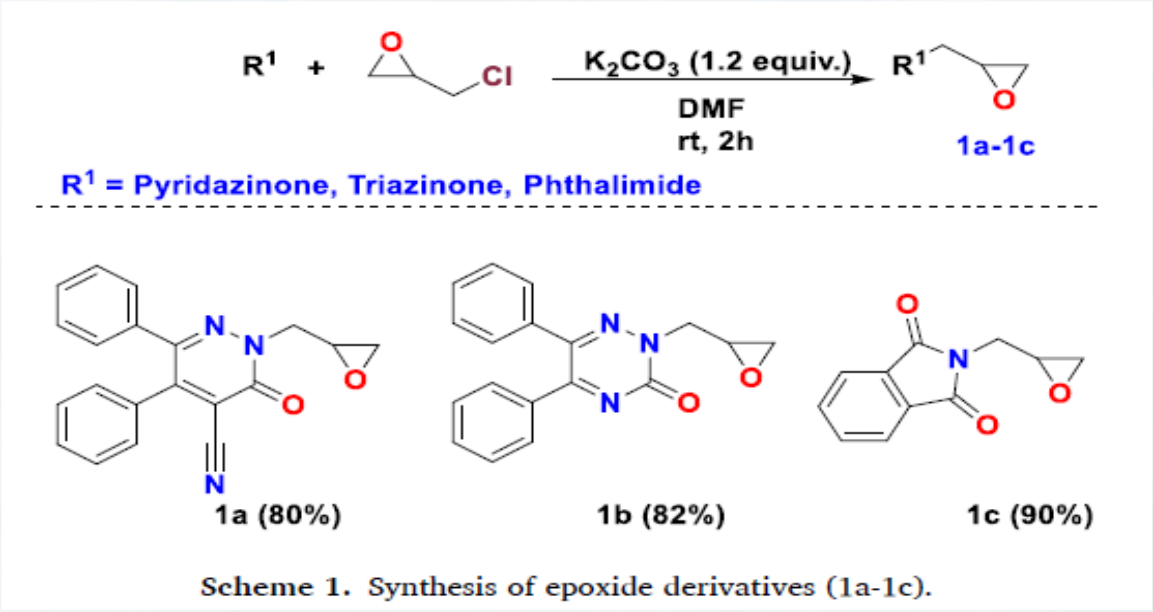
ABSTRACT

Under the influence of ultrasonic irradiation, pyridazinone, triazinone, or phthalimide containing 2-hydroxy dithiocarbamates, a biologically relevant novel organo-sulfur compound, was synthesized. Detailed characterization computational, and molecular docking studies are being investigated. Molecular interactions were studied using 3D Hirshfeld surfaces and corresponding 2D fingerprint plots. Theoretical (DFT) studies on themolecular structure, HOMO, LUMO, and quantum chemical descriptors were performed at the B3LYP/6–311++*G*(d,p) level of theory. At the same time, the interaction energy was computed using the B3LYP/6–31G(d,p) level of theory. The interactions of 2-hydroxy dithiocarbamate derivatives with the ligand-binding site of thetarget COX-2 (cyclooxygenase-2) enzyme were investigated using in-silico molecular docking experiments.Compared to the standard medicine celecoxib, the results showed that most synthesized derivatives had betterglide scores and interaction.



Scheme 1. Synthesis of epoxide derivatives (1a-1c).

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P-7

Development of Morita-Baylis-Hillman Reaction using *N*-Aryl Acrylamides as a Micheal acceptor

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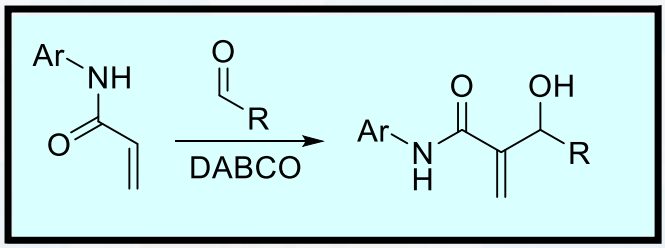
Abstract:

Despite being a popular method, Morita-Baylis-Hillman reaction suffers from slow reaction rate[1]. Although various Michael acceptors have been used, the use of acrylamide has been virtually missing from its domain. Here in we report a MBH reaction using *N*-aryl acrylamide as a Michael acceptor. Using DABCO as a catalyst and *p*-choro phenol as additive a rate accelerated MBH reaction was obtained. The reaction was widely applicable to a large number of substrates.



Keywords: Morita-Baylis-Hillman, Michael addition, DABCO, PhOH

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P-8

Stitching β-Ketothioamides with *N*-Tosylbenzoquinone imine: Transition-Metal Free Site-Selective Domino Synthesis of 2-Amino-3-aroyl-5-sulfonamide Substituted Benzo[*b*]furans

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Abstract:

Benzofuran derivatives are core components in a large number of biologically active natural and synthetic compounds. Herein, we present an easy-to-access and TM-free, one-pot, three-step synthesis of 2-amino-3-aroyl-5-sulfonamide substituted benzo[*b*]furans bearing many functional groups of different electronic and steric nature using thioamides (as a 2C synthon) and *N*-tosylbenzoquinone imine (as a CCO unit partner) at room temperature in open air. The reaction proceeds via deprotonation/Michael addition/cyclization/aromatization cascades forming two new (C–C and C–O) bonds and one ring, liberating only H_2S as a byproduct. HRMS study endorses the key intermediates involved during the course of reaction, validating excellent regio- and chemoselectivity. Among benzo-fused heterocyclic compounds, benzofurans are considered as privileged motifs, which are frequently encountered in many natural products[1-4]

Keywords: β-Ketothioamides • Transition-metal-free • Simple and mild conditions • Michael addition/cyclization • Regio- and Chemoselectivity

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P-9

Safety and Efficacy of a Classical formulation (Palashadi Basti) for PCOS Management: From Preclinical Toxicity Profiling to Clinical Validation

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Abstract:

Polycystic ovary syndrome (PCOS) is a complex endocrine disorder with limited safe long-term treatment options. Ayurvedic polyherbal formulations, rooted in classical texts, offer multi-target therapeutic potential through herb synergism; however, systematic safety evaluation is mandatory before clinical application. Palashadi Basti, selected from classical Ayurvedic literature, was subjected to standard physicochemical and pharmacognostic characterisation to establish quality benchmarks prior to experimental use. For preclinical safety assessment, female Charles Foster rats (150–200 g) were randomly allocated into six groups (n=10): vehicle control, low-, medium-, and high-dose, reversal vehicle control, and reversal high-dose. Palashadi Basti was administered rectally once daily for 28 days, with sacrifice on day 29. Reversal groups underwent an additional 14-day observation period (sacrifice on day 43) to assess delayed toxicity or recovery potential. Parameters evaluated included clinical signs, body weight, relative organ weights, hematological indices, blood and serum biochemical markers, and histopathological examination of major organs by H&E staining. In the clinical study, PCOS patients were divided into two groups: one receiving clomiphene citrate and the other treated with Palashadi Basti. The result demonstrated no mortality, adverse clinical signs, or treatment-related pathological alterations were observed in any preclinical group. All hematological and biochemical parameters remained within physiological limits and organ weights were comparable to controls, confirming an excellent safety profile with no delayed or irreversible toxicity. Comparative assessment of clinical and hormonal outcomes demonstrated favourable results with Basti therapy, indicating therapeutic equivalence or superiority in select parameters. Overall, Palashadi Basti may offer a promising complementary or alternative approach to PCOS management.

Keywords: Clinical study, *In vivo* toxicity assessment, Palashadi basti, PCOS.

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P-10

Metal-Free α-Sulfonylation of β-Ketothioamides: Access to α-Sulfonyl-β-Ketoamides

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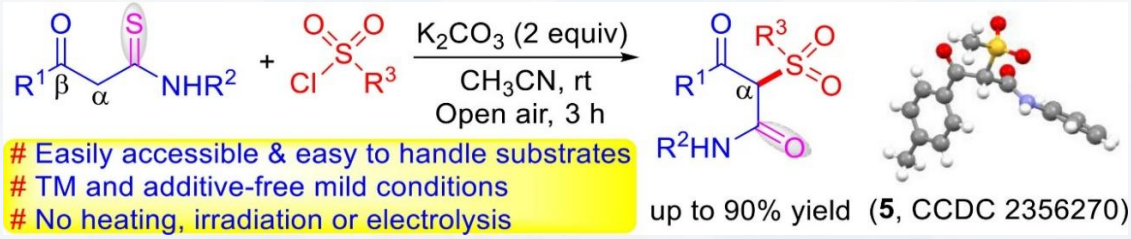
Abstract:

We report a metal and additive-free reactivity of β-ketothioamides with sulfonyl chlorides for the synthesis of previously unreported 2-sulfonyl-3-oxo-N,3-diarylpropanamides via in situ thioamide to amide conversion followed by dehydrohalogenative C−S cross-coupling at room temperature under open air. The process is simple, efficient, mild, and scalable, allowing for high yields of various a-sulfonyl-β-ketoamides. Furthermore, DFT and photophysical experiments confirmed the suggested mechanism, revealing a unique excitation-dependent emission linked with ESPT for the produced sulfones.



Keywords: β-ketothioamides; C−S cross-coupling

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P-11

Microenvironment-Regulated Self-Assembly Governs Tunable Emission for Targeted Lipid Droplet Imaging

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We report microenvironment-responsive fluorophores in which self-assembly governs tunable emission through a distinct structure–property relationship. The molecule exhibits strong emission in moderately polar solvents, while pronounced red-shift and fluorescence quenching are observed in highly polar and nonpolar media, indicating a strong dependence on the surrounding microenvironment. Gradual water fraction increase induces aggregation, leading to the appearance of a new red-emissive band, highlighting aggregation-mediated excited-state modulation.

The observed photophysical behavior is rationalized by the coupling of intramolecular charge transfer with self-assembly-induced restriction of intramolecular motion, enabling access to multiple emissive states across different environments. In the solid state, enhanced red emission further supports the role of intermolecular interactions in stabilizing low-energy excited states.

Importantly, the probe demonstrates selective localization in lipid droplets, where the hydrophobic microenvironment promotes emission enhancement. This study establishes a design principle for microenvironment-sensitive materials with tunable emission, offering insights into the development of functional luminescent systems for bioimaging and beyond.

A microenvironment-sensitive fluorophore exhibiting self-assembly-driven tunable emission is reported for selective lipid droplet (LD) imaging. The designed molecule shows strong emission in moderately polar media, while a significant red-shift accompanied by fluorescence attenuation is observed in highly polar and nonpolar environments, indicating pronounced sensitivity to the surrounding microenvironment. Systematic solvent studies reveal the emergence of a new red-emissive band in mixed solvent systems, attributed to aggregate formation. In the solid state, enhanced red emission further supports the role of restricted molecular motion and intermolecular interactions in modulating the photophysical behavior.

Mechanistically, the emission tunability arises from the interplay of intramolecular charge transfer and microenvironment-regulated self-assembly, leading to distinct emissive states in solution, aggregated, and solid phases. Notably, the probe preferentially accumulates in lipid droplets, where the hydrophobic and confined environment restricts intramolecular motion and stabilizes the emissive state, enabling bright intracellular fluorescence.

This work highlights a unified strategy integrating microenvironment sensitivity and self-assembly to achieve tunable emission, providing a promising platform for the design of advanced fluorescent probes for lipid droplet imaging and related bioanalytical applications.

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Visible-light induced C-N bond Formation from 6-Aminouracil and Aryl Iodide

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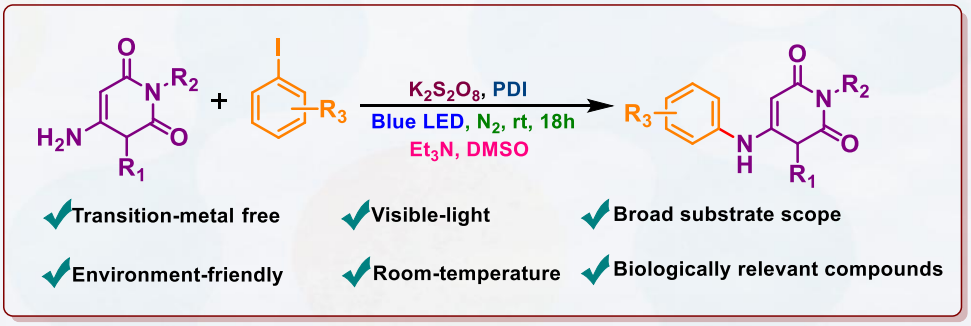
Abstract

A photocatalytic C-N coupling reaction utilizing 6-aminouracil and aryl iodide under visible light using N, N'-bis(2,6-diisopropylphenyl)-3,4,9,10-perylenetetracarboxylic diimide (PDI) as an organic photocatalyst have been developed which forms the N-arylated 6-aminouracil derivatives. These are valuable nucleobase analogues which are biologically important compounds. Notably, this method operates under mild reaction condition without the need for metal catalyst and highlights the potential of PDI-based photoredox catalysis under visible-light irradiation[1-3]. This method provides a sustainable and environment-friendly approach for the formation of C-N bond.



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P-13

Mapping the Variant Spectrum in β-Thalassemia: Insights from Targeted Next-Generation Sequencing of a Case–Control Cohort from Gujarat, India.

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β-thalassemia is one of the most prevalent inherited hemoglobinopathies in India, with particularly high carrier frequencies reported in western states such as Gujarat. Despite the identification of numerous pathogenic variants associated with β-thalassemia, the population-specific variant spectrum and its association with disease phenotype remain incompletely elucidated. Targeted next-generation sequencing (NGS) offers a robust approach for high-resolution characterization of genetic variants within clinically relevant genomic regions. A total of 298 peripheral blood samples were collected from individuals in Gujarat, comprising 215 clinically confirmed β-thalassemia cases and 83 healthy controls. Genomic DNA was subjected to targeted NGS using a custom amplicon panel designed to capture genomic regions implicated in hemoglobinopathies. Sequencing data were processed through a bioinformatics pipeline encompassing quality assessment, reference-based alignment, variant calling, and functional annotation, followed by stringent filtering of sequencing data. Association analysis was subsequently performed to evaluate variant–phenotype relationships which revealed multiple genetic variants across disease-associated loci within the cohort, several of which showed statistically significant associations with β-thalassemia. A cluster of highly significant signals emerged on chromosome 11, with rs33915217, rs12574989, and rs72869872 exhibiting the strongest associations. Additional variants in the region also demonstrated robust and consistent significance after multiple testing correction. Collectively, these findings advance the understanding of the population-specific genetic architecture of β-thalassemia in Gujarat and highlight the potential of targeted next-generation sequencing to strengthen molecular diagnostics, carrier detection, and preventive screening programs in high-burden settings.

P-14

The development of a robust folded scaffold as a fluorescent material using Butylidine-linked pyridazinone-based systems via aromatic π•••π stacking interactions.

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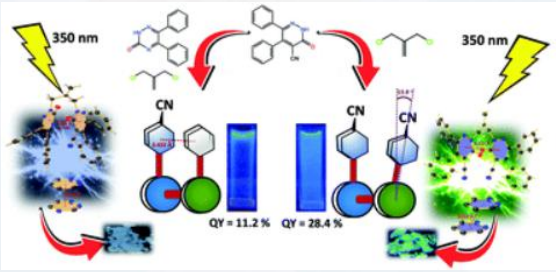
Abstract:

Fluorescence-capable robust folded pyridazinone-based homo- and heterodimers linked with butylidene linkers, whose crystals exhibit fluorescence with quantum yields of 11% (1CN) and 28% (2CN) due to intramolecular stacking, were synthesized. Previous reports state that intramolecularly folded/stacked compounds result in immediate quenching with no fluorescence, but we have designed two intramolecularly stacked compounds that show suitable emission spectra due to charge transfer between two conjugated heteroaromatic rings. Full spectral profiles and quantum yield of the organic solid-state emitters are reported. The optical behaviour of pyridazinone and the triazinone-related homo and heterodimers was rationalized based on time-dependent density functional theory (TD-DFT) studies, and the observed stacking interactions in crystals were studied in detail. This work demonstrates the significance of cyano aromatics in the design of solid-state organic fluorescent materials. Herein, we report that the intramolecular folding nature of organic solid-state materials has an important effect on their photophysical and charge transfer properties. Hence, our insights pinpoint the importance of charge transfer between pi-stacked folded dimers[1-3].



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P-15

Flower-like NiAl-LDH/$BiVO_4$ Z-Scheme Photocatalysts for Sunlight-Driven Degradation of Azo Dye: Performance and Mechanistic Insights

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Abstract:

Layered double hydroxide (LDH)-based materials have garnered significant attention as versatile photocatalysts for environmental remediation, particularly for the abatement of dye-laden wastewater, owing to their structural tunability, chemical robustness, and facile synthetic routes. In this context, a series of NiAl-LDH/$BiVO_4$ (NAL/BV) Z-scheme heterojunction nanocomposites were constructed by loading 5-15% (wt%) of $BiVO_4$ onto LDH via an ex-situ fabrication method, and evaluated for photocatalytic degradation of Congo red (CR), a typical azo dye, under solar irradiation. The structural, morphological, and optical attributes of the nanocomposites were meticulously elucidated through comprehensive analyses, including XPS, FTIR, PL, UV–DRS, FESEM, HRTEM, and BET surface area measurements. The optimized 5-NAL/BV composite exhibited a flower-like morphology with an augmented surface area, promoting efficient charge separation and enhanced photocatalytic activity. At a catalyst loading of 0.3 g L^{-1}, it achieved 94.3% CR degradation within 2 hours, with an apparent kinetic rate constant of 0.01673 min^{-1} and a synergy factor of 5.67. The effects of contaminant concentration, catalyst dose, pH, and light source on activity were systematically studied. TOC analysis confirmed 50% mineralization, while scavenging studies identified superoxide radicals as the primary reactive species. HRMS analysis elucidated degradation intermediates, and post-cycle characterization confirmed structural stability over six cycles. Moreover, a comparative analysis with previously reported studies demonstrates that this hybrid acts as a superior photocatalyst for the decomposition of hazardous dyes, highlighting the potential of NAL/BV nanocomposites for solar-driven wastewater treatment and environmental remediation(Kaur et al., 2025).

Keywords: Layered double hydroxides; $BiVO_4$; Z-scheme heterojunction; Congo red dye; Photocatalysis; Degradation; Wastewater treatment.

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P-16

Engineering Synergistic High-Entropy Spinel Oxide for Sustainable and High-Performance Oxygen Evolution Reaction

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Abstract:

Developing efficient and sustainable electrocatalysts for the oxygen evolution reaction (OER) is important for making clean hydrogen production more practical. In this study, three spinel-type high-entropy oxides $(Mn_{0.2}Ni_{0.2}Co_{0.2}Cu_{0.2}Zn_{0.2})(Cr_{0.5}Fe_{0.5})_2O_4$ (S-HEO-CF), $(Mn_{0.2}Ni_{0.2}Co_{0.2}Cu_{0.2}Zn_{0.2})(Fe)_2O_4$ (S-HEO-F), and $(Mn_{0.2}Ni_{0.2}Co_{0.2}Cu_{0.2}Zn_{0.2})(Cr)_2O_4$ (S-HEO-C) were prepared using a simple low-temperature hydrothermal method at 200 °C for 15 hours, followed by calcination at 400 °C for 2 hours, resulting in very small nanoparticles of around ~5 nm. Among these, S-HEO-CF shows the best OER performance, achieving a low overpotential of 265 mV at 10 mA cm^{-2}, which is clearly better than S-HEO-F (373 mV) and S-HEO-C (411 mV), as well as the standard RuO_2 catalyst. It also has a lower Tafel slope (81 mV dec^{-1}) compared to S-HEO-F (117 mV dec^{-1}) and S-HEO-C (127 mV dec^{-1}), indicating faster reaction kinetics. The intrinsic activity follows the same trend, with TOF values of 0.372 s^{-1}, 0.095 s^{-1}, and 0.048 s^{-1} for S-HEO-CF, S-HEO-F, and S-HEO-C, respectively. Electrochemical impedance spectroscopy (EIS) results further support this, showing lower charge-transfer resistance for S-HEO-CF (1.25 Ω) than for S-HEO-F (2.82 Ω) and S-HEO-C (4.5 Ω), indicating better electron transfer during the reaction. This improved performance comes from the combined (synergistic) effect of multiple metal elements, which helps tune the electronic structure and create more active sites. The catalyst also shows good stability, maintaining its performance for 48 hours with very little loss. Overall, this work presents a simple, low-cost, and efficient catalyst system for water-splitting applications.(Triolo et al., 2024; Zehtab Salmasi et al., 2025)

Keywords: Spinel HEO, Oxygen Evolution Reaction (OER), Electrocatalysts, Overpotential, Tafel Slope, Electrochemical impedance spectroscopy (EIS).

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P-17

From Preservative to Pathology: Sodium Benzoate Triggers Insulin Resistance and Muscle Atrophy

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Abstract

Sodium benzoate (SB), a widely used food preservative, has been reported to possess several therapeutic benefits (including treating neurodegenerative disorders) as well as negative effects (such as altering glucose homeostasis). However, limited attention has been given to its role in inducing insulin resistance (IR). Therefore, current study was designed to investigate the relationship between SB and insulin resistance using C2C12 myotubes and to explore the possible underlying mechanisms. Myotubes were exposed to SB (20mM) for 24h and glucose consumption and uptake assays along with confocal microscopy (GLUT4 translocation) were used to evaluate IR. Oxidative stress indicators *i.e.* reactive oxygen species (ROS), lipid peroxidation (LPO), and reduced glutathione (GSH) levels were also measured. Myotubes morphology along with atrophic markers (calpain activity) were evaluated. Data show that SB exposure induced IR in cultured myotubes by disrupting insulin-mediated GLUT4 translocation. Alteration in oxidative stress-related markers (*i.e.* elevated ROS and LPO levels, reduced GSH) were also observed in SB-treated myotubes. Furthermore, decrease in the fusion index, length, and diameter of myotubes along with upregulation of calpain activity and decrease in muscle protein were also observed. Study concludes that SB exposure not only induced IR but also caused atrophy and oxidative stress in the C2C12 myotubes.

Keywords: Sodium benzoate, C2C12, Insulin Resistance, Oxidative Stress, Atrophy

P-18

Visible-Light-Induced Flavin Catalysis: A Green Route to Naphtho[2,1-*b*] furans via an *o*-(Naphtho)quinone Intermediate

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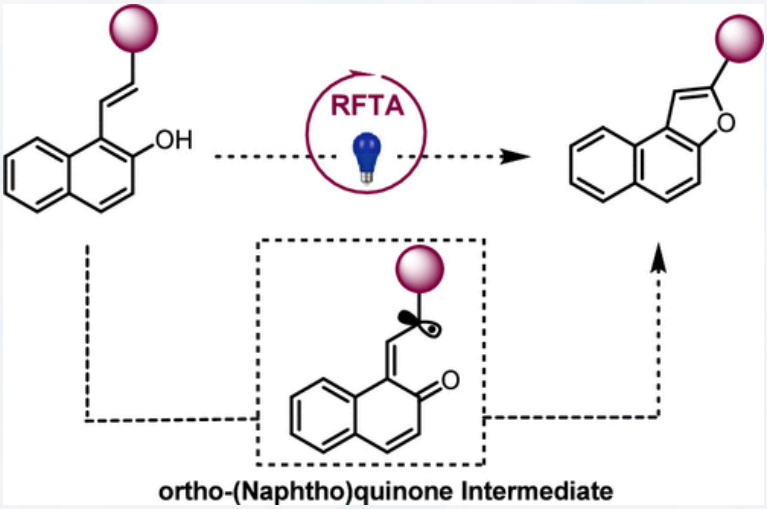
Introduction:

The significance of visible-light photocatalysis for sustainable chemistry and its extensive applications in organic synthesis have grabbed the attention of chemists in the past few years. Under mild reaction conditions, this catalytic method allows the formation of a variety of reactive species, often without a demand for stoichiometric activation chemicals.[1] Hetero- cyclic compounds are quite interesting to us in our daily life. Heterocyclic moieties are prevalent in agrochemicals, physiologically active compounds, natural goods, and medications.[2] To synthesize and functionalize heterocyclic compounds, we have been continuously involved in the development and implementation of photocatalytic systems and reactions. We outline our most recent discoveries and provide learnings from our research in this summary.A green and aerobic method for naphthofuran synthesis leverages riboflavin tetraacetate as a potent photocatalyst, accommodating diverse functional groups and a wide range of substrates. A comprehensive set of control experiments confirmed the involvement of o-(naphtho)quinone intermediates in the reaction mechanism, supporting the proposed catalytic pathway.



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P-19

Visible-light-Initiated decarboxylative acylation of unsaturated hydrocarbons with Keto acid via Csp2 –Csp2 cross-coupling

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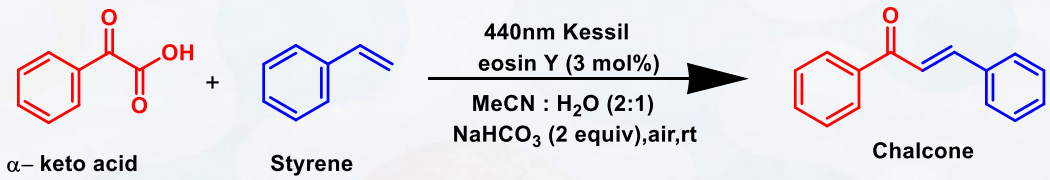
Abstract:

We present a simple and efficient method for the photocatalytic synthesis of chalcones via oxidative functionalization of unsaturated hydrocarbons. Organocatalytic decarboxylative cross-acyl coupling of Keto acid with styrene.Photoredox catalyst in visible light irradiation as a green energy input. Detailed mechanistic work shows that the changes happen via a radical mechanism. Furthermore, the wide functional group tolerance and compatibility with structurally complex and biorelevant substrates highlight the robustness and synthetic utility of the developed methodology. Such a methodology is highly attractive for late-stage modification of bioactive molecules and natural products.



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P-20

Nitrogen atom insertion into N=N double bonds: direct access to triazenes

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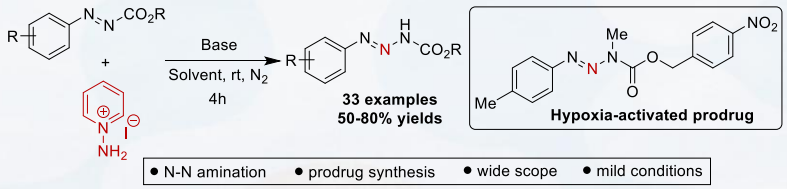
Abstract

Aryltriazenes, due to their versatile reactivity, are valuable synthons for constructing a broad array of heterocyclic frameworks and natural products. Moreover, aryltriazene derivatives display notable biological activities, serving as potent anticancer and antiviral agents Wang et. al. [1]. The present study describes the insertion of a single nitrogen atom into a diazene moiety, enabling direct formation of the triazene core. *N*-Aminopyridinium iodide was employed as single-nitrogen transfer reagent. This approach was further utilized in the synthesis of a hypoxia-activated triazene prodrug. Notably, the methodology features mild reaction conditions, operational simplicity, and broad substrate scope Rastogi et. al. [2].



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P-21

Designing DPP-4 inhibitors: Synthesis, characterization, in silico &in vitro evaluation, and theoretical calculation of flexible compounds linked via ortho xylyl spacers

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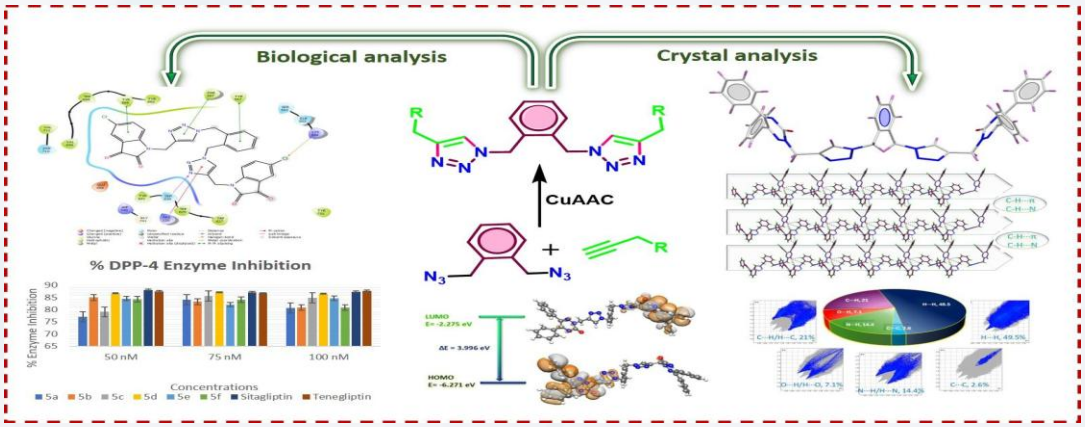
1,2,3-triazole-containing six symmetrical flexible dimer compounds (5a-5f) linked via ortho xylylspacers were synthesized using a copper-catalysed azide-alkyne cycloaddition (CuAAC) click reaction. Triazinone, isatin, and pyridazinone moieties were utilized to synthesize the heteroaromatic terminal alkynes (3a-3f). The structural characterization of all compounds was performed using spectroscopic techniques, including SCXRD, 1H and 13C-NMR, IR, and HRMS spectrometry. Among these compounds, compound 5a was crystallized, showing two twisted boat-type geometries at an angle of 43.98 degrees. Moreover, we investigated the intra- and intermolecular contact preserving the crystal packing in the solid state. Hirshfeld surface analysis and its related2-D fingerprint plots control the percentage contribution of intermolecular contact. The *in-silico* study of these compounds was conducted and revealed that 5d and 5c have good docking scores and interactions; further, all these compounds were validated by in vitro DPP-4 inhibitory activity. DPP-4 inhibition revealed that compound5d has an IC50 value of 1.57 Nm,similar to the standard drug sitagliptin. Compound 5d could be a potent DPP-4inhibitor with antidiabetic potential for further investigation.



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P-22

EFFECT OF ATLANTIS WEEDICIDE (MESOSULFURON METHYL 3% + IODOSULFURON METHYL SODIUM) ON MYCORRHIZAL FUNGI OF WHEAT CROP

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Abstract:

Wheat (Triticum aestivum L.) a primary dietary necessity in India, demands boosted output to guarantee sustenance stability. Weeds are the major substantial impediments in agriculture which not only decrease the yield and quality of wheat crop but also depleting essential nutrients simultaneously. Hence, weed control is essential for enhancing wheat production. Despite their weed-killing ability weedicides also adversely impact beneficial non-targeted soil microbes including arbuscular mycorrhizal fungi (AMF), which form one of the most widespread symbioses with plant roots on Earth. Atlantis is most widely used weedicide in Haryana, northern part of India to control weeds. Nevertheless, its consequences on mycorrhizal fungi are seldom highlighted. Therefore, the present investigation undertaken to assess the impacts of Atlantis weedicide on the mycorrhizal ecology of wheat crop. The study involved the application of three concentrations of Atlantis weedicide (the recommended dosage of 400g/ha, half the recommended dosage at 200g/ha, and a double dosage at 800g/ha) and the consequential effects on mycorrhizal fungi were evaluated on the 30th, 60th, and 90th day of treatment. Mycorrhizal spore isolation was achieved via wet sieving and decanting techniques, while rapid clearing and staining technique was used to analyze root colonization. The results evince that Atlantis weedicide exerted deleterious effects on mycorrhizal fungi, diminishing spore abundance and the extent of root colonization and effect that intensified commensurately with concentration. In our ongoing chemical campaign against weeds, it behooves us to minimize collateral damage to beneficial soil microbes. Therefore, the administration of high-dosage weedicides should be approached with circumspection and judiciousness.

Keywords: Wheat, Atlantis weedicide, Arbuscular mycorrhizal fungi

P-23

Preparation of 1T/2H MoS_2@g-C_3N_4 nanocomposites for electrochemical detection of chlorpyrifos pesticides

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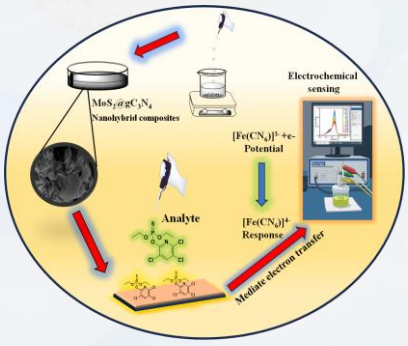
Abstract:

The report describes the production of a 1T/2H MoS_2@g-C_3N_4 hybrid nanocomposite for ultrasensitive electrochemical detection of pesticide contaminants.. Molybdenum disulfide (MoS_2) nanosheets have been linked onto graphitic carbon nitride (g-C_3N_4) frameworks using a simple hydrothermal synthesis procedure, resulting in a nanocomposite with multiple active sites, improved conductivity, and accelerated charge transfer kinetics. A comprehensive study using XRD, UV, SEM, TEM, FT-IR, and XPS demonstrates the successful fabrication and excellent properties of nanocomposites. [1-3] Electrochemical sensor electrodes made of 1T/2H MoS_2@g-C_3N_4 material show high sensitivity to "chlorpyrifos" pesticides, with detection limits in the nanomolar range and wide linear detection spans.[4] DPV sensing yields LOD values of 0.004577 µM/ml for higher concentrations and 0.03566 µM/ml for lower concentrations. Furthermore, the resulting electrode has great stability from 5 to 60 days, and the reaction time reveals a maximum current response at 10 seconds, indicating that the electrode responds rapidly and achieves its best sensing performance in only 10 seconds. 15 consecutive scans were performed to assess the reusability of complex matrices and their performance throughout multiple applications. Aside from that, the interference results indicates a minor change in current when heavy metals and urea are present, indicating that it is very selective for chlorpyrifos. Application studies involving real samples of fruits and vegetables i.e., tomato, brinjal and cucumber, which revealed high recovery rates, underscoring the sensor's practical viability. This work highlights the potential of 1T/2H MoS_2@g-C_3N_4-based electrochemical sensors as powerful tools for ensuring food safety and environmental health, paving the way for future integration into portable, on-site detection systems.



Keywords: 1T/2H MoS_2@g-C_3N_4, Chlorpyrifos Pesticides, Electrochemical sensing, Nanocomposites

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P-24

Metal-free visible-light-driven synthesis of amides from phenylglyoxylic acid and phenylhydrazine using eosin Y as a Photocatalyst

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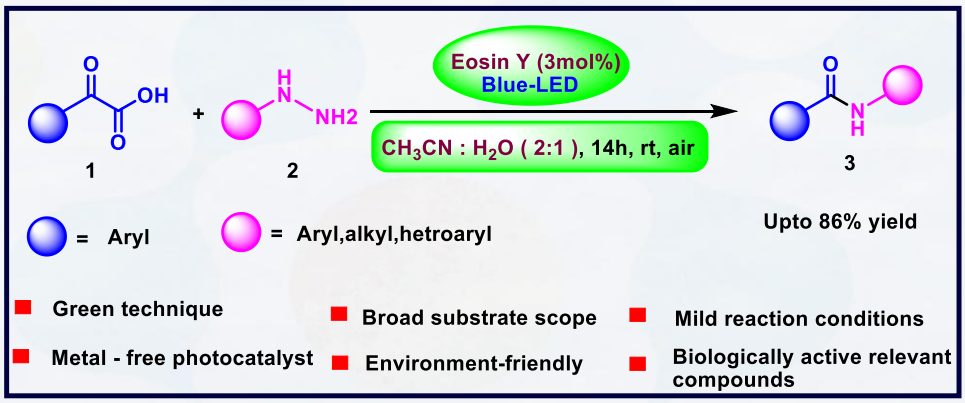
In this study, we report a metal-free and environmentally benign protocol for the synthesis of amides via decarboxylative amidation of phenylglyoxylic acids through C–N bond formation. This transformation is facilitated by eosin Y as an organic photocatalyst in a CH_3CN/H_2O mixed solvent system, with visible light irradiation as a sustainable energy source and molecular oxygen from ambient air serving as the terminal oxidant. The developed methodology demonstrates broad substrate scope, enabling the efficient conversion of various phenylglyoxylic acids and phenylhydrazines into the corresponding amide products. Overall, this protocol provides a practical and green synthetic platform for the preparation of biologically relevant amide-containing compounds.



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P-25

SEQUENTIAL COLORIMETRIC SENSING OF IODIDE AND GLUTATHIONE VIA ANTI-AGGREGATION AND AGGREGATION OF DIAZO-CAPPED GOLD NANOPARTICLES

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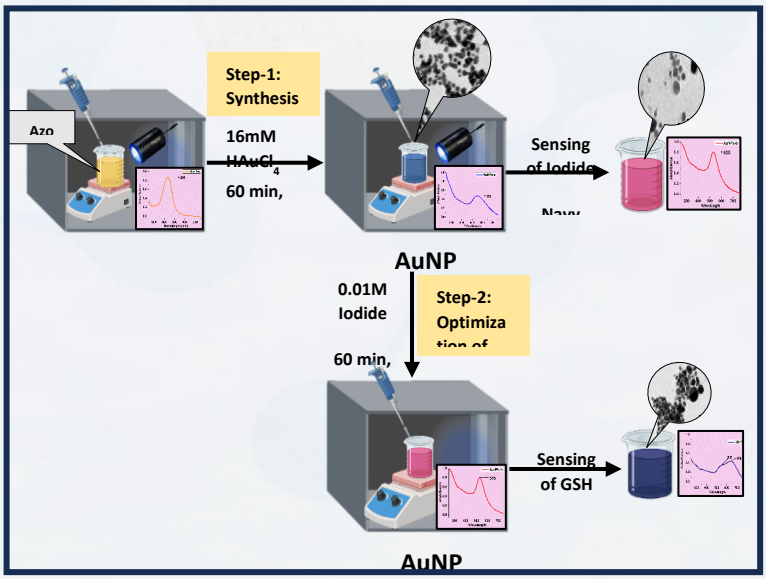
Iodide (I^-) and glutathione (GSH) play vital roles in biological systems, hence their rapid detection is important. Herein, we have synthesized an azo dye viz. 2-((4-nitrophenyl)diazenyl)benzene-1,3,5-triol as reducing and capping agent for the synthesis of stable navy-blue gold nanoparticles (AuNPs) via ultraviolet (UV) irradiation (370 nm) in an aqueous alkaline medium. The formation of AuNPs were confirmed through UV-Vis, FTIR, XPS, XRD, SEM, TEM, SAED, DLS and surface charge measurements. They exhibited surface plasmon resonance (SPR) band at 556 ± 5 nm, with average size range of 12–13 nm, and concentration of 10.21 nM. Also, they showed highly sensitive sequential detection of dual analytes i.e., I^- and GSH in the presence of several interfering analytes. The navy-blue AuNPs changed to magenta (535 nm) by preferential adsorption of I^- on AuNPs, thus corroborating anti-aggregation mechanism. Later, upon addition of GSH to this magenta colored AuNPs, its color changed to deep blue with bathochromic shift in UV–Vis spectrum (630 nm), indicating the aggregation of AuNPs. The limit of detection for GSH and Iodide has been successfully calculated. Also, its applicability was extended to spiked real samples viz., kelp and thyroxine for I^- detection, human saliva and blood for GSH detection with excellent recovery rates.



P-26

Design and Synthesis of Lawsone-linked N-Heterocyclic Hybrid Scaffolds as Promising Antimicrobial Agents

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Antimicrobial resistance has emerged as a global threat in the current era. It has necessitated the development of novel therapeutic agents with enhanced efficacy and diverse mechanisms of action [1]. In this context, hybrid pharmacophores have gained considerable attention due to their ability to integrate multiple bioactive moieties into a single molecular framework [2]. The present study focuses on the rational design and synthesis of novel Lawsone- linked N-heterocyclic hybrid scaffolds as potential antimicrobial agents. Lawsone (2-hydroxy-1,4-naphthoquinone), a naturally occurring bioactive compound, was strategically functionalized and conjugated with various N-heterocyclic moieties through Mannich bases to generate a series of amino derivatives of lawsone [3,4]. The synthesized compounds were characterized using standard spectroscopic techniques, including FTIR, ^{1}H NMR, ^{13}C NMR, and mass spectrometry, confirming their structural integrity. The antimicrobial potential of the synthesized hybrids was evaluated against a panel of Gram-positive and Gram-negative bacterial strains, as well as selected fungal species [2]. Further, the synthesized compounds were *in silico* assessed on the druggability parameters, including Lipinski's rule, Veber's rule, and ADMET. The select compounds showed strong binding affinity with the potential targets, playing a crucial role in microbial pathogenesis. Several compounds exhibited significant antimicrobial activity, with some derivatives showing enhanced potency compared to the parent scaffold, indicating a possible synergistic effect of the hybrid framework. In conclusion, the study demonstrates that lawsone-based N-heterocyclic hybrids represent a promising strategy for the development of multi-targeting, broad-spectrum antimicrobial agents, offering the potential to combat drug-resistant pathogens.

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P-27

Photoinduced Condensation of Methyl Arene with Active Methylene Compounds via C(sp3)-H Functionalization

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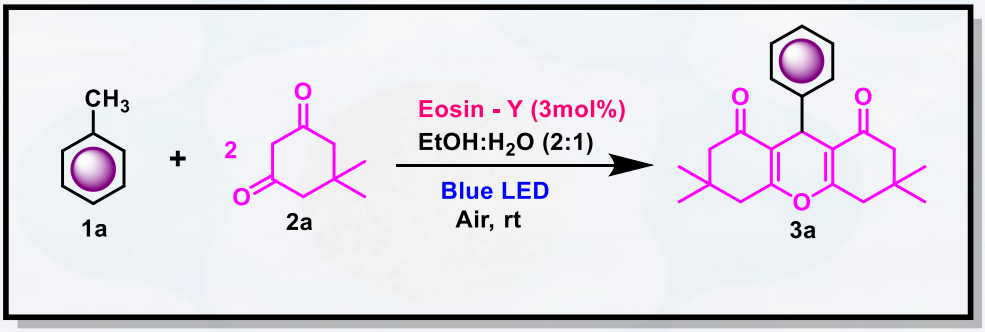
ABSTRACT:

Notable progress is being made in visible-light-driven C(sp3)-H functionalisation that results in the creation of carbon-carbon bonds and is enabled by a metal-free photocatalyst. Here, we report a metal-free approach to the condensation of methyl arenes with active methylene compounds, developing carbon-carbon bonds, using eosin-Y as a metal-free organic photocatalyst in the presence of atmospheric oxygen as the oxidant. This method demonstrated compatibility with visible light, a greener solvent, and metal-free conditions, thereby promoting environmental friendliness and broadening the substrate scope. This protocol's use in creating pharmaceutically relevant analogues and biologically active molecules is demonstrated by the transformation of methyl arenes and active methylene compounds into a variety of desirable substrates.



- Greener solvent
- Metal-free process
- Room temperature
- Visible light
- Air as an oxidant
- C-H functionalization
- Bioactive compound

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P-28

"Beyond Survival: Probiotic Resilience to Heavy Metal Exposure and Oxidative Stress"

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Abstract:

Members of the genera *Lactobacillus*, *Bacillus*, *Enterococcus*, and *Streptococcus* are well-established probiotic microorganisms integral to gastrointestinal homeostasis; however, their persistence and beneficial role in the gut can be significantly compromised by environmental stressors, particularly heavy metals and reactive oxygen species. In the present study, probiotic strains belonging to these genera were systematically screened for heavy-metal tolerance, and resistant strains were identified for further characterization. Minimum Inhibitory Concentration (MIC) determination was carried out to quantify the tolerance of the selected strains against a specific heavy metal, while IC_{50} values were determined to assess the concentration of metal at which 50% inhibition of growth was observed, providing a more precise measure of strain-level sensitivity. In addition, oxidative stress tolerance was evaluated across all probiotic strains to assess their capacity to withstand conditions physiologically relevant to the gastrointestinal environment. The metals investigated included arsenite (As^{3+}), cadmium (Cd^{2+}), mercury (Hg^{2+}), and nickel (Ni^{2+}). MIC and IC_{50} profiling revealed strain-specific variation in metal tolerance across strains of all four genera, indicating that individual strains employ distinct stress-adaptation mechanisms. Strains exhibiting higher IC_{50} values alongside higher MIC thresholds were identified as particularly strong candidates for probiotic applications, especially in contexts where the gut is simultaneously challenged by metal toxicity and oxidative damage. Further work will examine effect of stressors on probiotic traits relevant to the specific strains using the same panel of metals, with the aim of further elucidating the metal-management strategies of probiotics. Collectively, the findings demonstrate that the characterized probiotic strains possess robust adaptive potential, supporting their suitability as resilient probiotics for functional food and therapeutic applications, with particular relevance for populations subject to elevated environmental metal exposure.

Design, Synthesis and Biological Assessment of Anthraquinone *bis*-1,2,3-triazolyl Macrocycle and its Anticancer Application

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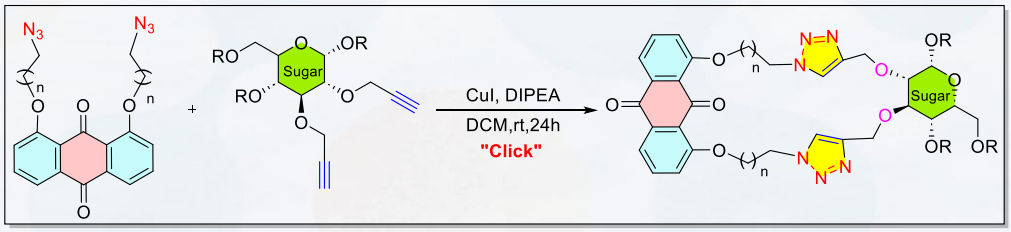
Macrocyclic compounds have attracted considerable attention due to their diverse structural features and significant biological activities.[1-2] In this study, an anthraquinone-based macrocyclic framework was designed and synthesized using a [3+2] cycloaddition strategy with sugar motifs. The synthetic approach involved the reaction of azide and alkyne functionalized precursors under optimized click chemistry conditions to afford triazole-linked macrocycles in good yields. The structures of the synthesized compounds were characterized using spectroscopic techniques NMR and mass spectrometry. Preliminary biological evaluation of the synthesized macrocycles was carried out against selected Hela cell lines, which revealed promising anticancer activity.[3] The results demonstrate that anthraquinone-derived macrocycles provide a versatile platform for the development of biologically active molecules and may serve as potential candidates for further pharmacological investigation.



Scheme 1. Synthesis of 1,2,3-triazolyl anthraquinone based macrocycle glycoconjugates *via* click protocol

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P-30

Stereoselective synthesis of Deoxy Sugar and Glycoside Assembly via Pd-Catalysed, TFA Activation and Lewis Acid Mediation

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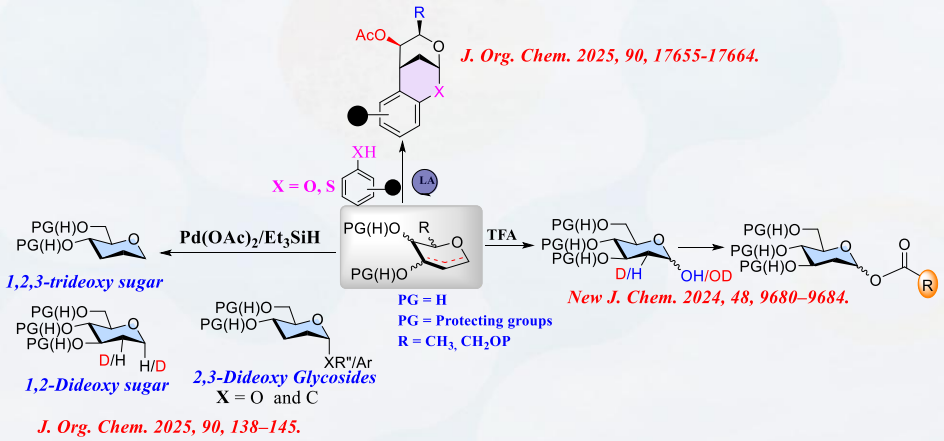
We report a versatile and efficient synthetic platform for the preparation of deoxy sugars and glycosides via selective hydrogenation and functionalization of sugar enol ethers and glycals. A $Pd(OAc)_2/Et_3SiH$ catalytic system enabled chemoselective reduction of diverse glycals and glycosides, affording 2-deoxy sugars in yields up to 96%. Application to both O- and C-glycosidic substrates provided rapid access to 2,3-dideoxy glycosides with excellent efficiency and stereo control.[1,2] An environmentally benign protocol further allowed direct conversion of protected and unprotected glycals to 2-deoxy sugars under ambient conditions, delivering products in yields up to 98%. Subsequent esterification with structurally diverse carboxylic acids, including pharmaceutically relevant agents such as indomethacin and tolmetin, furnished a library of 2-deoxy glycosyl esters.[3] Given the biological and medicinal importance of Deoxyglycosides, a complementary Lewis acid-promoted domino annulation was developed from protected glycals, including acetylated D-galactal, D-arabinal, and L-fucal derivatives. This transformation proceeded with remarkable regioselectivity, affording annulated 2-deoxyglycosides exclusively. Broad substrate scope encompassed naphthols, substituted phenols, and thionaphthalenes. DFT studies revealed preferential nucleophilic attack at the C-3 position of a transient oxocarbenium intermediate, consistent with isolation of a key intermediate.[4]



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P-31

N-(Arylthio)phthalimide as thiol alternatives in Csp2-S coupling reactions using aryldiazonium tetrafluoroborate salts

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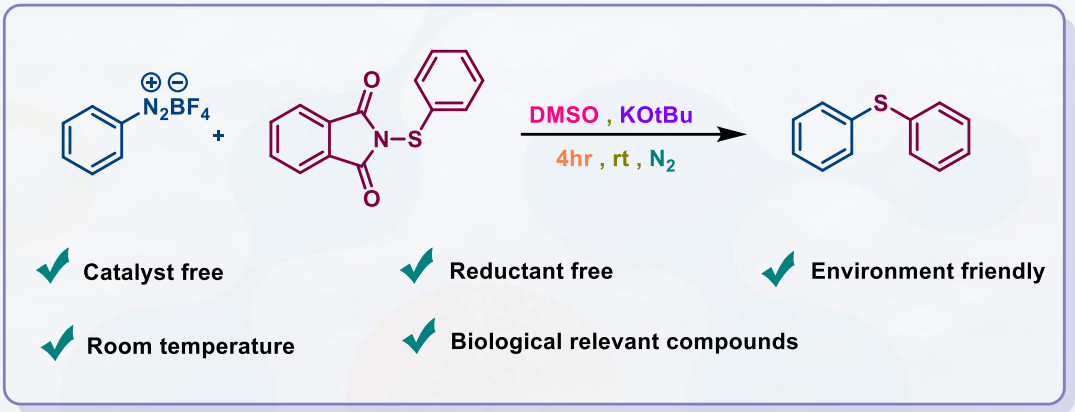
Diaryl sulfides are widely found in the pharmaceutical industry, organic synthesis, and materials sciences. We report an efficient approach to the synthesis of diaryl sulfides via C–S cross-coupling of N-(arylthio)phthalimide with aryldiazonium salts in the presence of base, without a catalyst. Here, N-(arylthio)phthalimide compounds have been employed as thiol replacements. The technique demonstrates a broad substrate range and good product yields.



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P-32

Redox-Neutral electrochemical Diazo Coupling: Controlled Synthesis of Olefins and Azines via modulating reaction conditions

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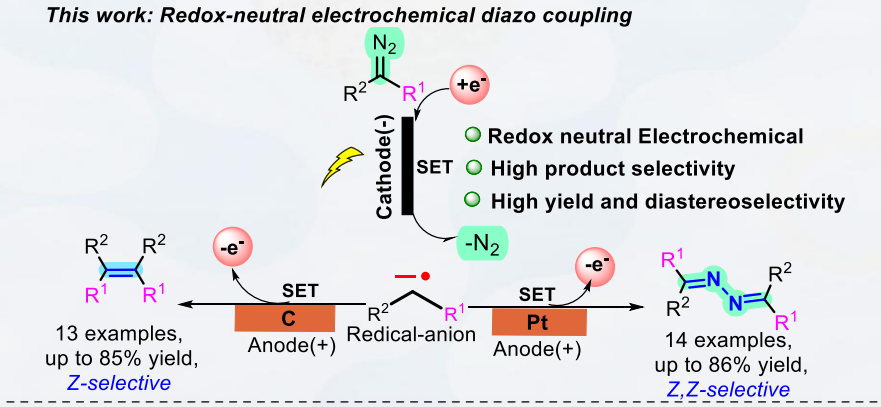
Abstract

We report a metal-free, linear, paired redox-neutral [1] electrochemical coupling of aryl diazoesters, enabling switchable, selective synthesis of tetrasubstituted azines or olefins through simple modulation of reaction parameters. While traditional catalytic approaches for diazo coupling often rely on transition metals or photocatalysts, which frequently suffer from limited substrate scope or selectivity, this electrochemical platform offers a sustainable, reagent-free alternative. Mechanistic investigations, including cyclic voltammetry and radical trapping experiments, reveal a cathodically initiated radical-anion pathway in which the electrode interface dictates the coupling manifold. Specifically, platinum electrodes favor N–N coupling to produce azines, while carbon electrodes facilitate C–C coupling to yield olefins.[2] The protocol exhibits a broad substrate scope, tolerating various ester groups and aryl substituents with good to excellent isolated yields and high diastereoselectivities. The methodology operates under a redox-neutral electron-catalytic regime, as evidenced by moderate Faradaic efficiencies. Successful gram-scale implementation further underscores the practical utility of this approach. Overall, this work demonstrates that the precise tuning of electrode materials and electrolyte environments provides a powerful, tunable tool for modern synthetic organic chemistry, circumventing the need for external catalysts while enhancing product control in diazo transformations.



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P-33

From Parent to Progeny: Computational Design and Evaluation of Nitrogen-Rich, Hydrogen-Free Energetic Materials Inspired by the Heat-Resistant TACOT Skeleton

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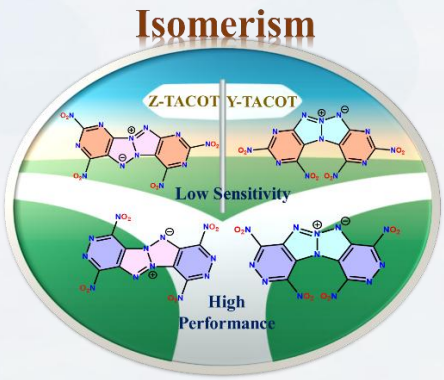
Abstract

In this study, we report the computational design of six hydrogen-free energetic compounds derived from heat-resistant and highly stable *y*-TACOT and *z*-TACOT frameworks, with the objective of achieving an optimal balance between detonation performance and sensitivity. [1] To improve the energetic performance and energy content of these frameworks while retaining their inherent thermal stability and low sensitivity, the fused benzene rings in the parent structures were systematically replaced with diazine heterocycles, namely pyrazine, pyrimidine, and pyridazine. Our findings reveal that substitution of benzene rings in the TACOT backbone with diazine moieties significantly enhances the energetic properties without compromising structural stability. Although *y*-TACOT and *z*-TACOT represent benchmark heat-resistant explosives, exhibiting decomposition temperatures (Td) above 400 °C, their practical applicability is limited by relatively poor detonation performance. [2] Therefore, the rational modification of such well-established energetic frameworks provides an effective strategy for developing advanced heat-resistant materials. By judiciously modifying the molecular backbone or functional groups of these benchmark systems, key properties such as density, heat of formation, oxygen balance, crystal packing, and intermolecular interactions can be finely tuned. This approach enables the optimization of the critical balance between high detonation performance and thermal stability, which is essential for next-generation energetic materials.

Keywords: Heat-resistant, TACOT, Sensitivity, Performance.



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P-34

Fusion of FOX-7 and HMX framework via diamino bridges: A DFT study on insensitive high-energy explosives

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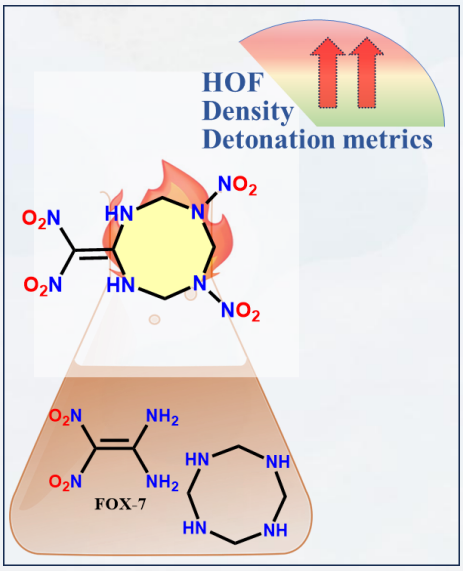
Abstract

Progress in energetic materials remains challenging because energy output and stability exhibit an inverse relationship: higher performance often diminishes stability [1]. In recent decades, significant research focus on structural modification on FOX-7, particularly the alteration of amino groups [2,3]. This work describes the structural alteration of FOX-7 (1,1-diamino-2,2-dinitroethene) by fusing it with the HMX framework, aiming to enhance its performance characteristics. The evaluated result indicates that the addition of the terazocane ring notably enhanced the heat of formation of the designed compounds than FOX-7 (-88.50 kJ/mol). Also, substituting nitro group on the ring fosters the detonation velocity (> 9.15 km/s) and pressure (> 39.54 GPa) of the designed compound as compared to FOX-7 (D= 8.80 km/s; P= 33.62 GPa) and HMX (D= 8.90 km/s; P= 38.39 GPa). ESP, NCI, Mayer bond order, QTAIM analysis, and planarity index were also examined and compared with FOX-7. Additionally, designed compounds show high C-NO_2 strength (> 219 kJ/mol), which indicates their thermal stability. The computed results reveal that the physicochemical, detonation and sensitivity parameter of FOX-7 lies between those of the designed compounds, highlighting their potential for continued research and practical application as thermally stable, high-density energetic materials.

Keywords: Energetic molecule, FOX-7, HMX, detonation, sensitivity



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P-35

In Silico Design and Energetic Performance Analysis of Dinitroheterocycle-Substituted Fused Furazan–Pyrazine System

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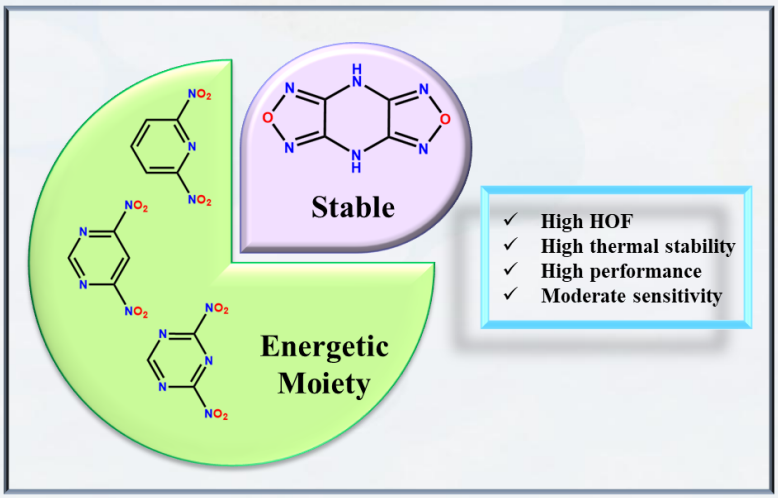
Abstract

In this work, three novel energetic compounds derived from 4H, 8H difurazano[3,4-b;3′,4′-e] pyrazine (DFP) were designed, and their heat of formation, physicochemical properties and sensitivity parameters were predicted. The variation in these properties with the changing substituent ring on the nitrogen atom of the pyrazine ring was comprehensively studied and analysed [1,2]. The results reveal that the designed compounds exhibit high positive heat of formation (>685.7 kJ/mol), high density (>1.80 g/cm^3), and good detonation performance (D> 7.68 km/s, P> 23.87 GPa), and the results were compared with the previously reported compounds. A detailed analysis of the performance and sensitivity parameters demonstrates that the designed compounds exhibit a favourable equilibrium between energetic performance and sensitivity. Aromaticity indices, LOLIPOP index and planarity parameters were also reviewed, and the stability of compounds towards thermal decomposition was evaluated by the bond dissociation energy (> 210 kJ/mol) of the trigger linkage, i.e., C-NO_2 bond [3]. Additionally, these compounds possess a moderate as predicted by specific parameters like impact sensitivity (> 29 cm), charge on nitro group (-Q_{NO2} >0.166 e), and maximum heat of detonation (Q_{max} <1378 cal/g). These outcomes validate that this work on furazano-pyrazine derivatives is a viable approach towards designing, screening, and identifying promising high-performance energetic compounds.

Keywords: Energetic materials, Fused heterocycles, Detonation, Heat of formation, Sensitivity.



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P-36

Engineered Single Nucleobase-Derived Bionanozyme with Oxidase-Like Activity for and Environmental Applications

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Abstract:

Oxidase enzymes are widely employed in biosensing and environmental technologies due to their high substrate specificity and catalytic efficiency under mild conditions. However, their practical applications are often constrained by limitations, including high production costs, poor operational stability, and limited reusability. To overcome these challenges, we report the development of a robust, eco-friendly bionanozyme derived from a single nucleobase and cobalt cofactor, synthesized via green, aqueous-phase self-assembly. The resulting black precipitate, B–Co bionanozyme, exhibits remarkable oxidase-like activity without requiring additional cofactors or mediators. Comprehensive characterization revealed superior catalytic stability across broad pH, temperature, and storage conditions, outperforming natural oxidase enzymes in harsh environments. Notably, the B–Co bionanozyme demonstrated high efficiency in the selective detection and differentiation of aminophenol isomers (o-, m-, p-AP)—persistent environmental toxins and precursors to carcinogenic dyes/pesticides—through distinct spectroscopic shifts and visual colorimetric changes, enabling naked-eye visual identification even at trace levels. This study introduces a cost-effective, sustainable alternative to natural oxidases and expands nucleobase-derived nanozymes for environmental monitoring platforms. The simplicity of synthesis combined with exceptional catalytic performance positions this bionanozyme as a versatile tool for environmental remediation technologies.

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P-37

Bi_2S_3 as an efficient Photocatalyst for enhanced photo-Fenton degradation of Ciprofloxacin

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Abstract

Antibiotics is one of the majors from medical waste and sewage treatment plants and pollutes the environment if they are not treated prior to disposal beside all these pesticides, insecticides, dyes used in agricultural sector and industrial sector respectively, are also the part of contaminants, therefore, treatment of waste water coming from these sources is a major concern. In this work, with the help of Bi_2S_3 nanoparticles, Photo-Fenton like process is utilized to degrade the toxic organic pollutants like antibiotics and dyes in simpler non-toxic components like H_2O and CO_2. Out of many metal sulfides, bismuth sulfide is one of the promising catalysts for degradation of pollutants by photo-Fenton like process. Bi_2S_3 was synthesized using simple solvothermal method. The synthesized photocatalyst was characterized by using techniques like XRD and UV-DRS. XRD data of Bi_2S_3 shows bismuthinite phase of Bi_2S_3. UV-DRS conforms the synthesis material have band gap of 1.43eV. FE-SEM images conformed that the synthesized material has nanorod like shape with average particle size of 98 nm. The synthesized Bi_2S_3 material show remarkable activity towards the degradation of ciprofloxacin (one of the major pharmaceutical pollutants) having turnover frequency of 121.993 μmol gm^{-1} h^{-1}.

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P-38

"Citric acid-functionalized Mo-doped $CoFe_2O_4$ nano-adsorbents for co-adsorption of organic pollutants: experimental and computational insights"

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Abstract

This research advances a dual organic pollutant adsorption strategy closely aligned with real-world wastewater treatment scenarios. In this context, citric acid-functionalized Mo-doped cobalt ferrite ($CoFe_2O_4$) nanoparticles were prepared with varying Mo doping levels (1, 2, 4, and 8%). Mo-doping modulates the electronic structure, introduces additional active sites, and enhances the adsorption affinity of $CoFe_2O_4$. Citric acid modification not only reduced particle size and increased surface area but also provided additional binding sites, while simultaneously tuning the ferrimagnetic behavior of $CoFe_2O_4$ toward superparamagnetic. Among the prepared materials, the 4% Mo-doped sample (CA/4MoCFO) exhibited the best performance at a near neutral pH (~6), with adsorption capacities of 28.68 $mg.g^{-1}$ for ciprofloxacin (CIP) and 129.61 $mg.g^{-1}$ for tetracycline (TET). These adsorption capacities are substantially higher than those exhibited by pure $CoFe_2O_4$. Equilibrium isotherm data were best described by the extended Freundlich isotherm, consistent with heterogeneous adsorption sites on the adsorbent. XRD and DFT analyses confirm that Mo dopants preferentially substitute Co(Oh) sites in the $CoFe_2O_4$ lattice, and XPS further reveals that, owing to Mo's higher electronegativity relative to Co and Fe, this substitution redistributes electron density to generate heterogeneous adsorption sites with tailored affinities for diverse adsorbates. DFT interaction energy calculations aligned with experimental results, confirming physisorption as the dominant mechanism. The synergistic effect of citric acid modification and Mo doping yielded nano-adsorbents with good recyclability up to 5 cycles. Overall, this is a cost-effective and sustainable strategy for simultaneously removing different antibiotics from water systems.

Keywords: Nano-adsorbents, Co-adsorption, DFT calculations, Adsorption isotherm

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P-39

A Facile Method for Oxyhalogenation of Thiols and Disulfides to Sulfonyl Fluorides

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Abstract:

Sulfonyl fluorides, one of the most important sulphur (VI) fluoride species, have attracted a fast growing research interest in recent year due to their inimitable properties and wide range of application, including material science [1], polymer synthesis [2], in chemical biology [3] as covalent protein modifier, drug discovery, protease inhibitor, antibiotic, lipoprotein lipase inhibitor, AChE inhibitor, activity based probe and in organic synthesis. One of the most notable features of sulfonyl fluorides is their strong electrophilic nature and the presence of covalent link highly electronegative fluorine atom to the sulphur atom which enhance its reactivity and allowing it to act as a powerful electrophile. Unlike to other sulfonyl group, sulfonyl fluorides are hydrolytic & thermodynamic stable, resistance to reduction and bond cleavage in metal catalysis. Due to the vast applications of sulfonyl fluorides, the syntheses for their preparation from abundant starting materials are highly desired. The most common strategy prepared by oxidation of thiols involves a chloride/fluoride exchange of Sulfonyl chlorides in the presence of aqueous solution of fluoride salts. However, Sulfonyl chlorides are less stable, hydrolyze and decomposed during workup hence these reagents not widely available and need to be prepared from the corresponding thiols. We, herein, report a facile process for efficient and one step preparation of sulfonyl fluoride through a direct oxyhalogenation of thiols and disulfides to sulfonyl fluorides. Our method involves the reaction of indigenously available thiols and disulfides with trichloroisocynuric acide (TCCA) for in situ generation of sulfonyl chloride which on further reaction with tetra butyl ammonium fluoride (TBAF) and 18 crown 6 in acetonitrile-water in same reaction vessel gives corresponding sulfonyl fluorides in single step. This method was found superior to the existing methods in term of time and yield.

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P-40

Trifluoromethoxy-Schiff base vanilloxyl mesogens: phase transitions and bioactivity

PALKESHBHAI NILESHKUMAR CHAUHAN

The homologous series of 4-(((4-(trifluoromethoxy)phenyl)imino)methyl)phenyl 4-alkoxy-3-meth oxybenzoate has been developed analyzed for structural elucidation using spectral analysis (FT-IR, 1H- and 13C-NMR, UV-visible), mass spectrometry (ESI-MS) and X-ray diffraction. Thermal stability and liquid crystalline (LC) phases have been determined by DSC polarized optical microscopy analysis, respectively. The studied samples (except K1 and K2) display a nematic mesophase with moderate thermal stability, showing an average transition temperature of~ 142°C. Computational calculations were employed to discuss energy and relevant parameters like polarizability, dipole moment, aspect ratio etc. The energy gap and anticipated thermal stabilities for titled molecules, K4 show the considerable gap and maximum stability, followed by other samples which have approximately equal values. Among the tested samples, K12 and K18 showed notable potency against the bacterial strains used in the experimental study, with activity compar able to standard drugs. Following a similar performance trend, samples K12 and K18 demonstrated higher binding affinities, suggesting their potential effectiveness as precursors for inhibiting protein receptor activity. The findings indicate that the© synthesised LC molecules hold promise as potential bacterial inhibitors, though optimization and validation in preclinical trials are required

SYNTHESIS AND CHARACTERIZATION OF 2,7-DICHLORO-6-FLUORO-3-(((SUBSTITUTED)HYDRAZONO)METHYL)QUINOLINE SKELETON AND THEIR BIOLOGICAL SCREENING

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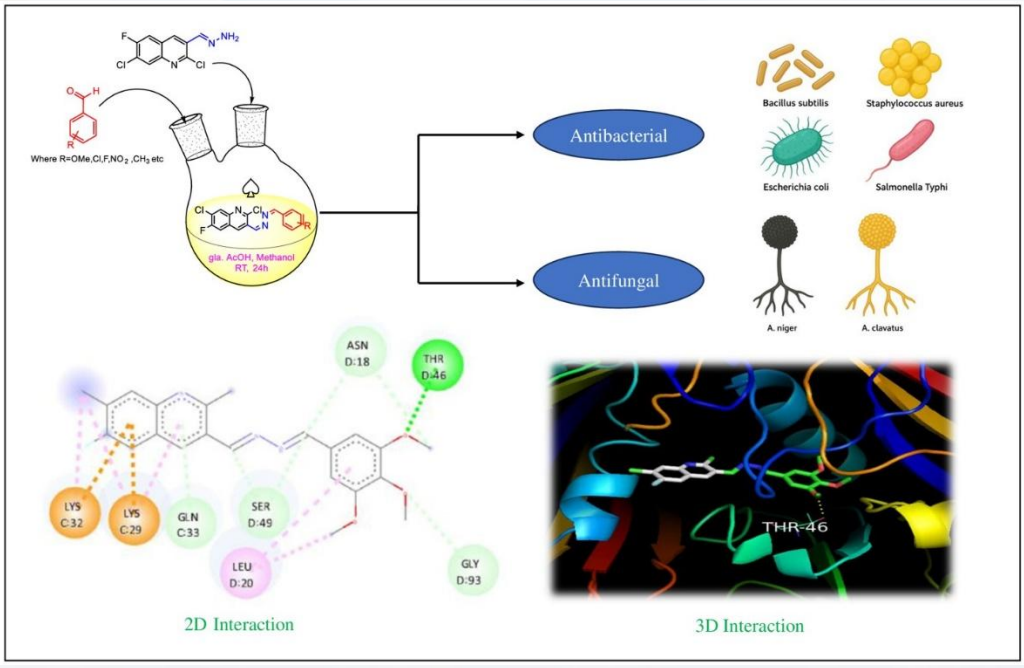
ABSTRACT

An efficient, simple and rapid synthesis method for the 2-chloro-5,6-dimethyl-3-(((((lower benzylidene)hydrazinylidene)methyl)quinoline. The one pot reaction of 2-Chloro-3(We found different organic compounds that act as antibiotics by reacting hydrazonemethyl)-7,8-dimethylquinoline with various substituted benzaldehydes in the presence of catalytic amounts of glacial acetic acid and methanol as a solvent to gives desired product. We synthesized various molecule which act as a antimicrobial agents and its showed moderate activity against the bacteria used.

KEYWORDS: Antimicrobial activity, SAR study, One-pot reaction



P-42

High-Resolution Characterization of Å-nm Scale Pores During the Electrical Breakdown of the Lipid Bilayer Membranes

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Lipid bilayer is a fundamental constituent of the cell membrane that facilitate the translocation of the selective molecules and ions through it when subject to external electric field, called electroporation. Here, we have studied the statistical defects in lipid bilayer which caused the short-lived pore formation in μs-ms time scale, and Å-nm range in size and rupture behaviour in the lipid bilayer membrane for four varieties of phospholipids DPhPC, POPC, DOPC and DOPG, each differing in their molecular structure. In a typical experiment, we have used the Montal-Muller method to form a vertical lipid bilayer membrane on a 100 μm Teflon aperture and applied a linear stepwise voltage ranging from 0 to 1 V with a 10 mV voltage step with a 20 ms step duration, while monitoring the ionic-current with pA current and μs time resolution in 1M KCl buffer solution. We found that the measured distribution of membrane breakdown voltage $V_{breakdown}$ follows the Weibull distribution, and its shape changes with the identity of the lipid molecule. Our analysis of the observed short-lived pores both during and prior to the membrane rupture suggests that the pores during the instantaneous rupture at $V_{breakdown}$ and the pores prior to the rupture occur independently and have different population of hydrophilic and hydrophobic pores. For DOPG lipid-bilayer, we observed a roughly 5-10 times faster rate of conductance change during rupture in comparison to the three lipids, which is likely due to the presence of a negatively charged glycerol group destabilizing the metastable pore during the rupture process.

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P-43

Emerging Small Organic Chemosensors for Optical Detection of Biorelevant Species

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Abstract:

Small organic chemosensors have emerged as powerful analytical tools for the optical detection of biorelevant molecules due to their significant advantages over conventional detection techniques. These sensors provide high sensitivity, selectivity and rapid response times. They enable selective detection of biologically significant analytes such as metal ions, reactive oxygen species, anions and other small biomolecules such as amino acids, carbohydrates and drugs in complex chemical and biological environments. (Kr et al., 2022) These chemosensors are designed in such a way that atleast one heteroatom is present in the molecular structure of the compound such as nitrogen, sulfur or oxygen. Generally, the heteroatoms present in the molecule acts as coordination sites thereby facilitating selective analyte binding. (Darwish et al., 2023) Moreover, the presence of different heteroatoms along with varying ring sizes enable precise tuning of their electronic properties, allowing precise modulation of absorption and emission responses. (Udhayakumari & Nanthakumar, 2025)Recent developments have emphasized both on colorimetric and fluorometric sensing techniques. These techniques serve as powerful alternatives to traditional sensing methods by providing excellent selectivity, sensitivity and ease of use for sensing of biorelevant analytes. Chromogenic techniques offer a useful blend of simplicity and adequate sensitivity, whereas fluorogenic techniques exhibit remarkable sensitivity, making them highly suitable for identifying trace amounts of biorelevant analytes in a wide range of environmental, biological and food samples. (Udhayakumari, 2020) Therefore, these sensors possess promising potential for real-time monitoring of biorelevant species in environmental and biological systems.

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P-44

Magnetically recyclable phytogenic MBC-ZnO nanocomposite for sustainable environmental cleanup

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Abstract

In this work, a green-synthesized MBC-ZnO nanocomposite (NCs) was developed and evaluated for photocatalytic. Murraya koenigii (curry leaves) powder was used to carbonize an iron-based precursor, forming a MBC-ZnO material. Comprehensive characterization using XRD, FT-IR, HR-TEM, FE-SEM, BET, XPS, MPMS, Mott-Schottky analysis, and UV–Vis DRS were performed to investigate the structural, morphological, surface, compositional, optical, and magnetic properties of the synthesized NCs. UV–Vis DRS revealed a reduced bandgap of 2.88 eV compared to 3.10 eV for pure ZnO, contributing to the enhanced photocatalytic performance. The MBC-ZnO NCs effectively degraded multiple dyes, including methylene blue (MB), methyl orange (MO), rhodamine B (RhB), and crystal violet (CV), achieving 88.17 % MB removal in 135 min and 92.45 % at pH 10 under optimized conditions. Their performance was further validated in pond and river water sample added with dyes, demonstrating efficiency in complex aqueous matrices.

Keywords: Nanocomposite (NCs), Magnetic biochar (MBC), Biochar (BC)

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One-Pot Access to Tetrasubstituted 2-Aminothiophenes via Regio- and Chemoselective Domino Reactions of Dithioesters with Fumaronitrile at Room Temperature

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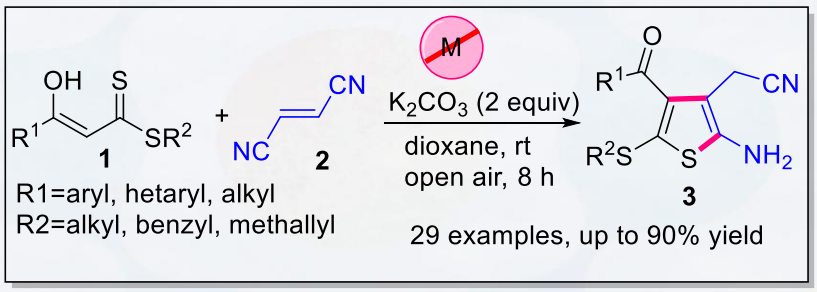
Abstract:

Herein, we report a one-pot viable protocol to synthesize tetrasubstituted 2-aminothiophenes engaging readily accessible α-enolic dithioesters and abundant fumaronitrile under transition metal-free conditions at room temperature in open air. The reaction proceeds via successive Michael-type addition/intramolecular cyclization/isomerization cascades. The added features are benign conditions, exclusive regio- and chemoselectivity, excellent atom-/step-economy, easy purification, and tolerance of wide range of functional groups of a diverse electronic and steric nature. This protocol not only provided a robust and modular approach to various 2-aminothiophenes in moderate to excellent yields, but also demonstrated the potential of dithioesters and fumaronitrile in the challenging intermolecular cross-coupling reactions widening the arsenal of synthetic methods.



Keywords: Michael-type addition; broad substrate scope; Metal-free; One-pot; 2-Aminothiophenes

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P-46

Strengthening Early Dengue Diagnosis Through Molecular Biomarker Development and Clinical Validation

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Abstract

Dengue virus (DENV) is an arboviral disease that is an alarming international health concern due to its rapid global spread. Dengue has four different serotypes (DENV-1 to DENV-4) and varies in severity from mild dengue fever to severe dengue haemorrhagic fever and dengue shock syndrome. The severity of the disease is influenced by viral type, the host's immune response to the virus, and secondary infections. Over 3.9 billion people in more than 130 countries are at risk of dengue, with the majority of cases occurring in tropical and subtropical regions. The WHO recommends serological and RT-PCR–based diagnostics for dengue; however, these methods are limited by reduced sensitivity during early infection and inadequate serotype differentiation. This study focuses on developing a universal detection strategy for dengue. Universal primers were designed using Primer3 based on conserved regions identified from 25 genomic sequences representing all four DENV serotypes, retrieved from the NCBI database and aligned using CodonCode Aligner. The validated assay demonstrated specific amplification in 100 clinical samples. This sensitive, serotype-independent approach enables early and accurate detection of DENV. This rapid and cost-effective diagnostic approach represents a significant advancement for improving disease management and outbreak response. This method holds significant value in health surveillance, supporting Sustainable Development Goal 3 by reducing infectious disease burden, improving health outcomes, and strengthening disease preparedness.

Keywords: Dengue, Biomarker, Serotype, Epidemiology.

P-47

Sustainable Advances in Nanomaterial-Enhanced Organic Rankine Cycle for Low-Grade Waste Heat Recovery

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ABSTRACT

Sustainable thermochemical energy conversion from low-grade waste heat sources represents a critical challenge in green chemistry and clean energy research. The Organic Rankine Cycle (ORC), offers an effective route for converting otherwise wasted thermal energy into useful. This study evaluates six conventional ORC modifications: ORC with internal heat exchanger (CYC1), regeneration (CYC2), reheating (CYC3), two turbines and internal heat exchanger (CYC4), regeneration with internal heat exchanger (CYC5), and internal heat exchanger with reheating (CYC6). All cycles are thermodynamically optimized using the Nelder-Mead method for low-grade waste heat sources operating over the 60–100 °C range. Isopentane (C_5H_{12}) was selected as the working fluid on the basis of its favourable molecular thermodynamic properties, ODP = 0, and global warming potential of only 5 (100-year horizon), establishing it as a chemically sustainable, naturally occurring alternative to phased-out synthetic hydrofluorocarbons. Results show that the basic ORC and CYC1 deliver the highest net work output (3.81 kW at 70 °C heat source temperature) and heat recovery efficiency (2.02%). CYC5, combining regeneration with an internal heat exchanger, achieves the highest thermal efficiency (4.78%), exergy efficiency (44.85%), and lowest total irreversibility (4.60 kW), demonstrating superior thermodynamic sustainability through entropy generation minimisation. Further limitations are minimized by integrating concepts from sustainable chemistry, particularly nanomaterials and catalysis. Nanomaterial-enhanced heat transfer fluids, nano-engineered surfaces, and catalytic interfaces are proposed to improve heat transfer, reduce entropy generation, and enhance overall system efficiency. A hybrid framework combining nanomaterial-enabled thermal energy storage with ORC is also proposed.

Keywords: Energy conversion; Organic Rankine Cycle; Exergy Efficiency; Waste heat recovery; Nanofluid enhancement; Cycle optimisation.

P-48

Cobalt-peptide based (Co-P) bionanozyme with catechol-like activity for chiral recognition

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Abstract

Enzymes are highly intricate catalytic entities that play vital roles in both biological systems and technological applications. However, their broader application in environmental contexts is limited due to factors such as high production expenses, limited stability under operational conditions, and complex recovery and reuse processes. As a result, the rational design of minimalistic biomolecular nanomaterials termed bio-nanozymes that can effectively replicate enzymatic functions while addressing these limitations has become a key objective in the field of biomolecular engineering. Here, we report a simple and highly active catechol enzyme mimicking cobalt-peptide (Co-P) bionanozyme comprising a dipeptide and a Cobalt atom, which converts 3,5-DTBC to 3,5-DTBQ and exhibits an absorption peak at 410 nm. Specifically, the elaboration of chiral Co-D arms results in higher catalytic selectivity over the chiral catechol substrate.

Keyword: Dipeptide, bionanozyme, Chiral, Enantioselective reaction

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P-49

Valorization of *Camellia sinensis* waste for recovery of bioactive phytocompounds and their antioxidant potential

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Abstract

The accumulation of brewed *Camellia sinensis* waste represents a significant underutilized biomass stream with considerable potential for the recovery of high-value bioactive compounds [1]. This study investigates a sustainable approach for the valorization of spent tea waste through solvent-based fractionation to isolate flavonoids, terpenoids, and caffeine. The extracted fractions were subjected to comprehensive phytochemical characterization using qualitative screening, Fourier-transform infrared spectroscopy (FTIR), and high-performance liquid chromatography (HPLC) [2]. FTIR analysis confirmed the presence of key functional groups associated with polyphenolic and terpenoid compounds, while HPLC profiling revealed a complex composition dominated by catechin derivatives, including catechin, epicatechin, and epigallocatechin gallate (EGCG), which are known for their strong biological activities [3]. Quantitative analysis indicated that the flavonoid fraction was the most abundant among the extracted phytochemicals, highlighting the significant retention of polyphenols in brewed tea residue. The antioxidant potential of the individual phytochemical fractions was evaluated using DPPH and ABTS radical scavenging assays. The flavonoid-rich extract exhibited the highest antioxidant activity (~50 – 52 % scavenging), followed by caffeine and terpenoid fractions, demonstrating the strong redox properties of polyphenolic compounds. The observed antioxidant performance is attributed to the presence of hydroxyl-rich catechins capable of hydrogen atom donation and free radical stabilization. Overall, the findings demonstrate that brewed tea waste remains a rich and viable source of bioactive phytochemicals with significant antioxidant potential. This study highlights the feasibility of transforming agro- tea waste into value-added functional ingredients, supporting sustainable resource utilization and circular bioeconomy principles.

Keywords: *Camellia sinensis* waste; waste valorization; phytochemical extraction; FTIR characterization; HPLC profiling; antioxidant activity

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P-50

Methanol Steam Reforming for Sustainable On-Site Hydrogen Production

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Abstract

Methanol steam reforming (MSR) is a critical technology in transition to carbon-neutral energy systems, providing a practical and affordable way to produce sustainable hydrogen. While hydrogen is accepted as a clean fuel, its widespread usage is hampered by issues with storage and transportation. The on-site generation of hydrogen can solve storage and transportation issues. Steam reforming of methanol (SRM) is considered a viable option for on-site generation of hydrogen due to its low reforming temperature and pressure. Further, it is easy to transport and safe to store. However, deasign or suitable catalyst and reactor is a major challenge fpor on-site generation of hydrogen and startup time and low CO selectivity are major challenge due to the poisoning of PEM fuel cell catalyst. Catalysts based on copper and noble metals, especially PdZn and Pt complexes, show significant catalytic activity. Cu, Fe, noble metals, etc., are the salient catalysts in SRM. The production of hydrogen and its selectivity are significantly influenced by the types of active sites, oxidation states, and metal-support interactions. In current work, advances in catalyst development is aimed to enhance catalytic activity, stability, and resistance to deactivation by utilising promoters, supports, and new materials such as metal-organic frameworks and perovskites. Ongoing research focused on optimising catalysts, understanding mechanisms, and improving system integration positions membrane steam reforming (MSR) as a promising option for clean, efficient, and on-demand hydrogen production.

P-51

Understanding the Behaviour of Knotted and Unknotted Proteins using all Atom MD Simulation

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Abstract:

Proteins containing topological knots exhibit unique structural stability and mechanical properties that influence their response to external perturbations such as temperature, pH, and electric fields. Nanopore sensing enables label-free, real-time single-molecule detection with high sensitivity to structural changes during protein folding and translocation. In this work, we are investigating the structural stability, unfolding behavior, and nanopore translocation dynamics of the YBEA protein using an all-atom MD simulation. The native YBEA protein contains a trefoil (3_1) knot in its backbone topology, which enhances its structural stability. To understand the role of this knot, an unknotted variant of the protein has been generated by removing the knot using PyMOL while maintaining the same amino acid sequence and overall structure. All simulations were performed using the GROMACS simulation package with a production run of 100 ns. Temperature-dependent simulations were performed for both the knotted and unknotted forms of YBEA to investigate thermal denaturation and compare their structural stabilities. The stability and conformational dynamics of the protein were analyzed using several structural parameters, including RMSD, RMSF, SASA, and Rg etc. With the help of temperature denaturation, it has been observed that knotted YBEA shows less deviation from the reference structure as compared to unknotted YBEA protein and as the temperature increases, the fluctuation in the respective proteins also increases. To further understand the influence of external forces on protein stability, electric-field-induced denaturation will be studied for both protein variants. Subsequently, the translocation behavior of the protein through a nanopore will be investigated to examine how the presence or absence of the trefoil knot affects the protein's stability and dynamics during nanopore passage.[1,2]

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P-52

Nitrate Electrosynthesis on Cation-Vacancy-Rich $FeSb_2O_4$ Microrods via Controlled Ammonia Dehydrogenation

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Abstract –

The growing demand for nitrogenous (NOx) products, particularly nitrate, necessitates the development of sustainable alternatives to the energy-intensive Ostwald process. Electrochemical ammonia oxidation (AOR) offers a promising route for nitrate synthesis; however, its practical application is limited by the lack of efficient and selective catalysts. Herein, we report $FeSb_2O_4$ as a highly selective catalyst for the conversion of ammonia to nitrate, achieving a Faradaic efficiency of 85% at a low potential of 0.8 V vs Hg/HgO. Electrolyte studies reveal that AOR conducted in Na_2SO_4 enhances nitrate selectivity compared to NaOH-containing systems. Temperature-dependent investigations (293–323 K) indicate a low activation energy of 19.52 kJ mol^{-1}, suggesting favorable reaction kinetics. Mechanistic insights obtained from in situ IR spectroscopy, RRDE experiments, and Koutecky–Levich analysis confirm a 6-electron transfer pathway with NO_2^- as a key intermediate. A kinetic isotope effect greater than 2 further indicates that proton abstraction from ammonia is the rate-determining step. This study demonstrates an efficient and selective catalytic system for sustainable nitrate synthesis and provides fundamental insights into the AOR mechanism.

P-53

Dual-Mode Fluorescent Sensors for Rapid Detection of Hydrogen Sulphide: Applications in Food Spoilage Monitoring

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Food safety is a major concern, with the WHO reporting 4,20,000 deaths every year due to the consumption of contaminated food[1]. Food spoilage is the major factor for this. Hence, there is a necessity for rapid detection methods. Hydrogen Sulphide is a key biomarker of food spoilage, and it also serves as a neurotransmitter[2]. Hence, we report the synthesis of a series of fluorescent sensors for detecting and quantifying sulphide. The developed sensors exhibit great selectivity over other sulphur-containing analytes. It exhibits dual-mode sensing via fluorescence via enhancement in fluorescence intensity under a UV lamp, and also distinct visible colour changes. We introduced structural variations by modifying the substituents, such as including an electron-donating group and a withdrawing group, into the sensors to see the effect on fluorescence. The sensors showed high sensitivity with low detection limits in the ppm range. These findings highlight the potential of the proposed systems for rapid, visual and real-time monitoring of food spoilage.

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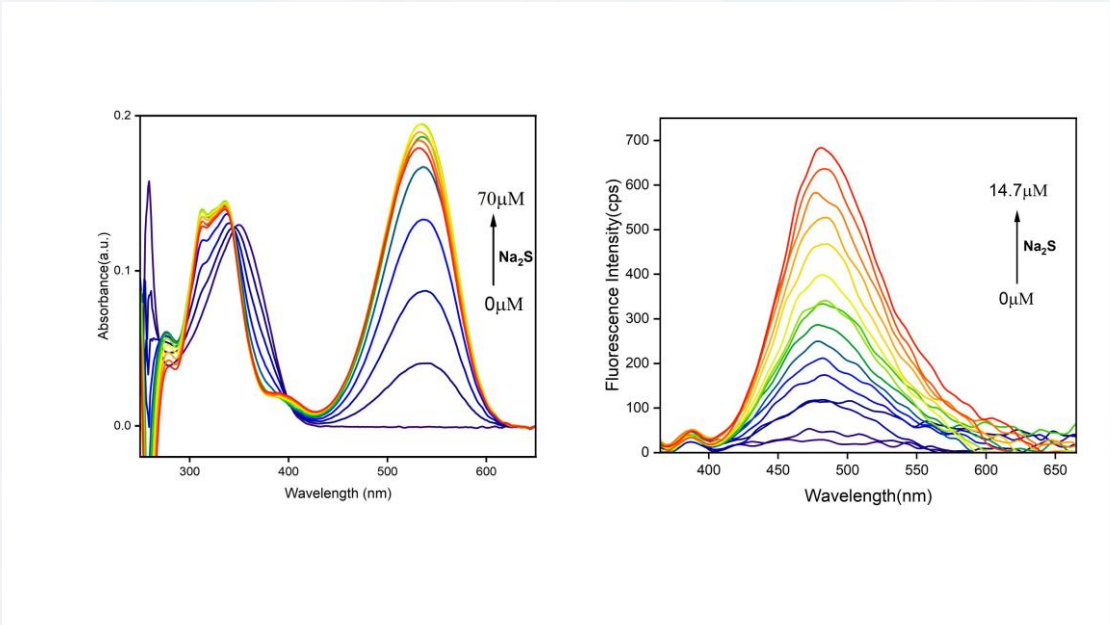

P-54

High Resolution Latent Fingerprinting by AIE-active Light Harvesting BODIHYs and pH-Induced Configurational Molecular Switching in Hydrazones

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Abstract

Latent fingerprint (LFP) detection is essential in criminal investigations, especially for identifying suspects. This study delves into the advancements in LFP imaging using artificial light–harvesting systems (ALHS). These systems demonstrate high energy transfer efficiency and the antenna effect of BODIHYs (**B1**–**B3**) when combined with Rhodamine 6G (R6G), which led to the generation of high resolution fluorescence images of LFPs, capturing details at levels 1–3 with great success. In these systems BODIHYs (**B1**–**B3**) serve as a donor while R6G as an acceptor. The BODIHYs were created from specific compounds: (*E*)-N'-(4-benzoylphenyl)picolinohydrazonoyl cyanide (**L1**), (*Z*)-N'-(4-benzoylphenyl)benzo[d]-thia-zole-2-carbohydrazonoyl cyanide (**L2**), and (*Z*)-ethyl 2-(benzo[d]thiazol-2-yl)-2-(2-(4-benz-oylphenyl)hydrazono)acetate (**L3**). The ligands and BODIHYs exhibit strong emission properties in solution, aggregate and solid states. Vital role of various interactions in aggregation induced emission (AIE; **L2** and **B1**–**B3**) and aggregation caused quenching (ACQ; **L1**) have been rationalized by X-ray single crystal analyses. Notably, the hydrazone **L3** contains a secondary hydrogen bond acceptor (–$COOC_2H_5$) and displays intramolecular hydrogen bonding, functioning as an effective molecular switch. Its ability to rapidly and reversibly transition between *E* and *Z* configurations under pH variations has been clearly demonstrated which has practical application in inkless writing.

P-55

Ultrasensitive detection of Uric acid via K-Intercalated MXene modified GCE

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Choice of mode- Poster

Abstract

For the selective determination of uric acid (UA) in biological fluids, a highly sensitive non-enzymatic electrochemical sensor was presented, which was based on potassium-intercalated titanium carbide (K-TC_{24}-4), a two-dimensional MXene (sareen et al. [1]). Potassium intercalation in MXene sheets enhances electrical conductivity and interlayer spacing, thereby improving surface adsorption, accelerating electron-transfer kinetics, and increasing sensing performance. The confirmation of structural and morphological features in K-TC_{24}-4 was done by XRD, XPS, FT-IR, FE-SEM, EDS and HR-TEM analyses. K-TC_{24}-4 was then applied to modify a glassy carbon electrode, enabling efficient UA oxidation at physiological pH (7). Ensuing experiments resulted in a low LOD of 382nM and LOQ of 1.27 µM, well below normal serum concentrations. The resultant sensor showed good stability, selectivity, and reproducibility.

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P-56

Fluorometric and Smartphone-Enabled Colorimetric RGB-Based Quantification of Au(III) Ions Using Fluorescein-Based Organic Compound

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Choice of mode- Poster

Abstract

A novel fluorescein-based, optically active chemosensor containing a 4-(Dimethylamino) cinnamaldehyde moiety is introduced, which can selectively identify Au^{3+} ions over other metal ions like Na^{+}, K^{+}, Ba^{2+}, Ca^{2+}, Hg^{2+}, Li^{+}, Cd^{2+}, Mn^{2+}, Mg^{2+}, Cu^{2+}, Pb^{2+}, Zn^{2+}, Co^{2+}, Ni^{2+}, Al^{3+}, Cr^{3+}, Fe^{2+}, Fe^{3+}, Pd^{2+} and Ag^{+}. The synthesized chemosensor exhibited aggregation-induced emission enhancement (AIEE) in a DMSO/Water medium. The sensing is performed using fluorometric, colorimetric and RGB methods. The degree of change in optical property varied linearly with Au^{3+} concentrations ranging from 0 – 13.15 µM, 0 - 9.9 µM and 0 – 13.15 µM with lower detection limits of 18.29 nM, 18.9 nM and 32.4 nM for fluorometric, colorimetric and RGB methods, respectively. The interactions of the chemosensor with Au^{3+} were revealed by Stern-Volmer plots, Job's plot, ^{1}H-NMR titrations, HR-MS and FT-IR. The proposed sensing assay successfully measured Au^{3+} ions in various water samples (tap, drinking, waste and river) with satisfactory precision and high recovery rates. FH-DMAC also provides a naked-eye qualitative analysis of Au^{3+} detection. Using a smartphone for RGB color analysis shortened the process, accelerated detection and introduced a more affordable method for real-time assessment of Au^{3+} levels in water samples.

P-57

Novel Ru(II)-Photo-antibiotics for Development of Infection-Resistant Mask Coatings

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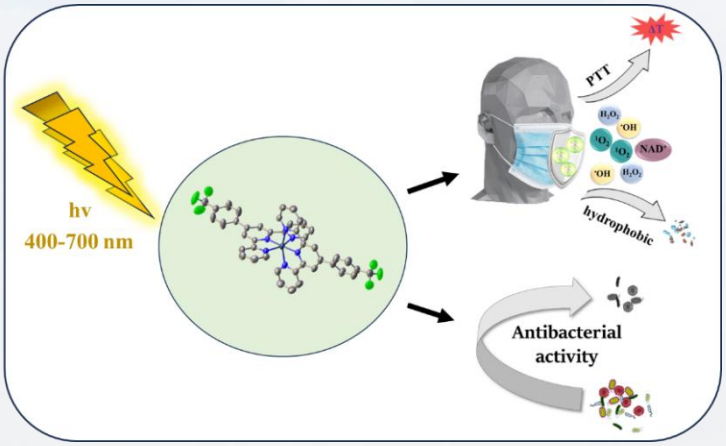
Abstract

Metal-based photoantibiotics can be a promising option for developing infection-resistant mask coatings, but this area has not yet been explored. To address this gap, we designed and developed a series of four visible light-activated Ru(II) photo-antibiotics $[Ru(CH_3\text{-Phtpy})_2](PF_6)_2$ (**Ru1**), $[Ru(NMe_2\text{-Phtpy})_2](PF_6)_2$ (**Ru2**), $[Ru(OH\text{-Phtpy})_2](PF_6)_2$ (**Ru3**) and $[Ru(CF_3\text{-Phtpy})_2](PF_6)_2$ (**Ru4**) (where CH_3-Phtpy = 4-(p-tolyl)-2,2′:6′,2″-terpyridine, NMe_2-Phtpy = 4-([2,2′:6′,2″-terpyridin]-4′-yl)-N,N-dimethylaniline, OH-Phtpy = 4-([2,2':6',2"-terpyridin]-4'-yl)phenol and CF_3-Phtpy = 4′-(4-trifluoromethylphenyl)-2,2’:6′,2″-terpyridine).[1] The complexes showed strong absorption in the 450-600 nm range due to MLCT, making them suitable for aPDT. Upon light exposure (400-700nm, 10 J cm^{-2}), **Ru1-Ru4** generated $^1O_2$ (quantum yield: 0.09-0.15) in PBS:DMSO (99:1 v/v, pH = 7.0) solution. **Ru2** efficiently oxidized NADH (TOF: *ca*. 41 h^{-1}) under light exposure, disrupting the NADH/NAD^+ balance. Upon light exposure, **Ru2** showed a Zone of Inhibition (0.60 cm) against E. coli, while its Minimum inhibitory concentration (MIC) values were as low as 0.05 µg/mL against S. aureus and 0.06 µg/mL against *E. coli*. **Ru2** showed significant bacterial reduction under light, with CFU decreasing to 1.2×10^6 (*E. coli*) and 4×10^5 (*S. aureus*).[1] Light-induced increase in contact angle (~131°) confirmed enhanced surface hydrophobicity, enabling self-cleaning and reduced bacterial adhesion.[1] Overall, these photoantibiotics exhibit potent antibacterial activity through combined oxidative stress induction and photothermal effects, and their surface hydrophobicity can be adjusted.

Figure: Schematic representation of a Visible-light activated Ru(II) complex for photodynamic antibacterial and self-sterilizing applications.



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P-58

Fluorescence Probes for On-Site Biogenic Amine Sensing: A Biomarker of Food Freshness

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Choice of mode – Poster

Abstract

One crucial area of research is the development and production of sensor probes to evaluate food quality and freshness. A rise in biogenic amine content is a sign of food deterioration and endangers food safety. Millions of individuals suffer from foodborne illnesses and food poisoning each year so it is necessary to evaluate the freshness and quality of food by measuring the concentration of biogenic amines. Conventional analytical techniques, including HPLC (Plakidi et al., 2020), GC-MS (Cunha et al., 2011), TLC (Lapa-guimarães & Pickova, 2004), cation exchange chromatography (Palermo et al., 2013), capillary electrophoresis (Sun et al., 2003) and enzyme-based biosensors (Corduneanu et al.)(Corduneanu et al., 2010) offer high accuracy but require sophisticated instrumentation, labour-intensive sample preparation, and skilled personnel, limiting their suitability for rapid or on-site applications. As a result, there is a need for the creation of a rapid, portable, and sensitive sensor for sensing biogenic amines in foodstuffs and biological materials. Fluorescence-based sensing has emerged as a powerful approach for measuring biogenic amines. This discussions focuses on reactivity-based small-molecule chemosensors and their metal complexes, discussing their design, synthesis, properties, and on-site detection capabilities, while outlining sensing mechanisms and broader applications in biogenic amine analysis. Because of its importance, this will be of significant interest to scientists working in related fields.

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P-59

Enantioselective [4+2] Annulation Reaction of C1-Ammonium Enolate and Azadiene for 3,4-Dihydroquinolinones Synthesis

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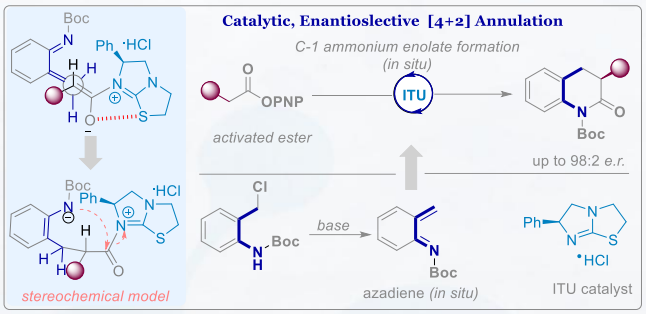

Abstract

Organic transformations mediated by the transient C1-ammonium enolate have demonstrated remarkable synthetic potential for the synthesis of enantioenriched three-dimensional molecules. Despite their importance in nature, enantioenriched 3,4-dihydroquinolinones and tetrahydroquinolines are rarely found in commercial small-molecule drugs, mainly due to the lack of efficient synthesis methods. Here, we describe a practical and mechanistically intriguing enantioselective synthesis of dihydroquinolinones through an asymmetric [4+2] annulation process utilizing an activated ester-derived transient C1-ammonium enolate and azadiene intermediates. Additionally, dihydroquinolinones may be further transformed into tetrahydroquinoline, dihydrothioquinolinones pharmacophores, and δ-amino ester building blocks through post-modification techniques. The method is practical and scalable, eliminates the use of transition metals or expensive catalysts, and provides the opportunity to access a variety of α-arylated enantioenriched dihydroquinolone and tetrahydroquinoline products with a variety of electronically diverse substituents.

Keywords: C1-Ammonium Enolate • Isothiourea organocatalysts • Enantiopure 3,4-dihydroquinolinones• [4+2] Annulation • Azadiene

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P-60

Screening of Surface-Active Microbial Strains Utilizing Hydrocarbon Substrates.

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Abstract

In the present study, samples were collected from the coastal mangrove ecosystems of Bhavnagar, Gujarat, characterized by extreme salinity and nutrient-rich conditions. Microbial isolation was performed, facilitating the isolation of both bacterial and fungal strains. These isolates were enriched in Mineral Salt Medium (MSM) supplemented with 1% crude oil as the sole carbon source, resulting in five promising bacterial strains designated as BHVBRW1, BHVBRW2, BHVBRW3, BHVBRW4, and BHVBRW5 further centrifugation was followed to obtain cell-free supernatant for biosurfactant screening, which reveals significant activity in oil displacement strong positive (++) activity in BHVBRW3, moderate (+) activity in BHVBRW4 and BHVBRW2, weak (-) activity in BHVBRW5, while BHVBRW1 showed comparatively lower response. Oil spreading assay demonstrated positive results in BHVBRW1, BHVBRW3, and BHVBRW4, whereas BHVBRW5 showed negative activity. The emulsification index (E24) was highest in BHVBRW3 (61.67%), followed by BHVBRW4 (46.67%) and BHVBRW1 (31.67%). BHVBRW3 exhibited a beta zone of hemolysis in blood hemolysis test, whereas BHVBRW4 and BHVBRW2 showed alpha zone of hydrolysis. On the Basis of Primary screening the Secondary screening test were performed using Lipase agar confirmed strong lipopeptide production in BHVBRW3, and biochemical assays including phosphate solubilization, Biuret, and phenol–sulfuric acid tests validated associated biomolecule production. Fungal isolates showing positive screening results were further characterized, with *Aspergillus* species identified through molecular analysis. Additionally, DCPIP assay demonstrated efficient hydrocarbon degradation by BHVBRW3. Overall, this study highlights the mangrove ecosystems of Bhavnagar as rich reservoirs of biosurfactant-producing and hydrocarbon-degrading microorganisms, with BHVBRW3 emerging as a promising candidate for bioremediation and sustainable environmental applications.

Keywords: Biosurfactant, Mangrove Microbiome, Crude oil degradation, E24 index, CTAB assay, DCPIP assay, Environmental Bioremediation

P-61

Evaluation of Tyrosine Kinase Inhibitors as a potential PPAR-γ modulator for the treatment of Type 2 Diabetes Mellitus using *in-silico* approach

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Background: Insulin resistance plays a central pathogenic factor in the progression of Type 2 Diabetes Mellitus. Peroxisome proliferator-activated receptor gamma (PPAR-γ) has been therapeutically targeted to enhance insulin sensitivity. However, its clinical application was discontinued owing to adverse effects. Emerging evidence indicates that tyrosine kinase inhibitors (TKIs) may interact with PPAR-γ receptors and modulate glucose homeostasis.

Objective: This study was designed to investigate the role of TKIs as a potential target of the PPAR-γ receptor through an integrated *in-silico* approach.

Methods: The Asinex library of Tyrosine kinase Inhibitors was downloaded, and virtual screening was performed to identify potential selective agonists of PPAR-γ, and compounds exhibiting higher binding affinities using AutoDock Vina 1.1.2 were shortlisted for ADMET (SwissADME and ProTox-II) and Molecular Dynamics simulation (GROMACS).

Results: nTZDpa and pioglitazone were used as reference compounds, showing binding affinities of -10.9 kcal/mol and -9.8 kcal/mol, respectively, against the A subunit of the PPAR-γ. In comparison, many promising molecules demonstrated significantly higher binding affinities, ranging from 13.1 kcal/mol to -11.0 kcal/mol. The stability of the interaction of TKIs and the PPAR-γ ligand binding site residues predicted by docking experiments was further assessed by molecular simulation studies.

Conclusion: In conclusion, our docking studies identified multiple derivatives with higher binding affinities compared to known full and partial agonists, including pioglitazone and nTZDpa. These compounds demonstrated strong interactions within the active site of a PPAR-γ, suggesting their potential as an effective activator.

Keywords: Type 2 Diabetes Mellitus, Insulin Resistance, PPAR-γ, Tyrosine Kinase Inhibitors and *in-silico*

P-62

Metal–Organic Framework (HKUST-1) as a Novel SERS-Active Substrate

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A copper-based metal–organic framework, HKUST-1 ($Cu_3(BTC)_2$), was synthesized via a solvothermal method and explored for the first time as an intrinsic Surface-Enhanced Raman Scattering (SERS) substrate without any external plasmonic metal decoration. This is the first report demonstrating pristine HKUST-1 as an active SERS platform for the detection of Methylene Blue (MB). The porous crystalline architecture and coordinatively unsaturated Cu(II) centers and π-conjugated BTC linkers of HKUST-1 facilitated strong analyte adsorption and efficient charge-transfer interactions, leading to significant Raman signal enhancement. The SERS spectra of MB revealed characteristic peaks, 1625 cm^{-1}, attributed to aromatic C–C stretching, 1398 cm^{-1}, corresponding to in-plane ring deformation coupled with C–N stretching, and 448 cm^{-1}, assigned to C–N–C skeletal deformation modes. These findings demonstrate that pristine HKUST-1 can act as a SERS-active substrate.

Keywords: HKUST, SERS, Methylene blue

P-63

Isolation and purification of phycocyanin from Nostochapsis lobatus HKAR-21

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Abstract:

The photosynthetic apparatus of cyanobacteria comprises light–harvesting antenna complex called phycobilisomes, consisting of different types of phycobiliprotein (PC, APC and PE). Phycocyanin (PC), a prominent blue -colored accessory photosynthetic protein-pigment complex found in cyanobacteria, has garnered significant attention due to its diverse biotechnological applications, including its reported anticancer and anti-inflammatory properties. The commercial viability of phycocyanin is heavily dependent on its purity and stability, necessitating efficient extraction and purification methods to maximise its utility. Our goals here are to extract the phycocyanin from cyanobacteria and reconstitute them in the liposomes. The extraction process generally involves cell wall disruption (sonication and freezing - thawing), removal of water -soluble colouring protein, and concentration and purification steps. We are exploring various methods for phycocyanin purification, which often involves ammonium sulphate precipitation, dialysis and sucrose density gradient to achieve an initial purity index, followed by advanced chromatography techniques. We found a UV absorption peak at 620 nm in the purified phycocyanin. A distinctive peak of fluorescence emission at 645 nm and excitation at 620 nm shows the functionality and stability of the phycocyanin protein structure. The ability to scavenge DPPH free radicals was used to assess free radical scavenging. Phycocyanin demonstrated dose-dependent antioxidative capabilities against free radicals. Because the phycobilisome is very luminous, it can be encapsulated in liposomes alongwith phycocyanin, for further characterisation using UV, fluorescence spectra, TEM and DLS.

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P-64

Synthesis, X-ray crystal structures and DFT calculations of Ru(II) complexes of dioxime, diimine and oxime-imine ligands derived from 2,6-diacetyl pyridine

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Presenting Author – Sumita Hazra (DOB – 06/09/1982)

Reaction of 2,6-diacetyl pyridine dioxime (dapdOH) with five different ruthenium precursors produced three different types of complexes of ruthenium: dioxime, diimine and mixed oxime-imine. $RuCl_3$ and Ru(terpy)Cl_3 form oxime complexes- **$[Ru(dapdOH_2)_2]Cl(PF_6)\cdot 2H_2O$** (**$1\cdot 2H_2O$**) and **$[Ru(terpy)(dapdOH_2)](PF_6)_2$** (**2**); Ru(bpy)$Cl_3$ and Ru(phen)Cl_3 produce imine complexes- **$[Ru(bpy)(dapdNH_2)Cl](PF_6).0.5H_2O$** (**$3\cdot 0.5H_2O$**), **$Ru(phen)(dapdNH_2)Cl](PF_6)\cdot H_2O\cdot 0.5C_2H_5OH$** (**$4\cdot H_2O\cdot 0.5C_2H_5OH$**) and $Ru(PPh_3)_3Cl_2$ forms the mixed oxime-imine complex- **$[Ru(PPh_3)_2$(dapOH-NH)$Cl](PF_6)$** (**5**) respectively. All the complexes were characterized by stansard spectroscopic techniques. Single crystal X-ray diffraction studies were performed on four complexes: **$1\cdot 2H_2O$, $3\cdot 0.5H_2O$, $4\cdot H_2O\cdot 0.5$ EtOH and 5**. Long iminomethyl (C=N) bond and correspondingly short C_{ipso}–C_{imine} bond in all the complexes indicate appreciable π-back bonding from Ru(II) to the π*-orbital of the imine moiety[1,2], which is supported by DFT calculations on **3** and **4**. In cyclic voltammetry Ru(II/III) oxidations are observed for all the complexes, whereas Ru(III/IV) oxidations has been assigned for complex **1**, **2**, **3** and **4**. Both the Ru(II/III) and Ru(III/IV) potential are highest for the di-oxime complex **1**. In the electronic spectra for all the complexes an MLCT band appears in the range 400-480 nm. DFT and TD-DFT calculations were performed on complexes **3** and **4** to understand the electronic structures and electronic spectra of the relatively rare diimine complexes.

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P-65

A Synthetic Antibiotic Class Targets Bacteria with a Two-Pronged Approach

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Antimicrobial resistance (AMR) has become one of the most pressing global public health challenges, underscoring the urgent need for novel antibiotics acting through distinct mechanisms.[1] The bacterial cell wall remains an attractive target as it is conserved throughout the bacterial species. Its biosynthesis relies on lipid pyrophosphates, that translocate the peptidoglycan precursors across the membrane.[2,3] Recently discovered natural antibiotics that target these lipid pyrophosphates remain limited by their structural complexity, poor stability, and costly production.[4-6] These scaffolds possess cationic macrocyclic and lipophilic features, enabling effective interaction with bacterial membranes and pyrophosphates. Guided by these principles, we designed a novel class of synthetic molecules featuring organic metallophores that are known for their strong affinity to pyrophosphates and a hydrophobic moiety.[7] A structure-activity relationship (SAR) optimization yielded a lead compound with potent activity against a broad spectrum of Gram-positive pathogens, including multidrug-resistant clinical isolates. While ineffective against Gram-negative bacteria due to membrane impermeability, co-administration with colistin or polymyxin B nonapeptide (PMBN) restored their activity. Lead compounds displayed low cytotoxicity, and no hemolysis up to 512 µg/mL. Leads also exhibited reduced resistance development and demonstrated robust antibiofilm activity. Mechanistic studies revealed a dual mode of action that are binding to lipid pyrophosphates and perturbing bacterial membrane. Notably, treatment with the compounds in a murine skin infection model resulted in a significant reduction in bacterial burden, demonstrating *in vivo* therapeutic potential. Altogether, this study introduces a promising new class of dual-targeting antimicrobial compounds that hold potential for treating multidrug-resistant infections.

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P-66

Elucidating the Synergistic Mechanisms of Pyocyanin and Vitamin C Formulations in Modulating Hyperpigmentation

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ABSTRACT

Hyperpigmentary disorders arise from dysregulated melanogenesis, primarily driven by tyrosinase activity, and remain a major dermatological concern. Developing effective and sustainable therapeutic strategies requires a deeper understanding of molecular interactions and the combinatorial effects of bioactive compounds [1,2]. In this study, we investigated the synergistic potential of vitamin C and pyocyanin formulations using an *in silico* and *in vitro* approach. Molecular docking studies were performed to evaluate the binding of vitamin C, pyocyanin, and their multi-ligand complex with human and mushroom tyrosinase. The combination exhibited enhanced binding affinity compared to individual ligands, suggesting cooperative interaction at the catalytic site. Density Functional Theory (DFT)-based geometric optimization further supported the stability and electronic compatibility of the combined formulation. ADMET profiling indicated favorable pharmacokinetic and safety properties, supporting its translational potential. *In vitro* validation using SK-MEL-1 melanocytes demonstrated dose-dependent cytocompatibility. Reactive oxygen species (ROS) analysis using DCFDA staining revealed that the combination effectively modulates oxidative stress, indicating a potential ROS-scavenging mechanism. Additionally, the cell-free anti-tyrosinase assay confirmed that the combined formulation exhibited enhanced inhibitory activity. Collectively, these findings demonstrate a synergistic interaction between vitamin C and pyocyanin in modulating melanogenesis via dual mechanisms: tyrosinase inhibition and regulation of oxidative stress. This study highlights the potential of combinatorial and biomolecule-based strategies as sustainable therapeutic approaches for hyperpigmentary disorders.

Keywords: Hyperpigmentation, Pyocyanin, Vitamin C, Melanogenesis.

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P-67

Electro-Catalysed Direct C-H Chalcogenation of Indolizine Frameworks

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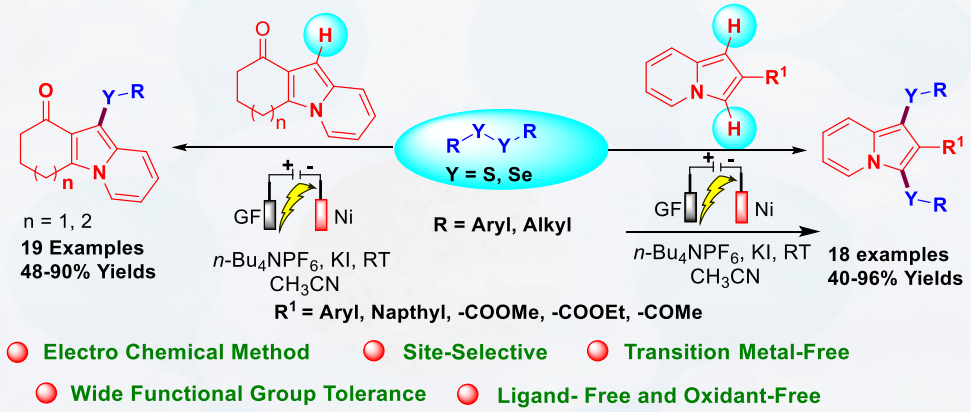
Abstract:

In recent years, the synthetic chemists who are regularly pursuit the green chemistry have promoted the use of electro-organic technique for the synthesis of value-added molecules.[1] Electrochemical synthesis is powerful and greener approach for direct chalcogenation of various chemical entities by obviating the use of stoichiometric amount of oxidants, catalysts, and ligands. In sharp contrast, we expand our research program on sustainable electrochemical synthesis of value-added molecules,[2] and recently developed first transition-metal-free, regio-selective direct C-H mono and bis-chalcogenation protocol for indolizine scaffolds using disulfides or diselenides as reaction partner via electro-organic synthetic strategy under catalyst-free conditions.[3]



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P-68

Superadsorbents: Wonderful Materials for Water Remediation

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Abstract

Water pollution from toxic contaminants, such as heavy metals, dyes, and inorganic ions, is a major environmental concern that requires efficient, sustainable treatment solutions. Superadsorbents have emerged as promising materials for wastewater remediation. Superadsorbents are especially important as they have been reported to offer excellent adsorption capacity. The adsorption capacities reported for the removal of hazardous dyes, such as methylene blue, Congo red, and crystal violet, were 2100mg/g[1] (Xiao-Sai Hu et al.). 2000mg/g[2] (Chao Liang et al.) and 1500mg/g[3] (Fakhreddine Ben Amara et al.). respectively. A biodegradable biopolymer-based superadsorbent composite was synthesised using chemical crosslinking and/or grafting techniques to enhance porosity, mechanical strength, and adsorption efficiency. The developed material exhibits excellent swelling behaviour and a strong affinity for various pollutants, owing to functional groups such as hydroxyl and amino groups. The composite was characterised using FTIR, XRD, SEM, and zeta potential analysis to evaluate its structural and surface properties. Adsorption studies revealed rapid and efficient removal of contaminants, as indicated by suitable isotherm and kinetic models. Overall, this work demonstrates that biobased superadsorbents are sustainable, cost-effective, and high-performance materials with significant potential for large-scale water remediation applications.

KEYWORDS: - Superadsorbents, Adsorption, Hazardous dyes, Bioadsorbent

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P-69

Unlocking the Potential of Biogenic Carbon Dots (CDs) as nano-carriers for enhanced drug delivery against breast cancer cells

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ABSTRACT

Nanotechnology, with special focus on carbon dots (CDs), has gained major attention in the field of therapeutics. Plant-derived carbon sources have emerged as promising substrates for the synthesis of biogenic CDs, offering sustainable, cost-effective, and eco-friendly alternatives to conventional carbon materials [1]. Research demonstrated the utilization of plants for the fabrication of sustainable CD synthesis [2]. Global research data show that breast cancer is a leading cancer, with metastasis being the major reason for huge deaths in women globally [3]. Since the treatment of metastatic cancer poses significant challenges like ineffective drug delivery [4], our research work aims to harness the anticancer properties of drug-conjugated biogenic CDs to abrogate breast cancer metastasis. This study included the synthesis of novel biogenic CDs and coating them with BSA. Both the CDs were characterized via techniques like DLS, UV-Spectroscopy, and FTIR, and were conjugated with less explored ion channel inhibitors (ICI). Drug release kinetics was performed, and the ICI-bCDs were examined in vitro for breast cancer cell lines like SUM-159 and MDA-MB-231 to check the effect on metastasis. The cytotoxicity was also determined on RPE1 (normal human cells). The molecular mechanism study of such anti-metastatic effect (if any) will be studied using CRISPR technology. Thus, integration of plant-derived CDs and repurposing less effective anti-cancer drugs can pave the path towards combating metastasis and improving healthcare outcomes in the future.

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P-70

Synthesis and Evaluation of Axially Modified Mn(I)-Tricarbonyl Complexes for Sonodynamic Cancer Therapy

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Carbon monoxide (CO) gas therapy is an emerging cancer treatment that delivers CO directly to tumor sites, inducing cytotoxic effects[1,2]. As an oxygen-independent approach, it is particularly effective against hypoxic tumor, where traditional photodynamic therapy (PDT) fails due to limited tissue penetration of light[1,2]. In contrast, ultrasound (US) offers deeper penetration (>10 cm), making it suitable for such conditions[1-3]. Therefore, a synergistic sonodynamic–CO gas releasing strategy represents a promising and innovative approach for treating hypoxic tumors. Here we have synthesized and characterized two Mn(I)complexes, *viz*., [Mn(Bphen)$(CO)_3$Br] (**Mn1**), [Mn(Bphen)$(CO)_3$X] (**Mn2**) (where, Bphen = 4,7-diphenyl-1,10-phenanthroline, X = 1,4-di(pyridin-4-yl) benzene). The X-ray structure of **Mn1** confirmed its distorted octahedral geometry. Under US irradiation, both complexes released CO (using the IR method & the Myoglobin method), generated singlet oxygen ($^1O_2$) (using the DPBF probe) as a reactive oxygen species (ROS) with quantum yield (Φ_{1O2}) values of 0.17 and 0.21, respectively. Among the two, the axially substituted **Mn2** was the most potent, showing a US-induced IC_{50} of *ca.*, 3.0 µM against HCT-116 cells, while **Mn1** displayed a higher US-triggered IC_{50} of around 10 µM. **Mn2** also demonstrated minimal dark toxicity and good selectivity toward cancer cells with the ultrasound toxicity index (UI) *ca.*, 6.7 for **Mn2** (UI = 6.7). Mechanistic studies confirmed ROS-mediated apoptosis via mitochondrial disruption and caspase activation, highlighting **Mn2** as a promising sonosensitizer. Overall, strong ROS-generating capability combined with the rapid CO releasing ability of **Mn2** might provide a bio-compatible anticancer SDT agent with a dual mode of action for hypoxic anticancer treatment.

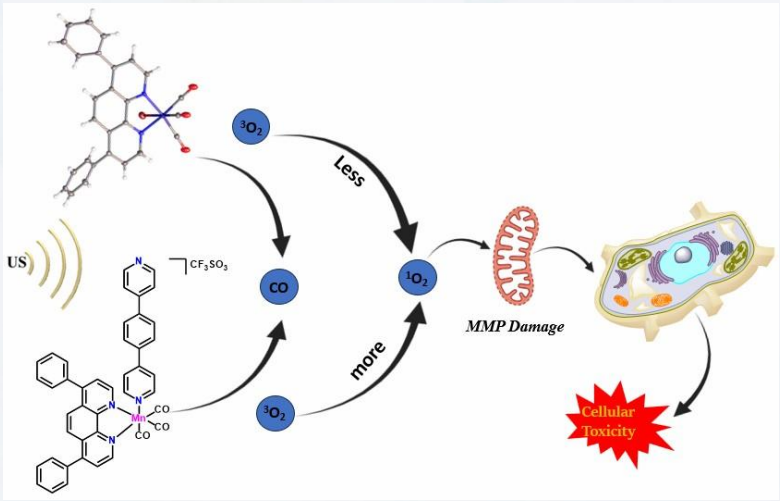

Figure: Schematic representation of Sonodynamic cancer therapy of Mn(I) tricarbonyl complexes

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P-71

Visible light photocatalytic ammonia production on single Cu entities attached to nitrogen-deficient functionalized BN sheets

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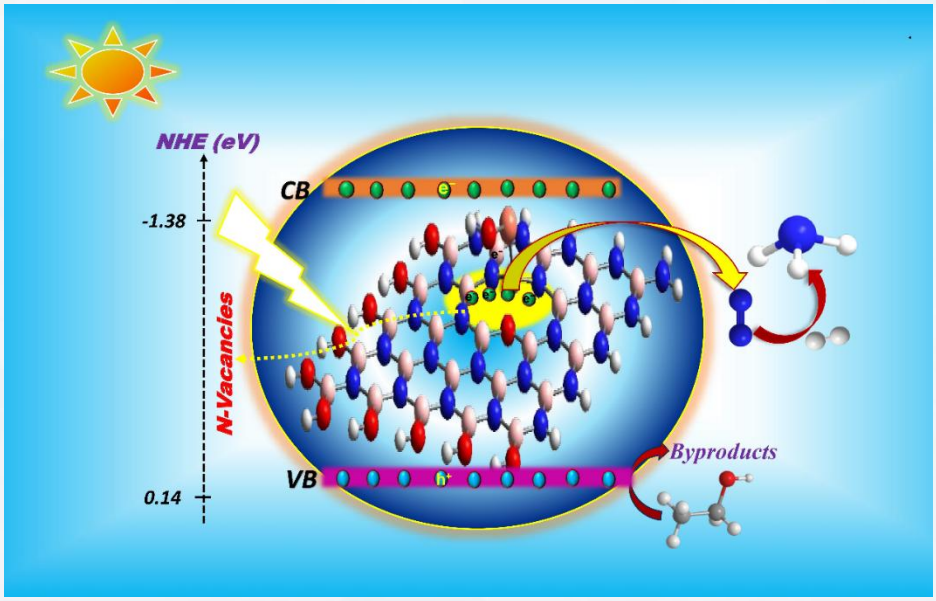
The present research involves the fabrication of a nitrogen-deficient functionalized BN material with isolated Cu–OH groups tethered to it. This material exhibits a visible-range indirect band gap (1.52 eV) with its conduction band position conducive to the 2-electron reduction of nitrogen to the N_2H_2 species. Overall, the nitrogen-deficient BN sheet with isolated Cu–OH entities exhibits enhanced visible light nitrogen reduction reaction (NRR) activity compared to many single-atom photocatalysts. Parallel to this, density functional theory (DFT) calculations are conducted to elucidate the interaction enhancement between nitrogen and the nitrogen-deficient BN sheet. Furthermore, it also points to photocatalytic charge transfer to N_2 through the Cu anchored to the nitrogen-deficient BN framework. Overall, this work highlights the potential of nitrogen-deficient BN systems as templates for novel single transition-metal-atom photocatalysts and their promise for efficient and sustainable ammonia production under ambient conditions.



Glass Formation Modulates the Charge Transfer Properties in CoFe-Prussian Blue Analog

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Abstract:

Prussian blue and its analogs (PB/PBA), a well-known coordination polymer, show metal-to-metal charge transfer (MMCT), modulating their electronic properties.[1,2] PB/PBA crystallizes in a cubic close-packed (ccp) or hexagonal close-packed system where the metal centers are interconnected through cyanide bridges.[3] The crystal structure of the PBA has a significant effect on the MMCT properties and hence the inter-metal electronic interaction.[1] Herein, we have transformed the crystalline (ccp) Co-Fe PBA into its glassy state by applying mechanical forces and evaluated the effect of glass formation on the overall charge transfer properties (MMCT and MLCT).[4] This leads to a significant change in the long-range order, but maintaining the short-range Fe-CN-Co connectivity.[5] Further, the structural evolution leads to a variation in the electronic distribution around the metal centers and a change in the Co/Fe-C, Co/Fe-N, Co-Fe bond distances (with a shortening of the Co-Fe bond compared to the crystalline analog), and cyanide vacancy. As a result, the glassy CoFe-PBA's redox behaviour is also different from its crystalline analog.

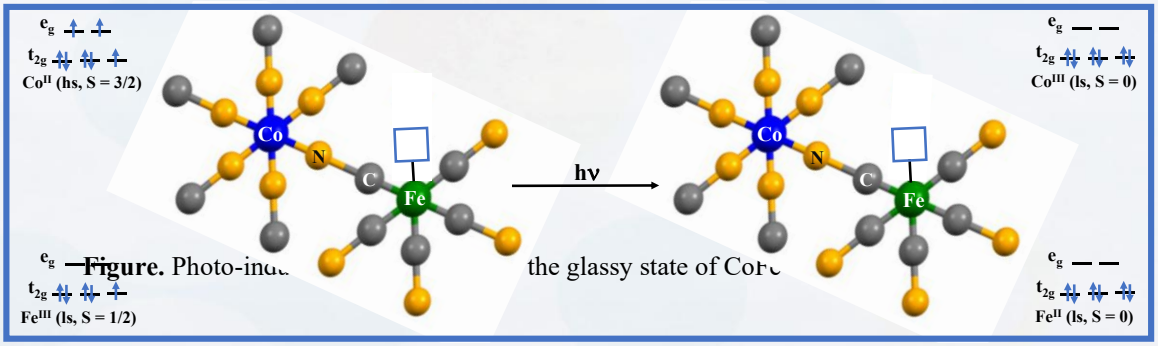

Figure. Photo-ind… the glassy state of CoFe

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P-73

Cyanide vs. Isocyanide Coordination of Fe in Cyanide-Bridged Polymers Modulates Structural Evolution to Active Water Oxidation Catalysts

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Abstract:

The chemistry of cyanate and isocyanate has been extensively studied in organometallic chemistry over the past decades. Notably, in the cyanide-bridged coordination polymer, the coordination behaviour of Fe in these two systems differs significantly, which directly influences their reactivity and catalytic properties in various chemical reactions.[1] Inspired by these findings, we applied the concept of different coordination modes in our work.[1-2] Here, we explored cyanide-bridged coordination polymers, Fe–NC–Ni–CP (CP = coordination polymer) and Ni–NC–Fe–CP, as precatalysts.[3] The distinct coordination environments in these two systems resulted in markedly different electrochemical activities, highlighting the critical role of coordination geometry in dictating catalytic performance.[3-4] The anodic activation of both forms Fe-Ni$(O)_x(OH)y$ as the active catalysts, having the same crystal phase but a wide variation in the local atomic and electronic structure. The XPS, EPR, and XAS studies showed the presence of $Ni^{2+/3+}$ and a mixture of low- and high-spin Fe^{3+} in the active catalysts.

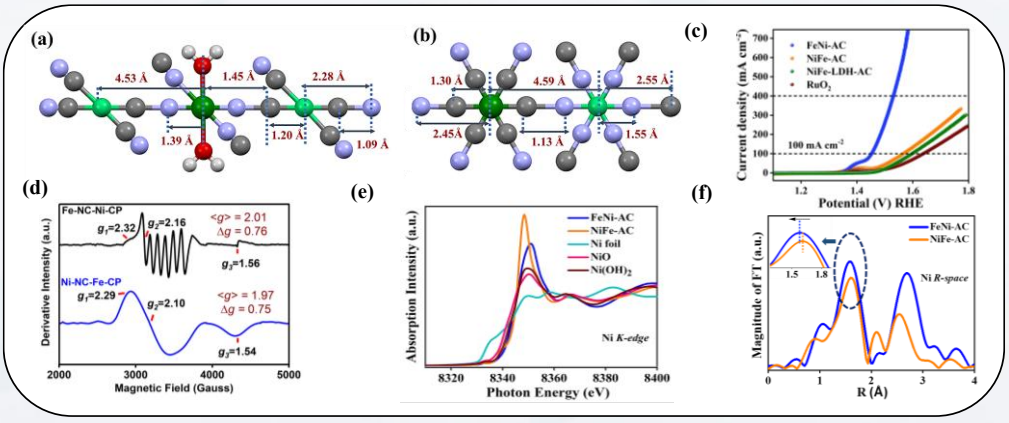

Figure. Coordination-Driven Structural Evolution and Oxidation State Modulation from Pre-Catalyst to Active Phase in Fe–NC–Ni–CP and Ni–NC–Fe–CP during OER.

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P-74

Streptococcal Surfaceome-Host Interactions Drive Adhesion, Invasion, and Divergent Inflammatory-Apoptotic Signaling in Oral Cancer Cells

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ABSTRACT

The oral microbiome plays a critical role in modulating tumor behavior in oral squamous cell carcinoma (OSCC), yet the molecular mechanisms by which individual microbial species influence cancer cell fate remain poorly understood [1]. *Streptococcus* species dominate the oral microbiota and express diverse surface-associated proteins that interact with host immune and death receptors [2]. In this study, we combined structural modeling, molecular docking, molecular dynamics simulations, and *in vitro* validation to investigate how pathogenic and commensal streptococci differentially influence oral cancer progression. Surface proteins from *Streptococcus mutans* and *Streptococcus oralis* were modeled and docked with host receptors, revealing strong interactions between *S. mutans* Antigen I/II and TLR2 (-14.7 kcal/mol) and between *S. oralis* penicillin-binding protein 1a and CD95 (-12.6 kcal/mol), which were further validated by molecular dynamics simulations. Functional assays in CAL27 cells demonstrated that *S. mutans* significantly enhances bacterial adhesion and invasion, induces necrotic responses, and triggers a ~7-fold increase in IL-6 secretion ($p < 0.01$), indicating a pro-inflammatory phenotype. In contrast, *S. oralis* exhibited reduced invasiveness but promoted reactive oxygen species accumulation, apoptosis, cell cycle alterations, and delayed cell migration, along with modulation of TGF-β1 levels. These findings reveal a commensal-pathogen dichotomy in streptococcal surfaceome interactions that governs adhesion, invasion, and divergent inflammatory versus apoptotic signaling in oral cancer. This study highlights microbial-host receptor interfaces as potential targets for microbiome-informed and sustainable theranostic strategies in oral cancer.

Keywords: *Streptococcus*, Oral Cancer, Dysbiosis, Surfaceome Interactions.

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P-75

Essential Oil–Loaded Core–Shell Nanofibermats with Antimicrobial Characteristic for Wound-healing Patches Application

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Abstract

Plant-derived essential oils and extracts have drawn a major attention Because of their inherent antibacterial, antioxidant, and fragrant qualities and are useful in biomedical materials, perfumery, and sustainable functional fabrics. In order to create multipurpose bioactive materials, essential oil-loaded nanofibrous mats were fabricated using the electrospinning technique. Electrospinning enables the production of ultrafine fibers with tunable porosity, high surface area and structural similarity to extracellular matrices, making them appropriate for use in biomedical applications. Polymer-1(name of the polymer) and Polymer-2(name of the polymer) are used as the supporting matrices to fabricate core-shell nanofiber morphology. The essential oil-based active chemical was incorporated into the fiber structure as core. The coaxial electrospinning setup is used for fabrication of matrix, wherein the polymer solution incorporated with the active molecules was introduced as the core, while the second polymer acted as the shell layer. Therefore a regulated encapsulation and sustainable release of the plant-derived bioactive molecule in the electrospun fiber assembly would be made possible by this arrangement, with increased fiber stability. The resultant nanofibrous mats exhibited uniform morphology and improved plant extracted essential oil loading efficiency. Thus fabricated electrospun fiber mats will be subjected to antimicrobial tests, followed by subjecting them for wound-healing patch application.

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P-76

Saccharomyces cerevisiae derived extracellular vesicles as nanocarriers for aminoglycoside delivery

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ABSTRACT

Aminoglycosides include broad-spectrum antibiotics such as Gentamycin which are critical in combating drug-resistant bacterial infections, especially Gram-negative bacteria; however, their efficacy is limited due to poor eukaryotic cell membrane permeability, restricting intracellular delivery [1]. To overcome this limitation, the present study explores using extracellular vesicles (EVs) derived from *Saccharomyces cerevisiae* - a GRAS organism - as biocompatible drug delivery vehicles, which are both permeable to eukaryotic cell and are able to release the drug within the host cellular microenvironment. To address this research gap, EVs were isolated from *S. cerevisiae* via ultracentrifugation and then subsequently characterized. Dynamic Light scattering (DLS) analysis of the isolated EVs was assessed which had a mean hydrodynamic diameter of 182.1 ± 3.345nm with a polydispersity index (PDI) of 0.227. Scanning Electron Microscopy (SEM) was performed to identify the surface morphology of the EVs, which confirmed the presence of spherical shaped vesicular structures. Nanoparticle Tracking Analysis (NTA) demonstrated a mean particle concentration of 1.78×10^8 particles/ml. Zeta potential measurements showed a surface charge of -37.04 ± 0.49 mV indicating high colloidal stability. Protein quantification using the Lowry-Folin assay was done to evaluate the vesicular protein content, supporting successful EV isolation. For encapsulation, EVs will be encapsulated with Gentamicin, a representative aminoglycoside using active loading methods such as electroporation. Encapsulation efficiency will be determined spectrophotometrically. Collectively, this study focuses on using *S. cerevisiae* derived EVs as therapeutic nanocarriers for enhancing intracellular delivery of aminoglycosides and improved treatment of intracellular infections.

Keywords: Extracellular vesicles, *Saccharomyces cerevisiae,* aminoglycosides, encapsulation, electroporation, intracellular delivery.

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P-77

Electric field driven protein translocation through single walled carbon nanotube embedded in lipid bilayer membrane

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Abstract

Cell membranes primarily act as boundaries that create distinct compartments, with each membrane separating an internal and external environment. One of the essential components of the physical structure of life is the lipid membrane. Carbon nanotube porins (CNTP) are short, nanoscale channels derived from carbon nanotubes that can spontaneously insert into lipid bilayers and mimic biological membrane proteins such as aquaporins. These synthetic channels demonstrated the selective transport of ions and even the translocation of single-stranded DNA, a DNA hairpin for single-molecule sensing. However, the application of these artificial channels for protein translocation has been envisioned but never been experimentally demonstrated. We will present the demonstration of the protein translocation through single-walled carbon nanotubes (SWCNTs). We have scissored long carbon nanotubes of the µm range to ultra-short length to 10-20 nm to incorporate it into the lipid bilayer. We have observed characteristic ionic current jumps in the single-molecule electrophysiology measurements due to spontaneous insertions of 10-20 nm long CNTs into the lipid bilayer membrane. Here, we report the translocation behaviour of cytochrome c protein induced by electric fields through a single-walled carbon nanotube of inner diameter ~ 1.3 nm. Electric field at the CNTP was found to sufficiently unfold the cytochrome c protein to facilitate the translocation, as confirmed by a decrease in the average residence time of the protein at the CNTP upon increasing the transmembrane potential.

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Nanoclay-based nanofungicides for controlled release and enhanced activity: A sustainable approach to pest management

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Abstract

Fungal plant pathogens cause significant crop losses, accounting for a 20–30% reduction in global yield and nearly USD 60 billion in annual economic damage. Although fungicides are widely used, only a small fraction (~0.1%) of the applied dose reaches the target organism, while the remaining portion contaminates soil, water, and non-target systems, posing risks such as neurological disorders, cancer, and organ toxicity. To address these limitations, nanofungicides have emerged as a promising and sustainable alternative. In the present study, nanoclay-biopolymer composite-based formulation of chemical fungicide, fludioxonil, were synthesized and evaluated for enhanced fungicidal performance against fungal plant pathogen, *Rhizoctonia solani*. LDH-based nanoclay was prepared using co-precipitation, followed by intercalation of the fungicide into the nanoclay layers and subsequent surface coating with a biopolymer, chitosan. Physicochemical and morphological characterization confirmed successful fungicide loading and coating, with an average particle size of 160 nm and a positive zeta potential of +20 mV. The encapsulation efficiency was high, reaching 94.6 ± 0.8% for nanoclay-fungicide and 97.0 ± 1.25% for the biopolymer-coated formulation. *In vitro* release studies demonstrated controlled release from nanoclay-fungicide and a more sustained release profile from the biopolymer-coated system. Furthermore, antifungal activity against *Rhizoctonia solani* was higher than that of the conventional fungicide. Overall, these findings indicate that biopolymer-coated nanoformulations improve stability, adhesion, and controlled release, thereby enhancing the overall antifungal efficacy. This approach holds significant potential for sustainable agriculture and aligns with global sustainability goals.

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Eco-friendly development of ZnO-based biopolymer (chitosan)-carbon nanocomposites for enhanced photocatalytic and antibacterial activity as a tri-nanocomposite

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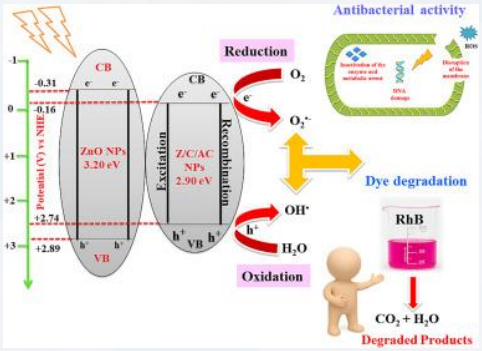
Abstract

A ZnO/Chitosan/Activated Carbon (Z/C/AC) nanocomposite was synthesized to develop an efficient and ecofriendly photocatalyst for wastewater treatment. The biopolymer chitosan provided structural stability and biocompatibility, while activated carbon enhanced surface area and adsorption capacity. The synergistic integration of these components significantly improved the photocatalytic degradation of Rhodamine B (RhB) under UV irradiation, achieving 97% degradation within 120 min. The optical band gap of the Z/C/AC nanocomposite was found to be 2.90 eV, indicating enhanced light absorption and efficient charge carrier separation compared to pristine ZnO. Kinetic analysis followed a pseudo-first-order model with a rate constant of 0.033 min^{-1}. The photocatalyst retained high degradation efficiency with only a slight decrease of about 10% after the fourth cycle, confirming its good stability and recyclability. Antibacterial studies revealed clear inhibition zones against E. coli and B. subtilis, demonstrating the material's dual functionality in water purification. Comprehensive characterization confirmed the formation of well-dispersed ZnO nanoparticles within the porous chitosan–carbon matrix. The study highlights a sustainable, biodegradable, and high-performance photocatalyst with enhanced dye degradation, stability, and reusability.



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P-80

Os(II) Complexes for Red Light-Activated Cancer Therapy

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Abstract:

Photocatalytic cancer therapy (PCT) has emerged as an alternative to chemotherapy with a novel catalytic MoA (NADH oxidation or NAD^+ reduction).[1,2] In this context, we developed novel Os(II)-based photocatalysts, $[Os(phtpy)_2](PF_6)_2$(**Os1**), $[Os(CF_3\text{-}phtpy)_2](PF_6)_2$(**Os2**), $[Os(OH\text{-}phtpy)_2](PF_6)_2$(**Os3**), $[Os(quinoline\text{-}tpy)_2](PF_6)_2$(**Os4**). **Os1**-**Os4** exhibited MLCT bands at 490-500 nm and additional spin-forbidden MLCT bands at 670-690 nm, making them suitable for red-light-triggered PCT.[3] Under red light (633 nm), **Os1**-**Os4** (5 µM) generated $^1O_2$ in DMSO-H_2O (1:99).[4] All photocatalysts efficiently photo-oxidized NADH (TOF:7.3-13.7 h^{-1}), disrupting NADH/NAD^+ balance, impairing mitochondrial function, and inducing cancer cell death.[1,2] **Os1**-**Os4** showed remarkable cytotoxicity against MDA-MB-231 TNBC, MCF-7 cells under red light. **Os4** showed the highest photocytotoxicity (IC_{50} =6.4±0.6 µM) against TNBC, and MCF-7 (20.3±0.9 µM) cells, likely due to enhanced pi-conjugation, leading to increased $^1O_2$ generation, NADH oxidation. *In vivo* studies using 4T1 tumour revealed that **Os4** reduced tumour volume in a dose-dependent manner upon exposure to laser (650 nm). Overall, red-light-triggered PCT offers a promising alternative for overcoming drug resistance by combining NADH photo-oxidation with ROS generation to kill cancer cells.

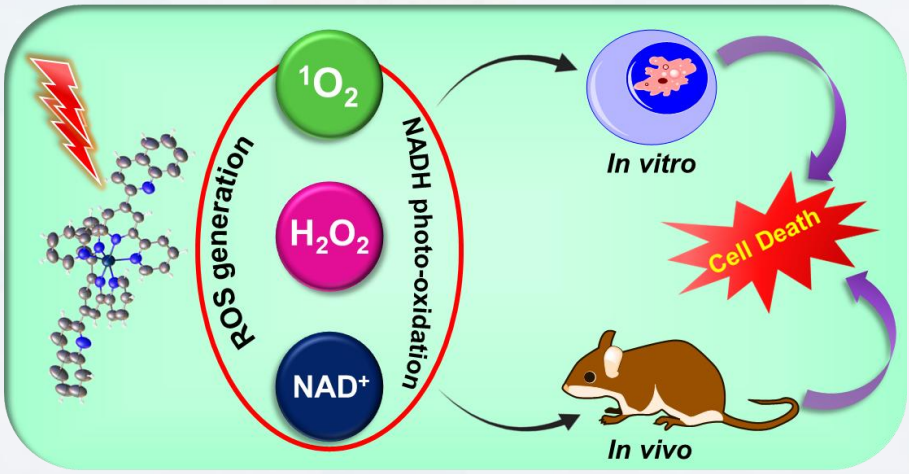

Figure: Schematic representation of anticancer activity of Os(II)-photocatalysts.

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P-81

Reengineering a Microbial Pigment into a Stable Nanoemulgel for Targeted Hyperpigmentation Therapy

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Abstract

Hyperpigmentation, driven by dysregulated melanogenesis, remains a common dermatological concern, often associated with limitations of conventional topical therapies such as irritation and poor patient compliance. The development of stable and biocompatible drug delivery systems is therefore essential. This study presents a pyocyanin-based nanoemulgel as a potential topical formulation for hyperpigmentation management. Pyocyanin, a microbial pigment derived from *Pseudomonas aeruginosa*, exhibits anti-tyrosinase activity [1] . A nanoemulsion was prepared using a low-energy emulsification method and optimized for droplet size, polydispersity index, zeta potential, and drug content. Stability studies demonstrated minimal variation in physicochemical parameters, while Fourier Transform Infrared (FTIR) analysis confirmed the preservation of functional groups. The optimized nanoemulsion was incorporated into a carbopol-based gel to obtain a nanoemulgel, which was evaluated for pH, rheology, spreadability, extrudability, and drug content uniformity. In vitro diffusion studies indicated sustained drug release. Biological evaluation demonstrated significant inhibition ($p < 0.01$) of mushroom tyrosinase along with good cytocompatibility ($p < 0.001$). The formulation also showed modulation of intracellular reactive oxygen species (ROS) and maintenance of glutathione (GSH) levels under oxidative stress conditions. Overall, the developed nanoemulgel represents a stable and promising topical system for targeting hyperpigmentation.

Keywords: Pyocyanin, Nanoemulgel, Hyperpigmentation, Tyrosinase inhibition, Topical drug delivery.

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Designing a sustainable & green heterogeneous catalyst for the valorisation of glycerol into glycerol carbonate

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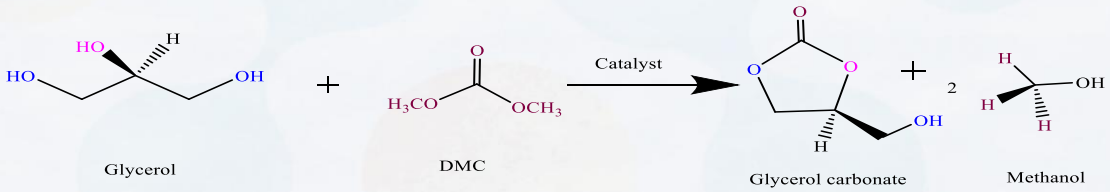
The global energy demand has led to the exhaustion of fossil fuels and environmental depletion, prompting interest in alternative bio-based renewable energy sources. Biodiesel is the most promising biofuel, obtained by transesterification of triglycerides with methanol, producing a surplus of glycerol as the main byproduct, which hampers biodiesel production profitability. Thus, the catalytic conversion of glycerol into value-added chemicals such as glycerol carbonate is a necessity. In the present study, we synthesise a silica-based catalyst from rice husk and then impregnate it with potassium and magnesium in different stoichiometric ratios. Under the best reaction conditions (85°C and 120 min, using 7 mol% of catalyst and a 1:3 ratio of GLY: DMC), a maximum 94.6% glycerol conversion was achieved with approx. 100% selectivity and 94% yield. Various characterisation techniques, including TGA, XRD, FTIR, XPS, BET, and SEM, have been used.

Reaction Scheme:



Different Applications:

- ✓ Pharmaceutical use
- ✓ Lithium-ion batteries
- ✓ Cosmetic industry
- ✓ Chemical intermediates

P-83

Regulation of the Second Coordination Shell of Ruthenium Single Atoms for Improved Acidic Hydrogen Evolution Reaction

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ABSTRACT

A precise control over the coordination environment of the atomic sites of a single-atom catalyst (SAC) was found to be crucial to achieve high electrocatalytic activity for hydrogen evolution reaction (HER). In this context, the modulation of the first coordination shell of the metallic sites has been extensively studied. Interestingly, the strategic modulation of the second coordination shell (surrounding the catalytic site but not directly bonded to it), exerted a significant contribution to the electrocatalytic activity by tuning the electronic properties, surface adsorption of the substrate and reaction intermediates, and proton-coupled electron transfer. Herein, we demonstrate Ru single atom anchored MnO_2 for the electrocatalytic acidic HER. The strategic modulation in the synthetic strategy produced $Ru_1@MnO_2$, Ru_1/MnO_2, and Ru_1-MnO_2 catalysts having different Ru–O–Mn coordination number for Ru-SAC (Figure a). Extended X-ray absorption fine structure (EXAFS) study revealed the detailed coordination environment of Ru and Ni in different catalysts. Ru_1/MnO_2 with four Ru–O–Mn coordination produced the best HER activity, achieving 10 mA cm^{-2} current density at an overpotential of 178 mV, far better than $Ru_1@MnO_2$ (267 mV), Ru_1-MnO_2 (203 mV), and MnO_2 (441 mV).

Keywords: Second coordination sphere · Single atom · Hydrogen evolution reaction · Modulation

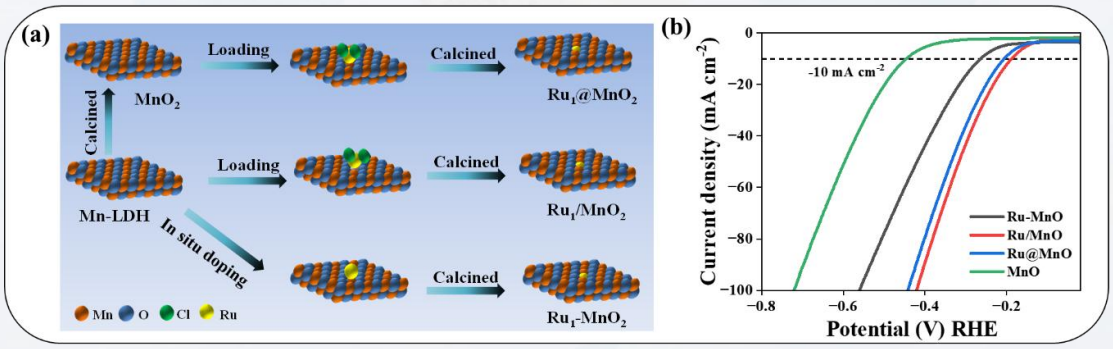

Figure: (a) Scheme for the synthesis of Ru_1-MnO_2 and MnO_2 with a modulated second coordination shell, and (b) LSV profiles for the hydrogen evolution reaction with the catalysts $Ru_1@MnO_2$, Ru_1/MnO_2, Ru_1-MnO_2, and MnO_2 in 0.5 M H_2SO_4.

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P-84

Photo-responsive Os(II) antibiotics for antibacterial therapy

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Antimicrobial resistance (AMR) has emerged as a major global health challenge, significantly reducing the effectiveness of conventional antibiotics.[1,2] In recent years, antibacterial photodynamic therapy (aPDT) has emerged as a promising strategy to address challenges associated with AMR.[3,4] In this context, three NIR emissive Os (II) based metallo-photoantibiotics, *viz.*, [Os(OH-phtpy)(thiophene-tpy)]$(PF_6)_2$ (**Os1**), [Os(OH-phtpy)(pyrrole-tpy)]$(PF_6)_2$ (**Os2**), [Os(OH-phtpy)(furan-tpy)]$(PF_6)_2$ (**Os3**), were successfully designed, synthesised and characterised. **Os1-Os3** exhibited intense absorption in the green region, making them suitable agents for light-triggered antibacterial applications. Single-crystal X-ray diffraction analysis of **Os2** confirmed a distorted octahedral geometry around the Os(II) centre with an OsN_6 coordination environment. Upon green light irradiation (525 nm, 50.4 J/cm^2), **Os1-Os3** revealed significant antibacterial activity against Gram-negative *Escherichia coli* and Gram-positive *Bacillus subtilis* by inducing oxidative stress via ROS generation (singlet oxygen, Φ_{1O2} up to 0.23) and NADH photo-oxidation TOFs up to 31.2 h^{-1}. Among the series, **Os1** (MIC_{90} = 50 µM) emerged as the most promising photoantibiotic, showing potent light-activated antibiofilm activity against mature *E. coli*. Moreover, **Os1** revealed biocompatibility in HEK cells, rat RBCs, and in the chicken egg model. Furthermore, in an *E. coli*-infected rat wound model, **Os1** under green light irradiation significantly accelerated wound healing. Overall, these findings demonstrated that Os(II) based metallo-photoantibiotics are potent light-triggered agents for the treatment of bacterial infections and wound healing.

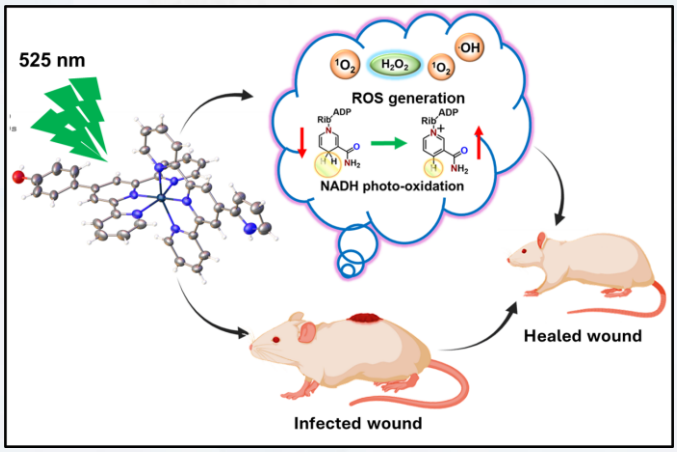

Figure: Schematic representation of antibacterial activity of Os(II) metallo-photoantibiotics.

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P-85

A naturally occurring 3D hydrophobic honeycomb structure for polarity-dependent microplastic trapping and plasmon-based sensing

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The detection of microplastics presents a fundamental challenge compared to conventional molecular sensing, owing to their particulate nature, heterogeneous distribution, and limited interaction with traditional sensing platforms. This constraint is particularly acute for ultrasensitive techniques such as Surface-Enhanced Raman Spectroscopy (SERS), which are inherently designed for molecular-level detection(1). To overcome this limitation, an effective strategy must integrate both particulate capture and molecular identification. In this work, we introduce a structurally optimised and intrinsically compatible SERS platform based on a naturally derived three-dimensional hydrophobic scaffold. A biodegradable substrate derived from natural sources is developed, exhibiting ~90% hierarchical porosity, ultralow density, and architecture-induced hydrophobicity(2). This unique combination creates a highly favourable microenvironment for the selective adsorption and enrichment of hydrophobic polymeric particles, enabling efficient interaction with plasmonic sites. Uniform in situ deposition of silver nanoparticles (AgNPs) throughout the porous network generates a high density of hotspots, resulting in significant enhancement of Raman signals(3). The Ag-shola substrate demonstrates superior performance compared to conventional planar substrates by simultaneously improving analyte capture and signal amplification. Environmentally relevant microplastics, including polyethene (PE), polyethene terephthalate (PET), polystyrene (PS), and polytetrafluoroethylene (PTFE), were successfully detected at low concentrations, even in complex matrices.

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P-86

Stimuli-Responsive Transition Metal Complexes: A Multimodal Platform for Anticancer and Antibacterial Applications

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The integration of stimuli-responsive medicinal inorganic chemistry has paved the way for highly targeted therapeutic interventions, notably through Photodynamic Therapy (PDT), Photocatalytic Cancer Therapy (PCT), and Sonodynamic Therapy (SDT). Photodynamic therapy (PDT), a non-invasive cancer treatment modality, offers appealing spatiotemporal control over drug activation and may overcome the problems of drug side effects and drug resistance in Pt-based clinical chemotherapeutics.[1] Whereas, Sonodynamic therapy (SDT) for cancer treatment is gaining attention owing to its non-invasive property and ultrasound's (US) deep tissue penetration ability (≤ 10 cm).[2] Our work focuses on developing and studying different types of metal complexes, using different transition metals such as iron, cobalt, nickel, manganese, ruthenium, rhenium, osmium, and iridium etc. These metals are chosen because they possess variable oxidation states and special properties that make the complexes highly active upon exposure to light or ultrasound. At first, the toxicity profile of the synthesized novel complexes was evaluated and used for *in vitro* and *in vivo* studies. In cancer or antibacterial treatment, these metal complexes can generate reactive oxygen species (ROS) or initiate catalytic processes (NADH oxidation, GSH depletion, etc.)[3] in the presence of light, which help kill cancer cells or bacteria while protecting healthy tissue. Overall, our research aims to develop new, effective treatments for anticancer, antibacterial studies using metal-based complexes with different ligand systems that respond to light/ultrasound effectively. By improving the efficiency of charge transfer and inter-system crossing, we aim to develop a flexible, multi-purpose approach for modern medicine.

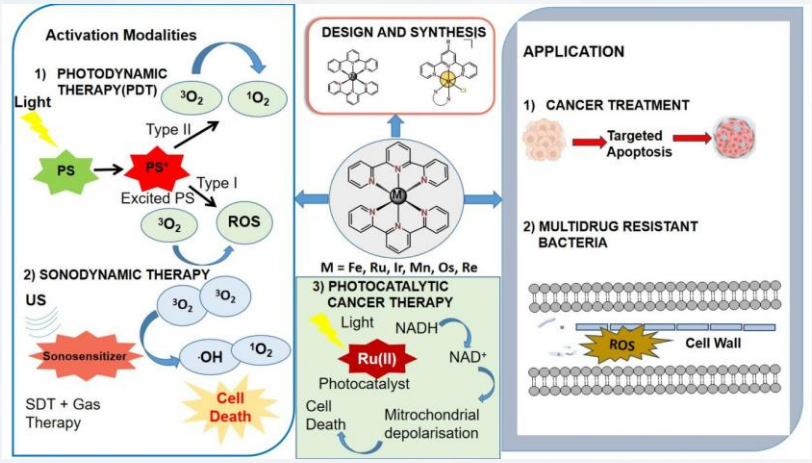

Figure: Schematic Representation of Multimodal Metal-Based Therapeutic Strategies.

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P-87

Electrochemical activation and functionalization of C-H bonds using transition metal-based catalysts

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Precise modulation of the Ru–Ru distance enables regulation of the catalytic pathway, favouring the more efficient adsorption of benzyl alcohol. Herein, we report a distance-modulation strategy for synthesising two types of dual-atom catalysts (DACs): one containing monomeric Ru species and the other comprising Ru dimer complexes homogeneously distributed on NiO nanosheets, denoted as Ru_1@NiO-DAC and Ru_2@NiO-DAC, respectively. Comprehensive structural and spectroscopic characterisations confirm the formation of an amorphous phase, along with strong electronic coupling and pronounced charge redistribution between the Ru-DAC and the NiO support. Notably, Ru_2@NiO-DAC exhibits markedly improved benzyl alcohol electrooxidation performance. Electrochemical studies reveal that the dimeric Ru complex exhibits significantly improved OER and benzyl alcohol oxidation activities compared to its monomeric counterpart. This improvement arises from the fixed Ru–Ru distance, which induces synergistic interactions, optimises benzyl alcohol adsorption, and ultimately improves the overall electrochemical performance.

Keywords: Oxygen evolution reaction · Dual atom · C-H activation · Value-added product

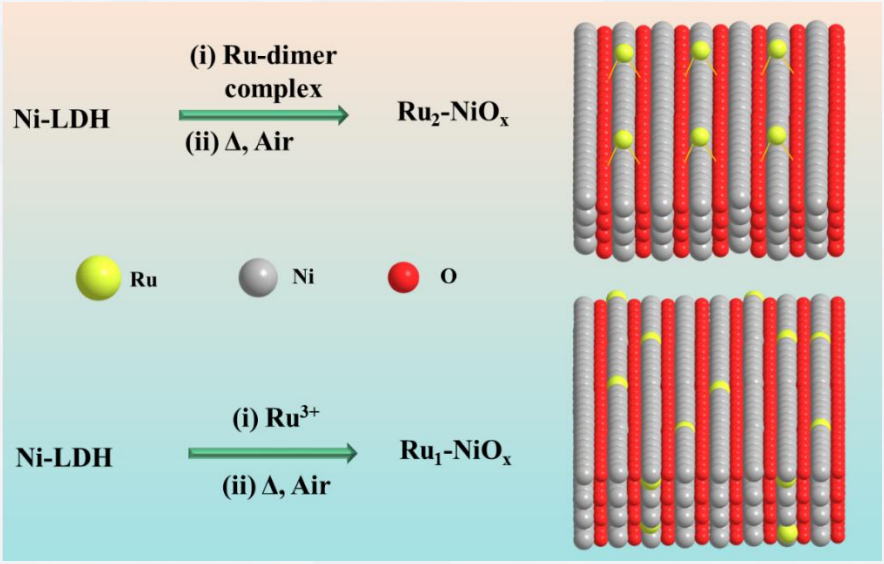

Figure: Synthesis of Ru_2@NiO_x and Ru_1@NiO_x

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P-88

Bacterial Serine Proteases as Modulators of Coagulation and Endothelial Function: An *In silico* and Cellular Approach

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Abstract:

Sepsis is a life-threatening syndrome with high global mortality, driven by dysregulated host responses, including endothelial dysfunction and coagulation abnormalities. While host inflammatory pathways are well studied, the role of bacterial virulence factors, particularly secreted serine proteases, remains underexplored [1,2]. This study aims to explore the interaction of Protease IV from *Pseudomonas aeruginosa* and EspP from *Escherichia coli* with key coagulation factors and their effects on endothelial cells. Protein-protein interactions of Protease IV and EspP with Thrombin, Fibrinogen, Factor V, Factor VIII and Factor X were analysed using ClusPro, refined with HADDOCK and evaluated for binding affinity using PRODIGY. The results indicated favourable binding interactions with key interface residues, highlighting a strong potential for these proteases to interfere with critical components of the coagulation cascade. Recombinant proteases were expressed and purified to facilitate downstream analysis. Human umbilical vein endothelial cells (HUVECs) were treated with purified proteins and cell viability was assessed using cytotoxicity assay. This assay demonstrated changes in HUVEC viability following protease treatment, suggesting a potential impact on endothelial cell integrity. Together, these findings provide a combined computational and cellular framework to better understand bacterial protease-host interactions in sepsis. Focusing on virulence attenuation rather than bacterial eradication represents a sustainable approach in sepsis management.

Keywords: Sepsis; Virulence Factors; Protein–Protein Interaction; Coagulation Factors; Endothelial Cells

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P-89

Molecular Insights into *Pseudomonas aeruginosa* Protease-Mediated Disruption of Wound Healing: An Integrative *In silico* And *In vitro* Study

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Abstract

Wound healing is a highly regulated process involving coordinated cell migration, proliferation, and extracellular matrix remodeling, which is often impaired during bacterial infections. Pathogenic bacteria such as *Pseudomonas aeruginosa* delay wound repair by producing tissue-destroying enzymes, endotoxins, and exotoxins that cause wound deterioration. Two major virulence proteins produced by the bacteria are pseudolysin and protease IV, which have been shown to cause detrimental effects on different cell types. In this study, *in silico* approach was employed to retrieve identify the key proteins involved in wound healing. Gene candidates were retrieved from the RNA Atlas and filtered to ensure biological relevance. Gene network analysis was performed and key proteins were identified. Further, functional enrichment analysis revealed significant enrichment in biological processes such as cell migration, angiogenesis, and extracellular matrix remodeling. Pathway analysis further highlighted the involvement of focal adhesion, regulation of actin cytoskeleton, and growth factor-mediated signaling pathways including FGFR, MAPK, and PI3K-Akt signaling. Further ClusPro, HADDOCK and PRODIGY was used to perform molecular docking for the key proteins with the proteases, which suggested stable binding of the proteins. *In vitro* studies using HaCaT cells demonstrated impaired migration and proliferation upon exposure to the proteases. Further validation through RT-PCR is proposed to confirm transcriptional modulation of the identified targets. Collectively, this study provides mechanistic insights into how bacterial proteases interfere with wound healing pathways and highlights their potential as therapeutic targets for improving chronic wound management.

Keywords: Wound healing, Virulence Factors, Protein-protein interaction, Molecular docking

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Development of Red light-activated Ru(II)-based Complexes for Antibacterial Application

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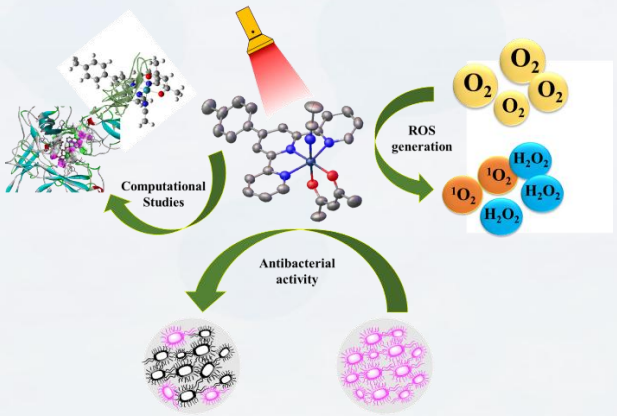
Abstract

Antibacterial photodynamic therapy (aPDT) has emerged as a promising strategy to combat multidrug-resistant infections [1]. However, most reported metal-based photosensitizers exhibit weak absorption in the phototherapeutic window (600–900 nm), limiting light penetration and restricting their effectiveness mainly to superficial tissues [2]. Therefore, developing red-light-responsive photosensitizers with high photodynamic efficiency remains an important research challenge. Here, we have synthesized and characterized a series of Ru(II) polypyridyl complexes containing acetylacetonate (acac)-based ligands *i.e.*, $[Ru(N,N,N)_2(acac)CH_3CN]PF_6$, where N,N,N = 4′-(4-Methylphenyl) 2,2′:6′,2″-terpyridine (**1**), 4′-(Naphthalen-1-yl)-2,2′:6′,2″-terpyridine (**2**), 4′-(anthracen-9-yl)-2.2′:6′.2″-terpyridine (**3**), and 4-(2,2':6',2"-terpyridinyl)] triphenylamine (**4**). **1-4** were synthesized and characterized by various spectroscopies. **1-4** exhibited MLCT transitions with maxima at 530 nm and 550 nm, respectively, that tail to *ca.*,750 nm, useful for red light-triggered aPDT application. Computational studies revealed the favourable HOMO-LUMO energy gaps, and optimum triplet excited state energy, enabling **1-4** as good photosensitizers for aPDT. Upon visible light irradiation (400-700 nm, 10 J cm^{-2}), **1-4** generated reactive oxygen species (ROS) through both type-I and type-II pathways and oxidized NADH. **1-4** generated singlet oxygen ($^1O_2$) with a quantum yield (Φ_Δ) of 0.13-0.17. Next, the light-activated antibacterial properties of **1-4** were evaluated against both *E. coli* and *S. aureus*, with minimum inhibitory concentrations (MICs) of 0.2-1.0 µg/mL. Notably, **1-4** showed no bacterial inhibition activity under dark conditions. Molecular docking studies further revealed favourable interactions of **1-4** with bacterial protein targets. Overall, the results suggested the potential of Ru(II) complexes as effective red-light-activated antibacterial agents.



Scheme 1. Schematic Presentation of red light-triggered antibacterial activity of Ru(II) Complexes.

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P-91

Visible Light-Driven Antibacterial Activity of Fe(III) Complexes via Singlet Oxygen–Mediated Membrane Disruption

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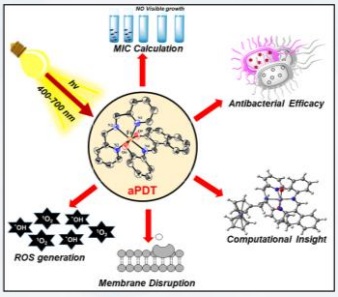
Abstract

The growing threat of antimicrobial resistance demands innovative therapeutic approaches beyond traditional antibiotics [1-4]. Antibacterial photodynamic therapy (aPDT), a non-invasive treatment strategy with a light-activated mechanism, has emerged as a promising alternative therapy [5-8]. In this study, four novel Fe(III) complexes, *viz.*, [Fe(dpa)(L1)]Cl (**Fe1**), [Fe(Fc-dpa)(L1)]Cl (**Fe2**), [Fe(dpa)(L2)]Cl (**Fe3**), and [Fe(Fc-dpa)(L2)]Cl (**Fe4**), where dpa = bis(2-pyridylmethyl)amine; Fc-dpa = N-(1-ferrocenyl)methyl-1-(pyridine-2-yl)-N-(pyridine-2-ylmethyl)methanamine; H_2L1 = (E)-2-((2-hydroxybenzylidene)amino)phenol; and H_2L2 = (E)-1-((2-hydroxyphenyl)imino)methyl)naphthalen-2-ol, were synthesized and characterized. **Fe1**-**Fe4** exhibit strong absorption in the visible region (~450 nm) and excellent photostability in biological media, making them suitable candidates for light-activated applications. Structural and computational studies revealed distorted octahedral geometries around the Fe(III) centre with a FeN_4O_2 core and favourable HOMO-LUMO energy gaps, enabling efficient photoinduced processes. Upon visible light irradiation (400-700 nm, 10 J cm^{-2}), **Fe1**-**Fe4** generate reactive oxygen species (ROS) through both type-I and type-II pathways. Biological studies demonstrated negligible antibacterial activity under dark, whereas remarkable activity was observed under light against both *S. aureus* and *E. coli*, with minimum inhibitory concentrations (MICs) as low as 0.2 µg/mL. Among the series, **Fe3** showed superior activity due to its enhanced electronic properties and ROS generation efficiency. Mechanistic studies indicated that ROS generation leads to oxidative stress and bacterial membrane disruption, as confirmed by membrane lysis assays. Overall, this study highlights Fe(III) complexes as promising, biocompatible photosensitizers for next-generation aPDT applications.



Scheme 1. Schematic Presentation of Light-Triggered Antibacterial Activity, Membrane Lysis, and MIC Calculation of Fe(III) Complexes.

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P-92

Vanadium-Doped CuFe2O4 as an Efficient Photocatalyst for Enhanced p-Nitrophenol Degradation via Photo-Fenton Process

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Abstract

P-nitrophenol (PNP) is a persistent, highly toxic micropollutant with carcinogenic nature. Here, we design and develop different compositions of vanadium-doped copper ferrite by a simple solvothermal method followed by calcination. A lower concentration of dopant results in lattice parameter contraction and band gap increase, while at a higher concentration of dopant, lattice expansion and a decrease in band gap is observed. TEM images confirm that the morphology of the CFO and 2VCFO is spherical. FT-IR spectra of CFO and 2VCFO photocatalyst confirmed the presence of -OH and C=O functional groups. The 2VCFO photocatalyst shows the best photo-Fenton activity towards PNP degradation at pH 3. The turnover frequency (TOF) and H_2O_2 normalized turnover frequency (HTOF) for the 2VCFO photocatalyst are 53.9 $\mu molg^{-1}L$ and 3.449 $mg^{-1}min^{-1}L$, respectively. This value is comparatively higher than the CFO photocatalyst and other reported photocatalysts in the literature. 2VCFO photocatalyst showed the PNP degradation 90.5% after the 5th cycle in the photo-Fenton process. The XRD pattern confirms no change in the phase of the 2VCFO photocatalyst after the 5th cycle of reuse. All these confirm that after V doping copper ferrite activity enhances towards PNP degradation in the photo-Fenton process.

Keywords: Doping, photo-Fenton, Organic pollutants, copper ferrite, solvothermal method

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One-Pot Synthesis of Sulfonyl hydrazones from Styrene via In Situ Benzaldehyde Formation

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In this study, we present a one-pot synthetic approach for sulfonyl hydrazones, where styrene serves as a precursor to benzaldehyde, which subsequently reacts with sulfonyl hydrazides to afford the desired products. These compounds are of significant interest due to their enhanced stability, versatile reactivity in organic synthesis, and improved biological activity compared to simple hydrazones. The developed protocol demonstrates a broad substrate scope and excellent functional group tolerance, enabling efficient synthesis and further functionalization of pharmaceutically relevant molecules.

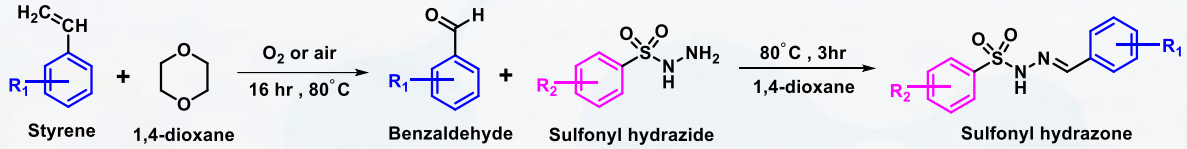

Figure 1. One-pot method for the synthesis of sulfonyl hydrazones.

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P-94

Review on Electro-organic Synthesis

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Abstract

Electro-organic synthesis has emerged as a sustainable and green approach for carrying out organic transformations by utilizing electrical energy instead of conventional chemical reagents. This method offers significant advantages such as reduced use of hazardous oxidants and reductants, improved selectivity, and environmentally tanign reaction conditions. The present work focuses on understanding the fundamental principles, mechanisms, and applications of electro-organic synthesis in modern chemistry.

In this study, various electrochemical techniques are considered, including anodic oxidation and cathodic reduction, carried out in suitable electrolytic cells under controlled conditions. The role of electrodes, solvents, supporting electrolytes, and current density in influencing reaction pathways and product selectivity is also discussed.

The results indicate that electro-organic synthesis provides higher efficiency, cleaner reaction profiles, and better control over reaction intermediates compared to traditional methods. Additionally, it supports the development of novel reaction pathways that are otherwise difficult to achieve.

In conclusion, electro-organic synthesis represents a promising and eco-friendly strategy for future organic synthesis, contributing significantly to green chemistry and sustainable chemical processes.

P-95

Topochemical Copper Nitroprusside Cathode Enables High Capacity and Cyclability Aqueous Proton Batteries

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Abstract:

Aqueous proton batteries (APBs) are emerging as a promising class of energy storage systems, particularly suited for grid-level renewable energy applications. Their key advantage lies in the intrinsic properties of protons-small ionic radius, lightweight nature, and high mobility, which enable fast ion transport and rapid charge-discharge capabilities. These characteristics offer rapid charge/discharge capabilities and high-power density. However, full-cell APB development is still constrained by limited energy density, rate capability, and cycle life. In this work, we present a high-performance APB system composed of an inorganic copper coordination polymer (CuFe-NP) cathode and an organic polyaniline (PANI) anode, operating in a 3.0 M H_2SO_4 electrolyte.

The CuFe-NP cathode, with its open-framework structure like a MOF, enables rapid and reversible proton intercalation, delivering a high capacity of 148.14 mAh g^{-1} at 2 A g^{-1} in half-cell testing. The PANI anode, relying on the reversible redox reaction due to its quinoid and benzenoid moieties, achieves a specific capacity of 117.77 mAh g^{-1} at 2 A g^{-1} and exhibits excellent stability.

The PANI//CuFe-NP full cell achieves a reversible discharge capacity of 100 mAh g^{-1} at 2 A g^{-1}, exceptional rate capability retaining 51.23 mAh g^{-1} at 20 A g^{-1}. Furthermore, the cell shows robust long-term cycling performance, maintaining 68% of its initial capacity and 72% energy efficiency over 6000 cycles at 10 A g^{-1}, outperforming many current APB systems.

This work demonstrates a promising pathway toward high-performance, scalable aqueous proton batteries by strategically integrating stable inorganic hosts with adaptive organic materials.

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P-96

Iodine-mediated pyrazolo-pyrimidine based nucleobase mimetics synthesis and structural studies

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Abstract

Nucleobases are the nitrogen containing heterocyclic compounds[1], which is important component of DNA (Deoxyribose nucleic acid) and RNA (Ribose nucleic acid)[2]. Structural modification of this nucleobase generally made it more prominent for therapeutic applications[3]. In this present study synthesized pyrazolo-pyrimidine analogue of purine nucleobase mimetics using iodine as a catalyst for the reaction, and their characterization using different spectroscopic technique's- ^{1}H-NMR, ^{13}C-NMR, High Resolution Mass Spectrometry, UV & IR, and structural studies for drug like property estimation.

Keywords: - Nucleobase mimetics, Pyrazolo-pyrimidine, structural studies etc.

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P-97

Progress in Electrochemical Biosensing using Graphitic Carbon Nitride, its Functionalized Derivatives and Composite Materials

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Abstract:

The metal-free, two-dimensional polymeric semiconductor material known as graphitic carbon nitride (g-C_3N_4) has gained significant interest in the context of electrochemical biosensing due to its exceptional physicochemical properties, such as superior chemical stability, adjustable electronic configuration, low toxicity, and facile synthesis (Majdoub et al., 2020). The g-C_3N_4 is mainly composed of nitrogen, which provides a large surface area for the adsorption of biomolecules. However, g-C_3N_4 has drawbacks, such as poor electrical conductivity and rapid charge-carrier recombination, which affect the efficiency of the biosensing mechanism (Zhang et al., 2024). Therefore, significant research has focused on modifying g-C_3N_4 through techniques such as heteroatom doping, surface engineering, and the design of g-C_3N_4-based composites with metals, metal oxides, carbon-based materials, and conductive polymers, which have shown significant improvements in the charge-transfer kinetics of g-C_3N_4-based electrochemical biosensors (Ansari et al., 2024; Kamble et al., 2024). Recent developments have shown that g-C_3N_4-based electrochemical platforms can achieve ultrasensitive detection of various analytes, including glucose, disease biomarkers, environmental pollutants, and pathogenic microorganisms, with low detection limits and fast response times (Chiu et al., 2025; Zhang et al., 2024). In addition, the use of g-C_3N_4-based platforms in combination with transduction methods, such as photoelectrochemical and hybrid sensing, has expanded their potential across different fields, including clinical diagnostics, environmental monitoring, and food safety. However, there are some challenges that need to be addressed. Thus, this article provides a comprehensive overview of recent advances in g-C_3N_4-based electrochemical biosensing platforms and outlines prospects for next-generation systems.

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P-98

Development of Low-GWP Ternary Refrigerant Blend (R32/R152a/R125) with Nano-Enhancement: Performance, and Sustainable Cooling Advancement

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The work involves systematic transition of conventional high-global-warming-potential (GWP) refrigerants to advanced nano-enhanced refrigerant systems with higher thermodynamic and environmental performance. Initially, basic vapor compression refrigeration system using R507C is demonstrated, highlighting its inherent limitations such as high GWP, zero ozone depletion potential (ODP), moderate coefficient of performance (COP), and environmental persistence due to its stable fluorocarbon molecular structure. The development of ternary refrigerant blend consisting of R32/R152a/R125 is then depicted using a compositional mixing framework at the molecular level, where intermolecular interactions, polarity differences, and vapor-liquid equilibrium behaviour contribute to optimized boiling characteristics, reduced GWP, and negligible ODP. The presence of hydrogen atoms in R32 and R152a improves air degradability over completely fluorinated compounds, improving sustainable development. A combination of nanoparticles (such as metal oxides or carbon-based nanostructures) into the optimal blend results in a nano refrigerant with different physical and chemical properties. Surface activation, van der Waals forces, and the application of surfactants all contribute to nanoparticle dispersion stability, resulting in little agglomeration and uniform suspension. At the nanoscale, phonon transport, Brownian motion, and interfacial liquid layering increase heat conductivity, while tribological processes like rolling and mending mechanisms reduce frictional losses in the compressor. Additionally, nanoparticle-refrigerant interactions may modify specific heat capacity and viscosity, which modifies heat transfer coefficients and flow behaviour. The integrated thermophysical and chemical effects minimize compressor effort, increase evaporator heat absorption, and improve exergy efficiency. Overall, the graphical progression demonstrates a reduction in environmental impact (GWP), improved chemical sustainability, and significant increase in COP from R507C to the ternary blend, and finally to the nano-enhanced refrigerant, indicating a viable path toward high-efficiency and environmentally friendly refrigeration systems.

Keywords: GWP; ODP; Nano refrigerants; Sustainable cooling; Thermodynamics; Performance

P-99

Ultrasound-assisted ring opening of epoxides in HFIP: THF: Synthesis, characterization, computational studies and molecular docking of novel 2-hydroxy dithiocarbamates

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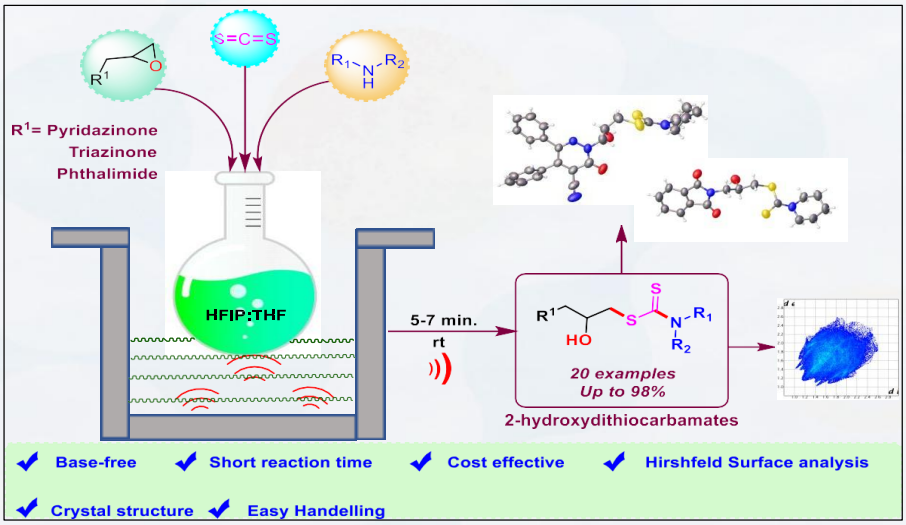
Abstract:

Under the influence of ultrasonic irradiation, pyridazinone, triazinone, or phthalimide containing 2-hydroxy dithiocarbamates, a biologically relevant novel organo- sulphur compound, was synthesized. Detailed characterization, computational, and molecular docking studies are being investigated. Molecular interactions were studied using 3D Hirshfeld surfaces and corresponding 2D fingerprint plots. Theoretical (DFT) studies on the molecular structure, HOMO, LUMO, and quantum chemical descriptors were performed at the B3LYP/ 6–311++G(d,p) level of theory. At the same time, the interaction energy was computed using the B3LYP/6–31G (d,p) level of theory. The FMO study revealed that molecules 4a and 4p in the gas phase have 3.545 eV and 3.263 eV HOMO-LUMO energy gaps, respectively, and they are hence kinetically stable. Quantum chemical calculations confirm the electrophilic character of compounds 4a and 4p, as the molecule is stable and highly electrophilic.



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P-100

Neutral pH Fenton and Photo-Fenton Activity of Starch stabilized W-doped FeS_2 particles

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Abstract:

Increased usage of chemical fertilizers, pesticides, dyes, and antibiotics pollutes the ground and surface water sources. Fenton and photo-Fenton processes are frequently used for treating organic pollutants in industrial wastewater/effluents. These chemical oxidation processes degrade/mineralize the organic pollutants in the wastewater into (small) non-toxic fragments. However, these processes have critical limitations like acidic pH, low H_2O_2 utilization efficiency for hydroxyl radical generation, recyclability, and iron sludge formation. In the current study, W doping of iron pyrite particles can enhance the photocatalytic activity. Starch stabilized FeS_2 (abbreviated as PF) and W-doped FeS_2 (WFS) materials were prepared by a solvothermal protocol[1–3]. XRD analysis shows that W doping enhanced the lattice parameters of FeS_2 and W substitutes the Fe^{2+}. After W^{4+} ion doping, the band gap of materials decreased. HR-SEM images confirm that the particle size decreased after doping. XPS spectrum of W 4f confirmed the W^{4+} ion doping. Fenton and Photo-Fenton para-nitrophenol (PNP) degradation at neutral pH was investigated on FS and WFS particles. The best photo-Fenton activity towards PNP degradation occurred at a particular W doping percentage. This photocatalyst exhibited high photo-Fenton turnover frequency, was stable under recycling, and the H_2O_2 required for these reactions was significantly lower than most reports at neutral pH.

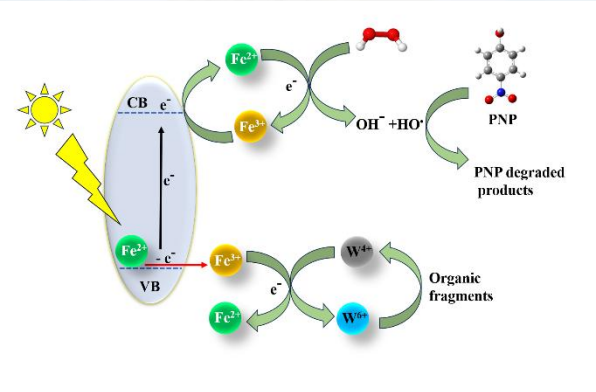

Figure 1. PNP degradation mechanism during the photo-Fenton reaction.

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P-101

Out-of-Equilibrium Bioinspired Hydrogels Enabling Fuel- and Light-Responsive Transient Conductive Properties

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ABSTRACT

The development of out-of-equilibrium supramolecular hydrogels, inspired by biological systems, has attracted considerable interest due to their potential applications in nanotechnology. Despite this, these transient hydrogels' (opto-)electronic properties remain elusive. This study introduces a bio-inspired dissipative hydrogel powered by a chemical fuel, exhibiting tunable semiconducting and photoelectronic functionalities. A bio-organic bolaamphiphile (PA) was designed and synthesized, integrating the optoelectronic characteristics of perylene diimide (P) with the reversible gel-triggered switching capabilities of aspartic acid (A). Precise temporal control over the supramolecular self-assembly and disassembly of the PA hydrogel was achieved by regulating the chemical fuel dimethyl sulfate (DMS). Results demonstrate that the PA-based dissipative self-assembly can reversibly switch between an insulating sol state and a semiconductive gel state, accompanied by nanostructural, fluorescence, and chiroptical switching. Furthermore, a thin film derived from the hydrogel exhibited light-responsive conductivity switching capability. PA's transient structural, chemical, and functional properties were extensively characterized using spectroscopic, microscopic, computational, and device fabrication techniques. This study not only elucidates the structure-property relationships in dissipative hydrogels but also paves the way for developing adaptive, life-like functional nanomaterials with promising applications in optoelectronics, nanotechnology, and soft robotics.

Keywords: Out-of-equilibrium hydrogels, Dissipative self-assembly, Fuel-driven supramolecular assembly, semiconductor, optoelectronic, Adaptive soft materials, Bio-inspired nanotechnology.

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P-102

Organotin(IV) Azo Hydrazonates as Lysosome-Targeted Anticancer Agents

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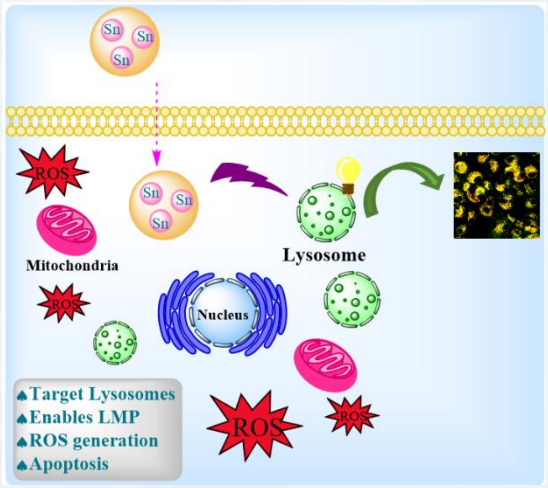
ABSTRACT

Following the success of cisplatin, several platinum-based anti-cancer metallodrugs were discovered, including carboplatin, oxaliplatin, and nedoplatin. Nevertheless, the severe adverse side effects associated with these Pt-based drugs have limited their widespread clinical use and prompted the hunt for non-Pt-based medication alternatives.[1] Metallodrugs with organotin(IV) compounds emerging as a potential alternative to platinum-based drugs have revolutionised the field of both diagnosis and therapy, offering enhanced anticancer efficacy and bio-imaging capabilities for targeting intracellular organelles.[2,3] Even though non-platinum metal-based complexes have been extensively studied as anticancer agents, their fast hydrolysis, reduced hydrolytic stability, and cellular absorption render them unsuitable for the development of standard anticancer metallodrugs.[4] In this presentation, we embarked on an effort to explore the theranostic potential of a new class of azo hydrazone-based organotin(IV) complexes $[Sn^{IV}L^{1-4}(Ph)_2]$ (1–4). The aqueous stability, hydrophobic character, and interaction of 1−4 with biomolecule (BSA and DNA) were examined. The speciation studies suggested the complexes possess exceptional hydrolytic stability. Further in-depth mechanistic studies revealed that they preferentially accumulate in the lysosome, damage lysosomal membrane potential, and upregulate intracellular reactive oxygen species (ROS), leading to apoptotic-mediated cancer cell death.



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P-103

Development of BiOBr/g-C_3N_4 S-scheme heterojunctions with Co-Ni_2P cocatalyst for enhanced photocatalytic dye degradation

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Abstract

The development of s-scheme (S-scheme) heterojunctions plays a crucial role in advancing photocatalytic processes by significantly promoting the separation and transfer of photocarriers. This enhancement directly contributes to improved redox activity, which is essential for efficient photocatalysis. A key factor influencing the effectiveness of these heterojunctions is the interface resistance, which can markedly affect the separation of electron-hole pairs and ultimately determine the photocatalytic activity of the system. To achieve this, BiOBr and g-C_3N_4 based S-scheme photoanode were developed and checked for photocatalytic dye degradation. As the electron-hole separation is poor and high recombination in BiOBr and g-C_3N_4 S-scheme heterojunction, we have modified the photoanode using cocatalyst Co-Ni_2P as an electron bridge to reduce recombination and the interfacial resistance for photocarrier transport between BiOBr and g-C_3N_4. The as-prepared BiOBr/Co-Ni_2P/g-C_3N_4 photocatalyst exhibited high visible-light photocatalytic performance for the degradation of of methylene blue, achieving 99% degradation efficiency. The high photocatalytic activity of S-scheme BiOBr/Co-Ni_2P/g-C_3N_4 was mainly attributed to the synergistic effects of the Co-Ni_2P cocatalyst and S-scheme heterojunction, which not only lowers the recombination but also reduces the interface resistance.

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P-104

Multifunctional Electrospun Polymeric Fiber Mats Embedded with Conductive Polymer and 2D materials for Antimicrobial Performance

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Abstract

Electrospun polymeric nanofiber mats have emerged as promising platforms for antimicrobial applications due to their high surface area, tunable porosity, and ability to incorporate functional nanomaterials. Their applications as membranes in clean water technology and as wound healing patches in the field of biomedical technology are inevitable. In this context, the present study focuses on the fabrication of composite nanofibrous mats using the electrospinning method. Herein, polyvinyl alcohol (PVA) is used as a base polymer, which is further combined with polyaniline (PANI), molybdenum disulfide (MoS_2), and titanium dioxide (TiO_2) to enhance its antimicrobial performance. The incorporation of conductive polymer (PANI) and inorganic nanomaterials (MoS_2 and TiO_2) aims to synergistically enhance antibacterial activity via reactive oxygen species (ROS) generation, membrane disruption, and electron transfer.

A comparative analysis was performed to evaluate the structural, morphological, and antimicrobial characteristics of various composite systems. The optimised composition of electrospun fibers exhibited uniform morphology with nanoscale diameters, confirming successful integration of the functional components in their matrices. Antimicrobial studies help in understanding the role of suitable mechanisms.

Based on the results obtained, we have highlighted the potential of multifunctional electrospun nanofiber mats as effective antimicrobial materials, particularly for biomedical and environmental applications. This comparative approach provides insights into the role of different nanofillers in tailoring the performance of polymeric nanofibers for targeted antimicrobial functionality.

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P-105

Evaluating P- doped transition metal selenide based electrocatalyst for oxygen evolution reaction

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Abstract:

In this study, to synthesize phosphorus-doped copper selenide hexagonal structure grown on a suitable substrate P-CuSe/NF as a highly efficient electrocatalyst for the oxygen evolution reaction (OER).The synthesize of CuSe nanoparticle (via hydrothermal method) and novel P-CuSe on nickel foam electrode and their physicochemical, electrochemical and operando spectro-electrochemical characterization towards oxygen evolution reaction (OER).The resulting P-CuSe nanostructure exhibit a strong synergistic effect, which enhance charge transfer kinetics, improve electrical conductivity, and provide abundant active sites. As a result, the catalyst demonstrated a low overpotential of 200 mV to achieved current density of 50mA cm-2, Tafel slope as low as 81 mV dec^{-1}. A small Tafel slope indicating favorable reaction kinetics, and excellent long-term stability. These finding highlight the practical feasibility of P-doped CuSe on NF for water splitting and offer a new approach foe efficiently preparing advanced electrocatalyst in future.

Keywords: Copper selenide (CuSe), Oxygen Evolution Reaction (OER), Electrocatalysis Water Splitting, P-doped CuSe, Transition Metal Selenides

P-106

Role of cation deficiency in Cr-doped NiO for developing superior for photocatalytic dye degradation.

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Abstract

Developing efficient, stable and economical catalysts is crucial for the dye degradation. Herein we report cation vacant Cr-doped NiO as a promising catalyst for the dye degradation. Nonprecious chromium dopant is incorporated into the cation vacant cubic rock-salt $Ni_{1-1.5x}Cr_xV_x''O$ ($0 < x < 0.2$; $V_x'' = Ni^{2+}$ cation vacancy) via a facile sol-gel method. We utilized the concept of inductive effect through doping with more electronegative/Lewis acidic Cr^{3+} in the NiO to improved photocatalysis of dye degradation. Doping of tri-valent Cr in NiO lattice generates cation vacancy which promotes higher activity by creating lattice vacancies on the surfaces for better adsorption of dye molecules. Among the compositions investigated, $\mathbf{Ni_{0.775}Cr_{0.15}O}$ is the most active as it exhibits excellent Photocatalyst for dye degradation. In this work, comprehensive characterization using XRD, FT-IR, HR-TEM, FE-SEM, XPS Mott-Schottky and UV-DRS Were performed to investigate the structural, morphology, composition and optical properties. The Cr-dopped NiO effectively degrade MG dye.

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P-107

Electronically Tuned Dipyrromethene and BODIPY Platforms for Selective Fluoride and Cyanide Detection

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Abstract:

Molecular engineering of rapid and highly selective sensing platforms for hazardous ions remains an open challenge due to their very low environmental thresholds. Hence, there is an urgent need for robust and efficient molecular systems capable of sensitive ion recognition in both solvent and solid states. To address this, we have developed two molecular scaffolds selective for either fluoride or cyanide detection. First, we designed a series of meso-aryl 1,9-bisbenzothiazole-substituted dipyrromethenes (DPMEs) as a fluoride-responsive system. Next, we converted DPMEs into their corresponding BODIPY derivative to generate a cyanide-trapping platform. To explore the influence of electronic effects on sensing behavior, various electron-donating and electron-withdrawing substituents were introduced at the meso-aryl position of the benzothiazole substituted DPME core. Interestingly, the 5-pentafluorophenyl-1,9-bisbenzothiazole DPME exhibited the highest selectivity toward fluoride ions, accompanied by a distinct color change from pink to blue. Sensing mechanism was further studied via absorption and fluorescence spectroscopy, that revealed a significant red shift upon addition of F^- ion. Notably, this sensing process with DPME derivate was fully reversible. NMR titrations confirmed that the pronounced optical response originates from strong interactions of fluoride with the pyrrolic N–H site. In BODIPY systems, the sensing preference shifted from fluoride to cyanide. In these BODIPY frameworks, nucleophilic attack of cyanide at the meso-position disrupts π-conjugation, leading to rapid fluorescence quenching. Overall, the robust and well-defined spectral responses highlight the promise of this tunable dipyrromethene/BODIPY system for environmental monitoring and safety-critical detection of fluoride and cyanide ions.

Keywords: Dipyrromethene and BODIPY sensor, fluorescence quenching, Pentafluoro benzothiazole, anion sensing, Optical spectroscopy.

P-108

Evaluating transition metal selenide based electrocatalyst for oxygen evolution reaction

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Keywords: Copper selenide (CuSe), Oxygen Evolution Reaction (OER), Electrocatalysis Water Splitting, pMF-R (polymerised melamine-formaldehyde resin), CuSe@pMF-R Composite, Transition Metal Selenides

Abstract:

In recent studies, metal selenides have demonstrated versatile electrocatalytic activity in the field of water splitting. Among them, copper selenide (CuSe) has attracted attention for its potential in the oxygen evolution reaction (OER). To enhance OER performance, we have developed three nanostructures: CuSe, pMF-R (polymerised melamine-paraformaldehyde resin), and the CuSe@pMF-R composite, where freshly synthesized CuSe nanostructures are anchored onto the pMF-R surface.

The formation of Cu–N bonds was confirmed, promoting efficient charge transfer channels and reducing the barrier between the glassy carbon (GC) electrode and the CuSe active sites. Due to the synergistic interaction between CuSe and pMF-R, the CuSe@pMF-R catalyst exhibited a low onset potential of 1.56 V and achieved a current density of 10 mA cm^{-2} at 1.608 V vs. RHE, indicating superior OER activity.

Operando spectroelectrochemical analysis revealed the participation of selenium, Cu^{2+}, and pMF-R as active sites in the generation of intermediate oxygen species, contributing to an exponential increase in OER kinetics. The reaction was found to be first-order, and the enhanced compositional and structural features of CuSe@pMF-R are credited for its outstanding electrocatalytic performance compared to conventional OER catalysts.

Charge-polarization-induced Photocatalytic Urea synthesis via Co-reduction of CO_2 and NO_3^-

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Urea remains the most widely used nitrogen-based fertilizer around the world and the industry follows Haber-Bosch process-a highly energy demanding reaction. In this context, the photocatalytic co-reduction of NO_3^- and CO_2 offers a sustainable approach for urea synthesis and environment remediation. In this work, we have explored a photocatalytic approach for the synthesis of urea using a Bi-based semiconductor. In the presence of light, the charge polarization in the semiconductor facilitates the charge separation and hence helps in the co-reduction of CO_2 and NO_3^- to urea (**Figure 1**). Over the time of the reaction, the activity of the catalyst is enhanced due to the surface reconstruction and defect formation. Therefore, this study provides new insights into polarization-mediated charge transfer dynamics and offers an effective strategy for advanced photocatalysts toward efficient solar-driven urea synthesis.

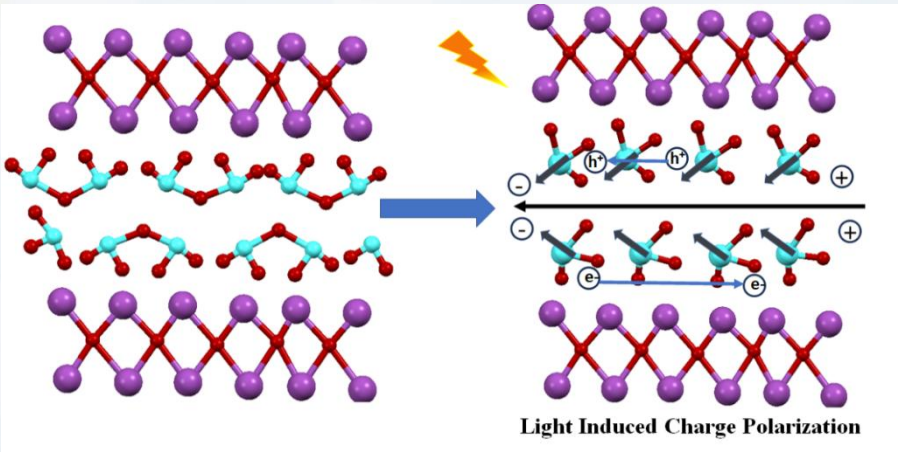

Figure 1. Light-induced charge polarization in the Bi-based semiconductor for photocatalytic urea production.

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P-110

SYNTHESIS AND CHARACTERIZATION OF BARIUM, CERIUM AND MISCH METAL BASED HETEROPOLY ACID CATALYSTS

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Abstract:

Heteropoly acids with Keggin structures are good popular oxidation catalysts [1,2]. Misch metal (Mm) is the raw mixture of lanthanide metals available in our earth. In this study we have prepared $H_3PMo_{12}O_{40}$, $H_xPMo_8M_4O_y$ (M=Ba, Ce, Mm), $H_xSiW_{12}O_y$, and $H_xSiW_8M_4O_y$ (M=Ba, Ce, Mm) heteropoly acids. Using misch metal, the raw mixture of rare earth metals, avoids the stringent and costly method of separation of individual rare earth metals. Thus usage of misch metal is a step forward in green synthesis march. We have characterized these compounds using XRD, IR spectroscopy and UV – Visible spectroscopy. XRD studies show Keggin type structures for these compounds with characteristic sharp diffraction peaks. IR spectra of these compounds show standard finger print peaks and few characteristic peaks in group frequencies. UV- Visible spectra of these compounds show characteristic main absorption peaks in ultraviolet region.

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P-111

Sol- gel synthesised CeO_2-TiO_2 Nanocomposite-grafted g-CN: an efficient photocatalyst for degradation of methylene blue under Visible-light.

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Abstract

The development of efficient photocatalysts for wastewater treatment remains a critical challenge in environmental remediation. In this study, a ternary **CeO_2-TiO_2/g-CN nanocomposite** was successfully synthesized via a facile sol-gel-calcination approach and evaluated for the photocatalytic degradation of methylene blue (MB) dye under visible light irradiation. The incorporation of CeO_2 and g-CN with TiO_2 was found to significantly enhance light absorption and suppress the recombination of photogenerated electron -hole pairs through the formation of a heterojunction structure. In this work, Comprehensive characterization using XRD, FT-IR, HR-TEM, FE-SEM, XPS, and UV-DRS were performed to investigate the structural, morphology, composition and optical properties.

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P-112

SMARTPHONE-BASED RGB COLORIMETRIC SENSING OF SITAGLIPTIN EMPLOYING MBTH AS A CHROMOGENIC REAGENT

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Abstract

The present study describes the development of a simple, rapid, and eco-friendly smartphone-based colorimetric method for the determination of Sitagliptin as such and in tablet formulation. The method is based on a complexation reaction between Sitagliptin and 3-methyl-2-benzothiazolinone hydrazone (MBTH) in the presence of $FeCl_3$, which produces a stable coloured complex suitable for quantitative analysis. Experimental parameters such as the concentration and volume of MBTH and $FeCl_3$ were carefully optimized to obtain the maximum analytical response. The developed method allowed the determination of Sitagliptin using three analytical approaches: spectrophotometry, digital image analysis through ImageJ software, and smartphone-based RGB colorimetric measurement. The method was validated according to ICH guidelines and showed good linearity, accuracy, precision, and reproducibility, confirming its suitability for routine pharmaceutical analysis. The proposed method was successfully applied to the determination of Sitagliptin in SITASON tablet samples with satisfactory recovery results. In addition, the environmental friendliness of the method was evaluated using RAPI and AGREE tools, giving scores of 72.5 and 0.86, respectively, indicating that the method is green, cost-effective, and suitable for routine quality control of Sitagliptin in pharmaceutical formulations.

Keywords: Sitagliptin, MBTH, digital colorimetry, RGB, AGREE, RAPI

P-113

Thermally Shrunk RuNi(O)x (P)y Electrocatalyst Enabling Ampere-Level Current Density for Efficient Alkaline Seawater Splitting

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ABSTRACT

The development of highly active and durable electro catalysts for alkaline seawater splitting is crucial for sustainable hydrogen production at an industrial scale. Herein, we report a thermally shrunk RuNi(O)x(P)y electro catalyst engineered to achieve ampere-level current density with excellent stability. The thermal shrinking strategy induces strong electronic coupling and structural reconstruction between Ru and Ni species, leading to the formation of abundant heterointerfaces and optimized active sites. These features significantly enhance the intrinsic catalytic activity for both the hydrogen evolution reaction (HER) and oxygen evolution reaction (OER). The catalyst demonstrates remarkable performance, delivering current densities exceeding 1 A cm^{-2} at low overpotentials in alkaline seawater conditions. Additionally, it exhibits outstanding durability under harsh chloride-containing environments, maintaining stable operation over extended periods. The presence of phosphorus further modulates the electronic structure, improving corrosion resistance and facilitating rapid reaction kinetics. Mechanistic studies reveal that the synergistic interaction between Ru and NiO phases promotes efficient adsorption and desorption of reaction intermediates, thereby accelerating overall water splitting.

Keywords: Second coordination sphere · Single atom · Hydrogen evolution reaction · Modulation

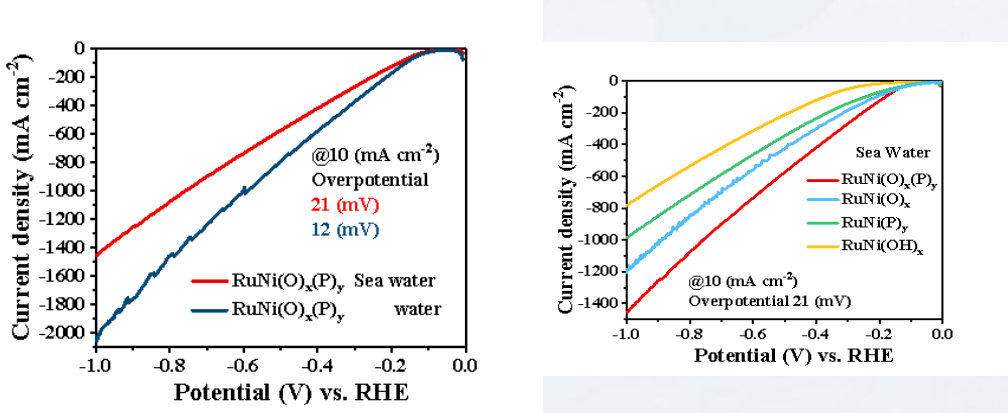

Figure: 12 mV at 10 mA cm^{-2} in 1.0 M KOH aqueous electrolyte 21 mV at 10 mA cm^{-2} in 1.0 M KOH seawater electrolyte

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P-114

The Role of the Hypoxic Pathway in the Bidirectional Correlation Between Myocardial Infarction and Affective Disorders

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The correlation between Myocardial Infarction (MI) and Affective Disorders (AD), including depression and anxiety, markedly elevates patient morbidity and mortality. People with major AD have a 40% to 60% higher risk of developing cardiovascular disorders and eventually having a MI. In India, a person with clinical depression has a 60% chance of having their first heart attack. Furthermore, 20% to 30% of the patients get AD, which makes them 2 to 3 times more likely to die in the next few months [1]. Recent evidence indicates a strong biological connection between MI & AD facilitated by the hypoxic pathway, in addition to behavioral factors. Present study investigates the role of oxygen deprivation as a mechanistic link between cardiac ischemia and psychiatric disorders.

During MI, acute myocardial hypoxia stabilizes Hypoxia-Inducible Factor 1-alpha (HIF-1α), which initiates an inflammatory chain reaction within the body. This promotes the release of pro-inflammatory cytokines that cause neuroinflammation once they cross the blood-brain barrier [2, 3]. This hypoxic stress disrupts neuroplasticity and monoaminergic signaling in brain regions that control emotional regulation. In relation, AD makes myocardial hypoxia worse by causing long-term problems with the HPA axis and too much activity in the sympathetic nervous system. The condition raises the oxygen requirement while also causing peripheral vasoconstriction and endothelial dysfunction, which makes the heart more vulnerable to ischemia [4, 5].

Understanding this hypoxic interaction is essential for clinical manifestation, implying that focusing on the HIF-1α pathway and reducing systemic oxidative stress could provide dual advantages in addressing both cardiac recovery and psychological stability. It is important to include psychiatric care in post-MI care to break this hypoxia-driven feedback loop and improve long-term cardiovascular outcomes.

Keywords: Myocardial Infarction, Affective Disorders, Hypoxia, HIF-1α, Neuroinflammation, Psychocardiology.

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P-115

Efficient Microwave-Assisted Synthesis and Biological Evaluation of Novel 1,4-Dihydropyrimido[1,2-a]benzimidazole Derivatives

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Abstract

The rapid development of new heterocyclic compounds with antimicrobial potential is an important objective in medicinal chemistry. In this study, a series of novel 1,4-dihydropyrimido[1,2-*a*]benzimidazole derivatives were synthesized through a microwave-assisted multicomponent reaction using substituted β-ketoamides, thiophene-2-carbaldehyde, and 2-aminobenzimidazole. The optimized microwave conditions significantly reduced reaction time to 15 minutes and provided excellent yields up to 95%, demonstrating the efficiency of the green synthetic approach. All synthesized compounds were characterized by FT-IR, ^{1}H NMR, ^{13}C NMR, and mass spectrometry techniques. The biological activities of the prepared derivatives were evaluated against selected Gram-positive bacteria, Gram-negative bacteria, and fungal strains using the broth dilution method. Several compounds exhibited promising antibacterial activity, while selected derivatives also showed moderate antifungal performance. The findings highlight microwave irradiation as a powerful strategy for rapid synthesis of biologically active fused benzimidazole scaffolds and indicate that these compounds may serve as useful leads for future antimicrobial drug development.

Keywords: Microwave-assisted synthesis; Benzimidazole derivatives; Heterocyclic compounds; Antibacterial activity; Antifungal activity; Green chemistry; Medicinal chemistry.

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Transition Metal Based Multimetal Electrocatalysts for Hydrogen Evolution Reaction

PRATIBHA ANANT

Abstract

The development of cost-effective and efficient electrocatalysts for the Hydrogen Evolution Reaction (HER) is crucial for sustainable hydrogen production. In this work, a multimetallic coordination framework comprising a quintet of transition metals (Mn, Co, Cu, Ni, and Zn) has been successfully synthesised using 2-methylimidazole as an organic linker. The incorporation of multiple metal centres is expected to induce synergistic electronic effects, enhancing catalytic activity and structural stability.

The synthesised material was systematically characterised using powder X-ray diffraction (XRD), Fourier-transform infrared spectroscopy (FTIR), thermogravimetric analysis (TGA), and CHNS elemental analysis. XRD results indicate the formation of a crystalline framework, while FTIR confirms the coordination between metal ions and the imidazole ligand. TGA analysis demonstrates good thermal stability of the material, and CHNS analysis validates the elemental composition consistent with the proposed structure.

Preliminary electrochemical investigations suggest that the material exhibits promising behaviour toward HER, likely due to the presence of multiple active sites and improved charge transfer characteristics arising from the multimetallic composition. Ongoing studies are focused on detailed electrochemical evaluation and mechanistic insights.

This study highlights the potential of multimetallic imidazole-based frameworks as tunable platforms for next-generation electrocatalysts in hydrogen energy applications.

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Chiral Supramolecular Charge-Transfer Organogels with Emergent Ferroelectricity for Soft Electronics

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Abstract:

Supramolecular charge-transfer (CT) systems offer a compelling route toward soft, biocompatible ferroelectric materials; however, achieving stable, non-centrosymmetric organization in such assemblies remains challenging. Here, we report a chiral organogel constructed from amino acid–conjugated aromatic donor–acceptor pairs that undergo spontaneous self-assembly in a fixed stoichiometric ratio. The integration of amide functionality and molecular chirality promotes cooperative non-covalent interactions, including hydrogen bonding and π–π stacking, leading to highly ordered supramolecular architectures. Charge transfer between donor and acceptor components generates collective dipoles, while synergistic CT interactions and hydrogen bonding drive gelation in a non-aqueous medium. Spectroscopic and microscopic analyses confirm the formation of a chiral, fibrillar network with distinct charge-transfer characteristics. Importantly, the system exhibits thermally robust mechanical properties and switchable dipolar alignment in a non-centrosymmetric arrangement, satisfying the criteria for ferroelectricity. These findings establish a generalizable strategy for designing supramolecular ferroelectrics and highlight their potential in soft electronic and memory devices.

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P-118

Traditionally used Plants by Sahariya Tribe in Jhansi district, Uttar Pradesh

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Abstract

Jhansi district in Bundelkhand regions lies between 25° 27' North latitude and 78° 35' East latitude and about 275 m above sea level. The district is intersected or bounded by three principle rivers, the Pahuj, Betwa, and Dhasan and is home to many important medicinal plants, have a great potential for their conservation and cultivation. A great deal of information about the traditionally used medicinal plants is still intact with the tribal and rural peoples of this region. This paper deals with some traditionally used medicinal plants used by Sahariya tribes in Jhansi district of Uttar Pradesh. The Sahariya tribe, a particularly vulnerable group in Uttar Pradesh, relies heavily on traditional, forest-based herbal medicine for healthcare and other forest products. The present study has revealed 20 species of plants used by Sahariya tribe of this region.

Keywords: Bundelkhand regions, traditionally used, rural peoples, Sahariya tribe, healthcare.

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Development and Evaluation of Trimetazidine and Platelet-Rich Plasma-Based Gel Formulations for Enhanced Diabetic Wound Healing

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Diabetic wound healing is considered as clinically significant challenge because of chronic hyperglycemia along with persistent inflammation, impaired angiogenesis and delayed tissue regeneration[1]. The current study aims to evaluate the therapeutic potential of repurposing both Trimetazidine, an anti-ischemic agent selected through docking, Platelet-rich Plasma (PRP) alone and their combination for enhancing wound healing in diabetic conditions[2], [3]. Diabetes was induced in Sprague-Dawley rats by administering Streptozotocin (35 mg/kg), ip, followed by incision of wound. Gels of Trimetazidine, PRP and their combination were formulated using DOE software and evaluated for physicochemical properties such as viscosity, spreadability, extrudability, pH and drug content. In vitro studies were performed on 3T3-L1 fibroblast cell lines which showed enhanced cell viability, proliferation and cell migration in treated wells. In vivo results demonstrated significant improvement in wound contraction and re-epithelialization in treated groups as compared to diabetic controls. Biochemical parameters assessed showed a reduction in the expression of pro-inflammatory cytokines including IL-6 and TNF-α and increased levels of angiogenic and regenerative markers like VEGF and FGF-10[4], [5]. Histological evaluation using H&E and Masson's Trichrome staining assured improved tissue architecture, collagen deposition and better extracellular matrix remodelling in the treatment groups. Furthermore, ICAM-1 and TGF-β levels were reduced suggesting reduced inflammation and improved cellular interactions. IHC of α-SMA and CD-31 showed positive results for collagen formation and angiogenesis. Also, hydroxyproline and hexosamine estimations were positive for collagen synthesis. Among all groups, combination therapy exhibited the most pronounced effects showing enhanced angiogenesis, reduced inflammation and accelerated wound healing.

Keywords: Diabetes, Diabteic foot ulcer, Angiogenesis

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P-120

Sustainability of Biological Effects in the Pharmaceutical Industry: A Comparative Analysis with India's Market Growth Trends

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Abstract

The pharmaceutical industry plays a pivotal role in advancing global healthcare, yet it faces increasing pressure to integrate environmental, economic, and social sustainability into its operations. This study examines the sustainability of biological production systems within the pharmaceutical sector and compares these findings with the recent growth optimize of the Indian pharmaceutical market. Evidence indicates that environmental sustainability assessments have been conducted for only approximately 0.3% of pharmaceutical products worldwide. Among the evaluated products, environmental impacts vary widely across production technologies, and major impact categories—such as carbon emissions, water usage, energy consumption, and toxicity potential—have not been consistently assessed. This limited and fragmented evaluation restricts a comprehensive understanding of the industry's overall sustainability performance.

This comparison reveals a notable imbalance: economic expansion is robust, yet systematic environmental assessments remain limited. While biological production of (semi)synthetic pharmaceuticals offers potential environmental advantages over conventional chemical synthesis, biologically produced monoclonal antibodies may exhibit higher impacts and require optimization. Aligning rapid market growth with sustainability objectives necessitates comprehensive life-cycle assessments, standardized reporting across impact categories, and coordinated policy and industry initiatives to foster responsible and sustainable development.

Keywords: Pharmaceutical Industry; Sustainability; Biopharmaceuticals; Biological Production; Environmental Impact Assessment; Life Cycle Assessment (LCA).

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P-121

SYNTHESIS AND CHARACTERIZATION OF NOVEL BARBITURIC ACID PIPERIDINIUM SALT DERIVATIVES VIA FOUR COMPONENT REACTION

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Abstract

A series of barbituric acid piperidinium salt derivatives was synthesized through multicomponent one pot green domino reaction involving aromatic aldehydes, 4- hydroxycoumarin, 1,3-dicyclohexylbarbituric acid, and piperidine in methanol. The mechanism likely proceeds through an initial Knoevenagel condensation followed by intramolecular hydrogen bonding, resulting in the formation of piperidinium salts as the exclusive products. Piperidine acted as both, the reactant and the catalyst. The products were formed in good yields for different aldehydes containing electron withdrawing and electron donating groups. The reaction proceeded in mild conditions, in short reaction time and the products were isolated without the use of column chromatography. The products were confirmed by spectroscopic techniques such as FT-IR, MS and 1H NMR.

Keywords: 4-hydroxycoumarin, 1,3-dicyclohexylbarbituric acid, Knoevenagel condensation, piperidinium salts

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Do the precursors used in gCN synthesis influence its ability to catalyze electrochemical water splitting?

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Amidst rising global energy demands and declining fossil fuel resources, hydrogen energy emerged as a clean, renewable and sustainable alternative form of energy. However, achieving high efficiency in hydrogen energy conversion depends on the development of efficient and stable electrocatalyst. Graphitic carbon nitride (gCN) has emerged as a promising non-metal electrocatalyst for electrochemical water oxidation ascribed to its structural, physical and chemical features and cost effectiveness. Its 2D polymeric structure with the unsaturated nitrogen atoms provides a large number of strong coordinating Electron-Donor-N-sites which enhances the catalytic efficiency. However, the electrocatalytic activity of gCN depends mainly on the precursors used for its synthesis, which dictate its composition and morphology. As a result, the purpose of this study was to investigate into how the precursors used in gCN synthesis affected its ability to catalyze electrochemical water splitting. Three major precursors, namely, urea, melamine, and melamine-cyanuric acid, were used. Among all, gCN derived from melamine - cyanuric acid complex exhibited better hydrogen evolution reaction (HER). At an optimal catalyst loading of 0.5mg cm^{-2}, it exhibits excellent HER efficiacy, achieving a low overpotential of ~220 mV and a high current density around ~0.88A cm^{-2} at a potential of -1.09 V(RHE) in 1M KOH solution with an excellent stability over 48 hours at 10 mA cm^{-2}.

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P-123

A COMPREHENSIVE REVIEW ON EMERGING TRENDS IN SPRINKLE PELLETS FOR PAEDIATRIC-FRIENDLY ANTIBIOTIC DELIVERY TO ENHANCE MEDICATION ADHERENCE

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ABSTRACT

Sprinkle pellets constitute an advanced multi-particulate oral drug delivery system engineered to overcome the specific challenges of paediatric antibiotic therapy. These dosage forms comprise small, discrete, drug-loaded pellets that can be administered either intact or sprinkled onto soft food vehicles without compromising their release profile. This design is especially advantageous for children who have difficulty swallowing conventional tablets or capsules, thereby enhancing patient compliance and simplifying administration. [1] The preparation of sprinkle pellets encompasses essential pre-formulation studies, selection of inert cores, drug layering, and application of functional polymer coatings to achieve effective taste masking and controlled drug release. A range of manufacturing techniques-including extrusion-spheronization, drug layering, hot-melt extrusion, cryopelletization, and various spray-based methods-are utilized to produce uniform, stable pellets possessing optimal physicochemical properties. [2] Although sprinkle pellets offer numerous benefits, they present certain challenges, such as difficulties in taste masking, issues with dose uniformity, potential stability concerns when mixed with food vehicles, and manufacturing complexity. These limitations can be mitigated through advanced coating technologies, optimized process parameters, and patient-centric formulation strategies. [3] Sprinkle pellets provide key advantages, including flexible dosing, improved bioavailability, reduced gastrointestinal irritation, and superior stability relative to liquid formulations. Their compatibility with modified-release technologies further establishes them as a versatile platform for paediatric drug delivery. [4] Future advancements in sprinkle pellet systems are directed toward personalized medicine approaches, the development of novel functional coatings, and integration with emerging drug delivery technologies to expand their clinical applicability. [5] In conclusion, paediatric-friendly sprinkle pellets represent a promising, flexible, and patient-centric solution for antibiotic delivery. They align with contemporary pharmaceutical and regulatory expectations while substantially improving therapeutic outcomes and medication adherence in children.

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P-124

Effective electro-catalyst for oxygen evolution reaction

Deepshikha

ABSTRACT

Heptazine-based carbon nitride frameworks have emerged as promising for electro-catalytic applications due to their tunable electronic structure and high nitrogen content. In this study, a heptazine ring-containing melem-Ag hybrid material was successfully synthesized and evaluated for its oxygen evolution reaction (OER) activity. The formation and structural evolution of the material from melamine to melem and subsequentlys to melem-Ag were systematically confirmed using X-ray diffraction (XRD) and mass spectrometry analyses. Optical properties investigated through UV-Vis diffuse reflectance spectroscopy (UV-DRS) revealed a progressive narrowing of the band gap, indicating enhanced visible-light absorption and improved electronic conductivity upon silver incorporation. The reduction in band gap from melamine to melem and further to the melem-Ag composite highlights the role of Ag in modulating the electronic structure of the heptazine framework. Electrochemical performance assessed via cyclic voltammetry (CV) demonstrated that the synthesized melem-Ag material exhibits significant catalytic activity toward the oxygen evolution reaction. The improved OER performance is attributed to the synergistic interaction between the heptazine network and Ag species, which facilitates charge transfer and enhances catalytic efficiency.

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Electrocatalyst based on Transition metal for Oxygen Reduction Reaction

Kumari Sadhana

Abstract

The development of efficient and low-cost electrocatalysts for the Oxygen Reduction Reaction (ORR) is essential for advancing energy conversion technologies such as fuel cells and metal-air batteries. In this study, a nickel ferrite ($NiFe_2O_4$)-graphitic carbon nitride ($g\text{-}C_3N_4$) composite has been successfully synthesized and explored as a potential ORR electrocatalyst. The integration of spinel nickel ferrite with $g\text{-}C_3N_4$ is expected to enhance catalytic performance through synergistic interactions, improved conductivity, and increased availability of active sites. The synthesized composite was systematically characterized using powder X-ray diffraction (XRD), Fourier-transform infrared spectroscopy (FTIR), thermogravimetric analysis (TGA), and CHNS elemental analysis. XRD analysis confirms the formation of crystalline $NiFe_2O_4$ with characteristic diffraction peaks, while FTIR spectra verify the presence of $g\text{-}C_3N_4$ and metal-oxygen bonding interactions.

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Novel Tacrine Analogs for Lung Cancer: *In Vivo* Efficacy and Toxicity Evaluation

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Telomerase is a highly promising molecular target for cancer therapy due to its essential role in sustaining the unlimited proliferative capacity of malignant cells. In this study, an integrated computational approach was employed to design novel tacrine-based inhibitors targeting telomerase for lung cancer treatment. Initially, a robust pharmacophore model was developed by identifying key structural and functional features required for effective telomerase inhibition. This model was then used for virtual screening to identify potential lead scaffolds with favorable binding affinity.

Based on these computational insights, a series of structurally distinct "dog-bone"-shaped tacrine analogs was rationally designed to enhance target interaction and biological activity. A total of 25 compounds were synthesized and subjected to preliminary in silico and in vitro screening. The most promising candidates were shortlisted, and the top three compounds were further evaluated through *in vivo* studies using ICR mice.

These compounds demonstrated significant anticancer activity in lung cancer models, including improvement in tumor alveolar architecture and modulation of key biochemical markers such as TNF-α, CRP, LDH, and GGT, compared to 5-fluorouracil and BIBR 1532. Acute toxicity studies, conducted as per OECD Guideline 420, confirmed their safety and helped determine the maximum tolerated dose. Overall, this study identifies a promising lead compound for further anticancer development.

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P-127

Chemoselective Intramolecular Rauhut-Currier reaction on a acyclic labile framework

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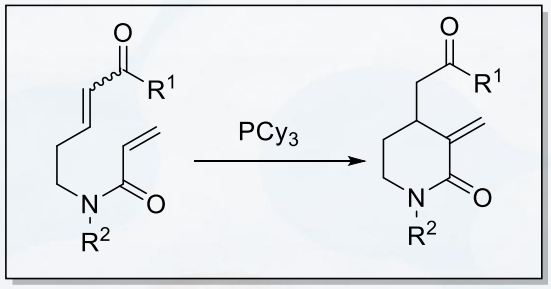
Abstract: Vinylogus version of the Morita-Baylis-Hillman (MBH) reaction is known as Rauhut-Currrier (RC) reaction.[1] intramolecular Rauhut-Currier (IRC) reactions, are popular methods for construction of carbcyclic or hetrocyclic framework. Herein we report an IRC reaction, on a acyclic labie framework using acrylamide as a source of initial enolate.[2] Tricyclohexylphosphine (PCy_3) was used as a stable, commercial, and easy to use nucleophilic catalyst.



Key words: Rauhut-Currier; Morita-Baylis-Hillman; phosphine

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Electrochemical access to the synthesis of Benzimidazo-quinazolinones fused Heterocycles and their biological evaluation

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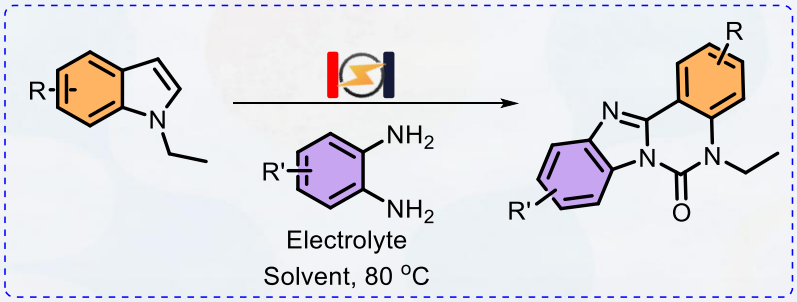
Abstract:

A one-pot, two-step electrochemical protocol has been developed for the synthesis of benzimidazo-quinazolinone (BZQ)-based tetracyclic heterocycles, providing an operationally simple, sustainable, and atom-economical route that obviates the need for traditional oxidants and metal catalysts. In an undivided cell equipped with carbon electrodes, indole is subjected to constant-current electrolysis in the presence of an appropriate electrolyte/solvent system under stirring at 80 °C. Subsequent addition of substituted phenylenediamines (PDAs) in the same cell furnishes the desired BZQ scaffolds in moderate to good yields, without any external oxidant or base. The products were purified by column chromatography and recrystallization, and their structures were unambiguously confirmed by HRMS, ^{1}H NMR, and ^{13}C NMR analyses. Given that BZQ-type heterocycles are well documented to exhibit potent biological activities, antimicrobial evaluation of the synthesized compounds is currently underway. In parallel, computational studies are planned to gain deeper insight into the structural and electronic features governing their properties.



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