33rd CRSI National Symposium in Chemistry and CRSI-ACS Lectures

Organised by
Dr. Reddy's Laboratories Ltd.

Hyderabad, India
July 4th - 6th, 2024

PROGRAM GUIDE

WELCOME

Dear CRSI National Symposium Attendees,

The Chemical Research Society of India (CRSI) was established in early 1999 as part of the 50th anniversary celebration of India's independence and has completed 25 glorious years! The main objectives of the CRSI are to recognize, promote and foster talent in Chemistry and Chemical Sciences and to improve the quality of Chemical Education at all levels.

We are delighted that the 33rd CRSI-National Symposium in Chemistry (CRSI-NSC-33) and the CRSI-ACS lectures will be held at Dr. Reddy's Laboratories Ltd., Bachupally Campus, Hyderabad, during July 4-6, 2024. This is the first NSC to be Organised by and in an Industrial setup, and we greatly appreciate the generous support of the colleagues at Dr. Reddy's Laboratories for organizing this event at their Leadership Academy venue. On behalf of the CRSI, I have great pleasure in welcoming all the participants of this symposium. CRSI also specially welcomes the participants invited through our strong partnership programme with the American Chemical Society.

NSC-33 will have several CRSI Medal lectures, Endowment lectures, Award lectures and CRSI-ACS lectures. Close to 100 young researchers/students will present posters covering all areas of Chemistry. CRSI and the organizers have put together an exciting programme and we hope that this would allow the participants build relationships to advance chemical science and allied fields in academics and in industry.

Sincerely,

Uday Maitra

Uday Maitra
President
Chemical Research Society of India

The Chemical Research Society of India (CRSI) was established in 1999 as part of the 50th anniversary celebrations of the country's independence. Currently, CRSI represents more than 3000 lifetime members, who participate in the study, practice, teaching and promotion of Chemistry. The main objectives of the CRSI are to recognize, promote and foster talent in Chemistry and Chemical Sciences and to improve the quality of Chemical Education at all levels. The CRSI organizes conferences, seminars, workshops, symposia and other related programs to facilitate and promote research in all branches of Chemistry. The society has active collaboration with the Royal Society of Chemistry (RSC), London, the American Chemical Society (ACS), Asian Chemical Editorial Society (ACES), the German Chemical Society (GDCh) and the French Chemical Society.

WELCOME

American Chemical Society is delighted to be a part of the 33rd Chemical Research Society of India's (CRSI) National Symposium on Chemistry in Hyderabad, well-known as India's pharma capital.

The symposium showcases the best of chemical sciences research and recent trends from India and across the world, bringing together eminent scientists, researchers and technologists from academia and industry.

The 33rd CRSI-National Symposium is being hosted by Dr. Reddy's Laboratories, India's leading pharmaceutical company, at its Leadership Academy, Bachupally campus, Hyderabad from July 4th to 6th, 2024, under the auspices of the CRSI.

ACS is one of the world's largest scientific organizations with more than 2,00,000 individuals in our global community across 140 countries. Our objective is to promote advancement of the chemical enterprise and its practitioners for the benefit of Earth and all its people. In India, we cherish our partnership with the CRSI, a leading chemical society.

We would like to congratulate CRSI for completing 25 years and are happy to be part of its 25th anniversary celebrations this year. On this celebratory occasion, we are proud to announce a special collection across different ACS journals, showcasing research in chemistry and allied sciences from India as well as a special collection of articles from Journal of the American Chemical Society (JACS) from the last 25 years.

The symposium will feature ACS lectures by leading scientists, Professor Erick M Carreira, Editor in Chief: JACS, Professor Shana J Sturla, Editor-in-Chief: Chemical Research in Toxicology and Professor Praveen Linga, Executive Editor: Energy & Fuels.

We would like to thank Dr. Rakeshwar Bandichhor of Dr. Reddy's Laboratories, Dr. Srinivas Oruganti of Dr. Reddy's Institute of Life Sciences, Professor Uday Maitra, President, CRSI, Professor N Jayaraman, Secretary General, CRSI, and other colleagues at CRSI & Dr. Reddy's Laboratories for their support in organizing this symposium.

Wish you a stimulating and productive symposium.

Deeksha Gupta.

Deeksha Gupta
American Chemical Society

The American Chemical Society (ACS) is the world's largest scientific society, with nearly 157,000 members representing 140 countries. With services and programs spanning research, publications, professional development, grants and scientific meetings, ACS is at the forefront of the evolving worldwide chemistry enterprise.

ACS has become the premier professional home for chemists, chemical engineers and related professions around the globe through its nearly 50 peer-reviewed journals, Chemical and Engineering News, research discovery applications like SciFinder®, 185 local sections, 32 technical divisions, 17 international chemical sciences chapters and more than 10 scientific meetings offered each year. ACS has also established seven strategic alliances and partnerships with international chemical societies. With a professional chapter in Mumbai and student chapters throughout the country, ACS is connecting chemical professionals and expanding its services to members in India and the region.

WELCOME

Dr. Reddy's Laboratories Ltd. is delighted and honoured to host the 33rd Chemical Research Society of India National Symposium in Chemistry (CRSI-NSC-33) being held at our Leadership Academy, Bachupally Campus, Hyderabad from July 4th — 6th, 2024. The symposium would bring together eminent scientists, young researchers and technologists from across academia and industry to provide a platform for presenting and discussing their achievements and newer research directions in the chemical and allied sciences with aims to contribute towards pursuit and promotion of chemistry for service to humanity. This conglomeration would serve to create opportunities to build long-lasting collaborative endeavors in the frontier areas of chemistry.

Dr. Reddy's Laboratories Ltd. is an integrated pharmaceutical company committed to providing affordable and innovative medicines for healthier lives across the world, driven by the purpose "Good Health Can't Wait" that signifies our empathy towards patients' globally unmet medical needs. We leverage our research and development expertise based on sound scientific principles and in-depth knowledge, end-to-end manufacturing know-how and progressive digital technology to deliver on our promises to patients and make the world a healthier place. The company is headquartered in Hyderabad, India and currently serves over half a billion patients worldwide. The company is working aggressively towards target of reaching over 1.5 billion patients by-2030.

Dr. Reddy's Laboratories Ltd. is proud to be part of the event and welcomes all eminent scientists and researchers, council members and dignitaries from CRSI and ACS. We would like to take this opportunity to congratulate CRSI for completing 25 years and are happy to be part of its 25th anniversary celebrations this year.

My best wishes to CRSI, ACS and Dr. Reddy's for organizing an extremely important event for scientists and researchers across academia and industry.

Sincerely,

Sushrut Kulkarni
Global Head – Integrated Product Development Organization
Dr. Reddy's Laboratories Ltd.

Dr. Reddy's Laboratories Ltd. (NYSE: RDY) is an integrated pharmaceutical company committed to providing affordable and innovative medicines for healthier lives and is headquartered in Hyderabad, India.

Through its three businesses - Pharmaceutical Services & Active Ingredients, Global Generics and Proprietary Products - Dr. Reddy's offers a portfolio of products and services including APIs, custom pharmaceutical services, generics, biosimilars and differentiated formulations.

Our major therapeutic areas of focus are gastrointestinal, cardiovascular, diabetology, oncology, pain management and dermatology. Dr. Reddy's operates in markets across the globe. Our major markets include the USA, Russia and CIS, and India.

AGENDA

Dr. Reddy's Laboratories, Leadership Academy

DAY 1: THURSDAY, 04 JULY	
8:00 AM - 9:00 AM	Onsite Registration, Tea and Networking.
Inauguration	
9:00 AM - 9:05 AM	Welcome of Dignitaries
9:05 AM - 9:10 AM	Lightening of the Lamp
9:10 AM - 9:25 AM	Welcome Address by Dr. Rakeshwar Bandichhor, Vice President and Head of Chemistry-API, Dr. Reddy's Laboratories.
9:25 AM - 9:40 AM	Remarks from Chief Patron, Mr. G. V. Prasad, Co-Chairman & Managing Director, Dr. Reddy's Laboratories Ltd.
9:40AM - 9:50 AM	General Remarks by Prof. Goverdhan Mehta, UOH.
9:50 AM - 10:00 AM	Remarks from Patron, Mr. Sushrut Kulkarni, Global Head of IPDO, Dr. Reddy's Laboratories Ltd.
10:00 AM - 10:10 AM	Remarks from Dr. James Milne, President, ACS Publications.
10:10 AM - 10:20 AM	Remarks from Dr. Deeksha Gupta, Director, Global Strategy for Society Programs, ACS.
10:20 AM - 10:25 AM	'About CRSI' by Prof. N. Jayaraman, Secretary General, CRSI.
10:25 AM - 10:55 AM	Presidential Address by Prof. Uday Maitra, President, CRSI.
10:55 AM - 11:00 AM	Remarks from Dr. Srinivas Oruganti, Director, DRILS, Hyderabad.
11:00 AM - 11:30 AM	High Tea and Networking
Session 1: **Chair of the Session: Prof. Jitendra K. Bera, IIT Kanpur**	
11:30 AM - 12:10 PM	**Chemistry in the Extreme Quantum Regime** By Prof. Balakrishnan Naduvalath, University of Nevada, USA (CRSI Medal)

AGENDA

12:10 PM - 12:40 PM	**Strained Ring Systems for the Construction of Heterocyclic Compounds** By Prof. T. Punniyamurthy, IIT Guwahati (Silver medal Lecture)
12:40 PM - 1:00 PM	**Sillen Aurivillius phases for energy harvesting** By Prof. Ujjal K. Gautam, IISER, Mohali. (Bronze Medal Lecture)
1:00 PM - 2:00 PM	Lunch and Networking
2:00 PM - 3:00 PM	General Body Meeting.
2:00 PM - 4.00 PM	**Poster Session 1** **Evaluation Committee** **Chair Persons: Prof. Nitin Patil (IISER, Bhopal) and Prof. Rupam Dinda, NIT, Rourkela.** Prof. V. Sridharan, University of Hyderabad. Prof. Raja Angamuthu, IIT, Kanpur Prof. Vidya D. Avasare, Ashoka University Prof. T. J. Dhilip, Kumar IIT Ropar. Prof. Oruganti Anjaneyulu, Central university of Karnataka Prof. Sivapriya Kirubakaran, IIT Gandhinagar
4:00 PM - 4:30 PM	Tea Break and Networking
Session 2: Chair of the Session/Coordinator: Prof. Uday Maitra, IISc, Bangalore	
4:30 PM - 5:15 PM	**Interactive Session on "The Future of Scientific Meetings"** Prof. Goverdhan Mehta, University of Hyderabad Prof. Erick M. Carreira, ETH Zurich Dr. Rakeshwar Bandichhor-Dr. Reddy's laboratories Ltd.
5:15 PM - 5:45 PM	**A Sustainable Approach to Store CO2 Permanently via Clathrate Hydrates** By Prof. Praveen Linga (National University of Singapore) - ACS Lecture
5:45 PM - 6:05 PM	**Rapid Estimation of Kinetic Barriers in (Bio)Molecular Systems** By Prof. Neelanjana Sengupta, IISER Kolkata. (Bronze Medal Lecture)
7:00 PM - 9:00 PM	Dinner

AGENDA

DAY 2: FRIDAY, 05 JULY

Session 1: **Chair of the Session: Swagata Dasgupta, IIT Kharagpur**	
9:15 AM - 9:45 AM	**Research led innovation: The Role of Publicly Funded Institutions** Talk by Dr. Radha Rangarajan, Director, CDRI, Lucknow.
9:45 AM - 10:15 AM	**Targeting the Tumor Immune Microenvironment with Small Molecules for Cancer Therapy** By Dr. Murali Ramachandra, CEO, Aurigene Oncology, Bangalore.
10:15 AM - 10:45 AM	Talk by Prof. Erick M. Carreira, ETH Zurich. (ACS Lecture)
10:45 AM - 11:00 AM	Talk By Pharmadem Representative
11:00 AM - 11:30 AM	Tea and Networking
Session 2: **Chair of the Session: Prof. V. Chandrasekhar, TIFR, Hyderabad**	
11:30 AM - 12:00 PM	**Mapping chemical landscapes in the genome: from oxidative stress and toxicants to cancer drugs** By Prof. Shana J. Sturla, ETH-Zurich, Switzerland (ACS Lecture)
12:00 PM - 12:30 PM	**Ligand-Enabled Gold Redox Catalysis** By Dr. Nitin T. Patil, IISER, Bhopal (CNR Lecture)
12:30 PM - 12:50 PM	**Applications of N-heterocyclic Germylenes** By Prof. S. Nagendran, IIT Delhi (Bronze Medal Lecture)
12:50 PM - 2:00 PM	Lunch Break
2:00 PM - 4:00 PM	**Poster Session 2** **Evaluation Committee** **Chair Persons: Prof. Anil Kumar (BITS Pilani) and Prof. Vinod Kumar Tiwari (BHU, Varanasi)** Prof. V. Sridharan, University of Hyderabad. Prof. Raja Angamuthu, IIT, Kanpur Prof. Vidya D. Avasare, Ashoka University Prof. T. J. Dhilip, Kumar IIT Ropar. Prof. Oruganti Anjaneyulu, Central University of Karnataka Prof. Sivapriya Kirubakaran, IIT Gandhinagar
4:00 PM - 4:30 PM	Tea Break and Networking

AGENDA

Session 3: Chair of the Session: Prof. A. T. Biju-IISc, Bangalore	
4:30 PM - 4:50 PM	**Spin-State Switching in Dynamic Molecules** By Prof. Sanjit Konar, IISER, Bhopal (Bronze Medal Lecture)
4:50 PM - 5:30 PM	**Regio- and Stereoselective Synthesis of Functionalised N-Heterocycles and Carbocycles and Synthetic Diversification of Remdesivir** By Prof. Vibha Tandon, Director, IICB, Kolkata (AVR Lecture)
5:30 PM - 5:50 PM	**Surface and Interface Chemistry of Nanocrystals for optoelectronics** By Prof. R. Geetha Balakrishna, Jain University-Bangalore (Bronze Medal Lecture)
5:30 PM - 6:10 PM	**Polymer Crystallization-Driven Functional Two-Dimensional Assemblies** By Prof. Anindita Das, IACS, Kolkata (ACES-CRSI Early Career Award)
6:10 PM - 6:30 PM	**Complexes for Efficient Catalysis and Sustainable Energy Harvesting** By Prof. Maheswaran Shanmugam, IIT Bombay (Bronze Medal Lecture).
7:00 PM - 9:00 PM	Dinner

AGENDA

DAY 3: SATURDAY, 06 JULY

Session 1:
Chair of the Session: Dr. Rajeev Rehani Budhdev, Head, API R&D, IPDO, Dr. Reddy's Laboratories Ltd.

9:15 AM - 9:55 AM	**Advanced energy materials for clean energy conversion** By Prof. Tharamani C. Nagaiah, IIT Ropar (AVR Lecture)
9:55 AM - 10:15 AM	**Sustainable Synthesis of Next Generation of Responsive Polymers** By Prof. Sanjib Banerjee, IIT Bhilai (Bronze Medal Lecture)
10:15 AM - 10:45 AM	**The Role and Relevance of Chemistry in the Industry 5.0 Driven Interdisciplinary Space** By Prof. Narahari Sastry, IIT Hyderabad (Silver Medal Lecture)
10:45 AM - 11:05 AM	**Hierarchical Structure Formation in Poly(lactides): Role of Polymer Chain Packing on the Emissive Properties of Chromophore Embedded Poly(Lactide)s** By Dr. Bhoje Gowd Erathimmanna, CSIR-NIIST, Thiruvananthapuram (Bronze Medal Lecture)
11:05 AM - 11:30 AM	Tea Break and Networking

Session 2:
Chair of the Session: Prof. Akhila Kumar Sahoo, University of Hyderabad

11:30 AM - 12:00 PM	**Deciphering Methyl Transferase Mediated Mechanism of Antibiotic Resistance** By Prof. Ruchi Anand, IIT Bombay (Charusita Chakravarty Lecture)
12:00 PM - 12:20 PM	**Vinylogy for Enantioselective Desymmetrization** By Prof. Ravi Prakash singh, IIT Delhi (Bronze Medal Lecture)

AGENDA

12:20 PM - 12:40 PM	**Metal-Free Synthesis of Bioactive Molecules** Prof. Satyendra Kumar Pandey, BHU (Bronze Medal Lecture)
12:40 PM - 1:00 PM	**Synthesis of Functional π-Conjugated Small Molecules: From Structure to Function** By Dr. Surya Prakash Singh, IICT, Hyderabad (Bronze Medal Lecture)
1:00 PM - 2:00 PM	Lunch Break
Announcement of Awards and Medals Presentation	
2:00 PM - 2:20 PM	Announcement of Awards (Medal lectures and Posters)
2:20 PM - 2:40 PM	**Vote of Thanks** By Prof. N. Jayaraman, Secretary General, CRSI. By Dr. Rakeshwar Bandichhor, Convenor of the CRSI National Symposium in Chemistry. By Dr. Srinivas Oruganti, Co-convenor of the CRSI National Symposium in Chemistry

SPEAKERS

FEATURED SPEAKER

Prof. Balakrishnan Naduvalath
Professor, Department of Chemistry,
University of Nevada, Las Vegas

04 July | 11:30 AM - 12:10 PM

Chemistry in the Extreme Quantum Regime

Profile: Dr. Balakrishnan Naduvalath is Professor of Chemistry at University of Nevada, Las Vegas (UNLV). He received Ph.D. in Theoretical Chemistry from Indian Institute of Technology, Kanpur (1993) under the supervision of Prof. N. Sathyamurthy and carried out postdoctoral research at University of Copenhagen with Prof. Gert Billing (1993-1996) and at Harvard-Smithsonian Center for Astrophysics with Prof. Alexander Dalgarno (1996-2001). He has authored/co-authored over 160 peer-reviewed publications and several book chapters. His research interests are directed to the description of atomic and molecular collisions and chemical reaction dynamics in overlapping areas of Chemistry, Physics and Astrophysics. He is an elected Fellow of the American Physical Society (since 2009).

Abstract: A central goal in chemistry is the absolute control of quantum states of both reactants and products. This is not achievable at normal temperatures due to a thermal population of internal quantum states. By cooling atoms and molecules to temperatures close to absolute zero and confining them in electromagnetic traps controlled chemistry experiments can be performed between trapped atoms and molecules in the deep quantum regime. This allows unprecedented level of control over initial quantum states, molecular orientation, and even final states in certain cases. I will discuss recent theoretical progress in describing chemical reactions and molecular interactions in this regime and the prospects and challenges ultra-cold molecules offer in uncovering many aspects of chemistry that are yet to be revealed at its most fundamental level.

SPEAKERS

FEATURED SPEAKER

Prof. T Punniyamurthy
Indian Institute of Technology, Guwahati

04 July | 12:10 PM - 12:40 PM

Strained Ring Systems for the Construction of Heterocyclic Compounds

Profile: Prof. Punniyamurthy completed his graduate studies from Bharathidasan University and Ph.D. from IIT Kanpur under the supervision of Prof. J Iqbal (1995). He pursued postdoctoral research at North Dakota State University (Prof. M P Sibi), Kyushu University (Prof. T Katsuki) and Montpellier University (Prof. A Vioux and Prof. J E E Moreau). In 2001, he joined IIT Guwahati and served as the Head, Department of Chemistry, Dean of Faculty Affairs and Chief Vigilance Officer. His research interest is focused on stereoselective heterocycle synthesis using strained ring systems and directed C-H functionalization. He has guided 9 postdocs, 29 Ph.D. scholars and 39 M.Sc. students till date. He has published 190 research papers and edited a book on "Transition-Metal-Catalyzed C-H Functionalization of Heterocycles", Wiley, and special topic on "C-H Bond Functionalization of Heterocycles", Synthesis. He is visiting Professor at Oxford University, Kyushu University and The Scripps Research Institute, San Diego, and recipient of various prestigious fellowships such as UKIERI, JSPS, Fulbright and J C Bose National Fellowships. He is an elected Fellow of Indian Academy of Sciences (2015), The National Academy of Sciences, India (2018), Indian National Science Academy (2022) and Royal Society of Chemistry (2014). He received the CRSI Bronze (2015) and Silver (2023) medals and presently serves as Associate Editor of SynOpen.

Abstract: Transition-metal-catalyzed directed C-H functionalization provides an effective synthetic tool for the regioselective carbon-carbon and carbon-heteroatom bond formation. Further, cycloaddition of strained rings, more specifically, asymmetric cycloaddition, has been widely exploited for rapid construction of bio-relevant cyclic frameworks. Our group has made a significant contribution in these active topics since the past decade. Consequently, our research topic focuses on showcasing miscellaneous methodologies and their subsequent incorporation in fabricating hetero-atom embedded cyclic structural motifs. Further, using metalla-photoredox catalysis as an alternative sustainable and greener aspect of accomplishing C-H bond functionalization would be an interesting topic to anticipate and expand our area of research.

SPEAKERS

FEATURED SPEAKER

Dr. Ujjal K. Gautam
IISER Mohali,

04 July | 12:40 PM - 1:00 PM

Sillen Aurivillius phases for energy harvesting applications

Profile: Dr. Ujjal K. Gautam is an Associate Professor at the Indian Institute of Science Education and Research (IISER) Mohali. He completed his master's studies in Chemistry from IIT Delhi in 1999 and Ph. D. from the SSCU, IISc in 2006. Thereafter, he was a postdoctoral researcher at National Institute for Materials Sciences, Tsukuba, Japan for two years before joining a tenure track ICYS independent researcher position at the same institution. Dr. Gautam joined Jawaharlal Nehru Centre for Advanced Scientific Research in 2011 as a Ramanujan Fellow and worked until 2015. In 2015, he joined IISER Mohali as an Assistant Professor. His research interest revolves around developing high-quality nanostructured materials for renewable energy harvesting and environmental remediation. He has published over 120 papers in high-quality peer-reviewed journals and also owns about 8 patents. He has given over 50 invited talks at national and international conferences. Dr. Gautam recently received the prestigious MRSI Medal 2023.

Abstract: Sillen-Aurivillius oxyhalides (SA), consisting of layers of fluorite [Bi2O2], perovskite [An–1BnO3n+1], and halide [X] (A: Sr2+, Bi3+, etc.; B: Nb5+, Ta5+, etc.; n = 1,2,3, etc.) have immense structural flexibility and narrow band gaps. Using these, I will counter two common notions: (i) that photocatalysts degrade upon use by taking two reactions: H2O2 photo-production and rhodamine-B (RhB) photo-degradation; (ii) that the degradation of RhB lacks commercial prospects even after 54 years of research by showing that SA phases convert RhB to expensive Rhodamine-110 (Rh110) and while doing so, it continues to improve its activity for 300 h due to 'self-activation'. The commercial production Rh110 is challenging due to the formation of side-products, leading to high costs. We have been able to produce Rh110 using Bi4TaO8Br as a photocatalyst. The catalyst is not just stable over 30 catalytic cycles but also gets activated in successive cycles to produce 88% yield. Similarly, we used them to convert O2 to H2O2 with a high photon conversion efficiency of 17%. Here too, the catalyst gets activated continuously to increase the H2O2 yield by ~200% to >6 mmol/h/g.

SPEAKERS

FEATURED SPEAKER

Dr. Praveen Linga
Professor, Department of Chemical and Biomolecular Engineering, National University of Singapore

04 July | 5:15 PM - 5:45 PM

A Sustainable Approach to Store CO2 Permanently via Clathrate Hydrates

Profile: Praveen Linga is a Professor in the Department of Chemical and Biomolecular Engineering at NUS. He holds a Ph.D. from the University of British Columbia under the supervision of Professor Peter Englezos. He obtained his Bachelor's degree from University of Madras and Master's degree from IIT Kharagpur in chemical engineering from India. His research interests are in the areas of clathrate (gas) hydrates, storage and transport of fuels, carbon dioxide capture, storage & utilization (CCS & U) seawater desalination, and recovery of energy. Up to date, he has published more than 170 research articles and delivered more than 100 invited talks and seminars. He is recognized among the World's Most Influential Scientific Minds and Highly Cited Researcher in Engineering by Clarivate Analytics, recognized as Young Alumni Achiever by IIT Kharagpur and received Outstanding Asian Researcher and Engineer Award by the Society of Chemical Engineers Japan. Currently, he serves as an Executive Editor in Energy & Fuels journal of ACS publications. He is also an invited Editorial Advisory Board member of several journals: **including Applied Energy, Current Opinion in Chemical Engineering.**

Abstract: Climate change is known to be dominantly caused by the increased concentration of greenhouse gases in the atmosphere, in particular carbon dioxide (CO2). The clathrate hydrate process has been demonstrated over the years as promising technology for innovative applications like natural gas storage, carbon dioxide capture, seawater desalination, cold energy storage etc. CO2 hydrate, a solid compound made of molecular CO2 enclathrated in crystalline lattices formed by water molecules, is an attractive option to capture and for long-term CO2 sequestration. Methane (CH4) hydrates in oceanic sediments have been stable for millions of years. As a natural analog, is it possible to store CO2 in the form of hydrates oceanic sediments forever? In this presentation, the state of the art on clathrate hydrate technology pertaining to carbon capture and storage will be discussed in detail. Furthermore, future research and development opportunities and pathways for commercialization will be discussed.

SPEAKERS

FEATURED SPEAKER

Dr. Neelanjana Sengupta

IISER Kolkata

04 July | 5:45 PM - 6:05 PM

Rapid Estimation of Kinetic Barriers in (Bio)Molecular Systems

Profile: Neelanjana Sengupta adopts a multi-disciplinary approach to probe physico-chemical underpinnings of (bio)molecular structure, function, thermo-kinetics and dynamics. She obtained her M.Sc. at the Univ. of Burdwan, and her PhD at UC Irvine, USA. She joined CSIR-NCL as a scientist in the Physical Chemistry Division (2008), and began her independent theoretical and computational explorations. She moved to IISER Kolkata in 2016. She has been awarded the CSIR-Raman Research Fellowship (2015) and the Humboldt Fellowship in the Experienced Researcher Category (2020). Vigyan Prasar recognized her contributions in “Future Hopes” in the Vigyan Vidushi compendium (2023).

Abstract: A persistent challenge in protein structure-function studies is the accurate and efficient capture of high transition barriers in complex energy landscapes. Our recent algorithm, Expectation Maximized Molecular Dynamics (EMMD) incorporates a statistical inference-based approach for rate-limiting transitions. The algorithm demonstrates significant efficiency in predicting experimentally recognized patterns in diverse systems such small biomolecules, intrinsically disordered proteins, kinases, and membrane associated proteins. Further efforts focus on automated collective variable search and seamless implementations in multi-component biomolecular systems.

SPEAKERS

FEATURED SPEAKER

Dr. Radha Rangarajan

Director, Central Drug Research Institute, India.

05 July | 9:15 AM to 9:45 AM

Research led innovation: The Role of Publicly Funded Institutions

Profile: Dr. Radha Rangarajan is currently Director, Central Drug Research Institute, a constituent laboratory of the Council of Scientific and Industrial Research, India. She has been involved in translational research and product development, with antimicrobial resistance (AMR) as a focus, for the last two decades.

Dr. Rangarajan worked in the Drug Discovery division of Dr. Reddy's Laboratories between 2003 and 2009. Thereafter, she co-founded Vitas Pharma, an antibacterial drug discovery and development company. She leveraged public-private partnerships to build a highly efficient innovation platform delivering optimized candidates, patents and companion diagnostics. In 2020, she took on the role of Chief Technology Officer at HealthCubed, a medical devices company, where she was responsible for product development, clinical validation, manufacturing and regulatory affairs.

Dr. Rangarajan received the "Biotech Startup of the year" award at the Bengaluru Tech Summit (2021), the Federation of Indian Chambers of Commerce and Industry (FICCI) Award of Excellence for Women in R&D (2019) and the Discovery Award from the Longitude Prize Committee, UK for Vitas Pharma (2016).

Dr. Rangarajan has served as an expert for CARB-X, a global non-profit organization that supports antibacterial innovation. She is on the Board of Governors of the Tres Cantos Open Lab Foundation and a member of the selection committee for the Sree Padmavathi Venkateswara Foundation for grants in Translational Biomedical Sciences. She is a member of the Hub Governing Body of BITS BioCyTiH Foundation, domain expert for TIFAC in the areas of Chemical, Pharmaceutical, Healthcare and Medical Sciences, member of the selection Committee for DST INSPIRE Faculty Fellows and member of the scientific program committee of iHub-Data, IIIT, Hyderabad.

Dr. Rangarajan obtained her B.S degree in Biology from Stanford University and Ph.D. from the Rockefeller University. She was a postdoctoral fellow at the Harvard School of Public Health.

Abstract: Drug discovery and development have generally been considered to be the bastions of large, multinational pharmaceutical companies. While this view is true for the most part, alternate models exist. They include startups and academic institutions who pursue novel ideas and license the IP to pharmaceutical companies. CSIR- Central Drug Research Institute has been a pioneer in the field of drug discovery and development and has developed multiple drugs in the past. The most famous is Centchroman, a non-hormonal contraceptive that was developed in the 1990s and is sold in the market under brand names Saheli and Chhaya. However, the model of public institutions being able to develop drugs has come under serious challenge in the last 2 decades, with changes in Regulatory regimes, funding priorities and industry focus. There is now a renewed interest on both sides, industry and academia, as the innovation ecosystem has matured in India. I will present two case studies from CDRI to demonstrate the role of public institutions in research and development, the need for greater linkages with industry and how such models have the potential to deliver products of value to India and the world.

SPEAKERS

FEATURED SPEAKER

Dr. Murali Ramachandra

CEO, Aurigene Oncology Limited, Bangalore

05 July | 9:45 AM to 10:15 AM

Targeting the Tumor Immune Microenvironment with Small Molecules for Cancer Therapy

Profile: Dr. Murali Ramachandra is the CEO at Aurigene Oncology Limited, a subsidiary of Dr. Reddy's Laboratories Limited. Murali received his PhD from the University of Idaho (USA), and post-doctoral training from the University of Kansas Medical Center and DuPont Experimental Station. Prior to his current role, he was the Chief Scientific Officer at Aurigene Oncology, and positions of increasing responsibility at Schering-Plough Pharmaceuticals, USA and the US National Cancer Institute. He has contributed to the identification of 21 innovative drug candidates that are undergoing global clinical development and the first globally approved adenoviral gene therapy product for cancer, ADSTILADRIN. Murali has co-authored more than 75 scientific publications and holds 30 granted international patents.

Abstract: Cancer therapy has witnessed significant advancements with the recognition of the tumor immune microenvironment (TIME) as a critical player in tumor progression and response to treatment. The TIME comprises various immune cells, stromal cells, signaling molecules, and extracellular matrix components, all of which interact with tumor cells to influence the disease course. Targeting the TIME offers a promising strategy for enhancing anti-tumor immunity and improving therapeutic outcomes. In this presentation, our approaches to target TME with novel small molecule agents will be discussed.

SPEAKERS

FEATURED SPEAKER

Prof. Shana J. Sturla
Department of Toxicology, ETH Zurich

05 July | 11:30 AM - 12:00 PM

Mapping chemical landscapes in the genome: From oxidative stress and toxicants to cancer drugs

Profile: Shana J. Sturla is Full Professor of Toxicology at the ETH Zurich, the Swiss Federal Institute of Technology. Professor Sturla was born in New York, USA and studied Chemistry at the University of California at Berkeley and the Massachusetts Institute of Technology. She carried out a postdoctoral fellowship at the University of Minnesota Cancer Center, and was an Assistant Professor at the University of Minnesota. The goal of her research is to promote chemical, food and drug safety by elucidating the chemical basis of mutagenesis and toxicity, and to promote innovative bioanalysis strategies to link chemical structures and reactivity with molecular responses. Key areas include environmental toxicants related to human disease, DNA damage and mutagenesis, drug resistance in cancer therapy and biotransformation of xenobiotics by human gut microbiota. Professor Sturla is President of the Swiss Society of Toxicology, Chair of the Platform Chemistry of the Swiss Academies of Science, Editor-In-Chief of Chemical Research in Toxicology, and former Chair of the ACS Division of Chemical Toxicology. Her website is **www.toxicology.ethz.ch.**

Abstract: Unravelling the mechanisms governing reactions between small molecules and DNA, our research explores resulting non-canonical DNA base modifications and their interactions with DNA repair proteins, and cellular responses. These reactions provide a roadmap for deciphering mutational signatures in cancer, biomarkers of aging and cancer drug action. The talk will introduce diverse strategies for chemical-specific mapping of genome-wide base modifications, offering new insights into the genome-wide distribution of DNA oxidation and alkylation products. Within this framework, we delve into several examples, including the imprints of oxidative stress in human cells, and the aftermath of exposing cells to cancer drugs. The data shed new light on how environmental carcinogens shape mutational landscapes, linking in vitro damage maps to mutational signatures in human cancers, and offer new tools for precision oncology. This research leverages genome-wide profiling in order to provide new insight into early chemical interactions that drive cellular responses and disease phenotypes.

SPEAKERS

FEATURED SPEAKER

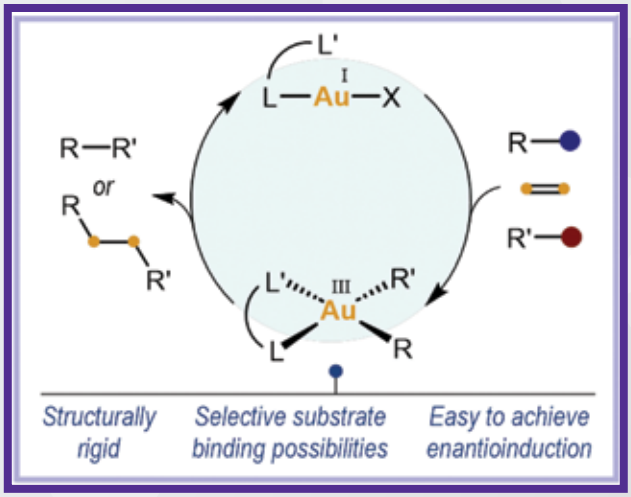
Prof. Nitin T. Patil
IISER Bhopal

05 July | 12:00 PM - 12:30 PM

Ligand-Enabled Gold Redox Catalysis

Profile: Nitin T. Patil was born in Jalgaon (Maharashtra), India, in 1975. He completed his doctoral studies from the University of Pune in 2002 under the supervision of Prof. Dilip D. Dhavale. Subsequently, he joined Prof. Christoph Schneider's group as a postdoctoral fellow at the University of Goettingen, Germany. In November 2002, he moved to Tohoku University, Japan, as a JSPS postdoctoral fellow to work with Prof. Yoshinori Yamamoto, where later on he was appointed as an Assistant Professor. In June 2006, he joined Prof. K. C. Nicolaou's laboratory at ICES, Singapore, and later at The Scripps Research Institute, USA. He began his independent career in September 2008 at CSIR-IICT, Hyderabad, and subsequently moved to CSIR-NCL, Pune, in August 2013. In July 2017, he joined IISER Bhopal as an Associate Professor and he attained the rank of Professor in October 2023. His research group focuses on understanding the unique reactivities of gold complexes and their utilization in developing organic transformations.

Abstract: In recent years, ligand-enabled gold-catalyzed organic reactions have emerged as a valuable tool, allowing for the use of aryl halides as cross-coupling partners. In this talk, I will discuss our most recent work in the area of alkene functionalization employing cross-coupling reactivities under ligand-enabled gold redox catalysis.



SPEAKERS

FEATURED SPEAKER

Prof. S. Nagendran
Department of Chemistry, IIT Delhi

05 July | 12:30 PM - 12:50 PM

Applications of N-heterocyclic Germylenes

Profile: S. Nagendran is an inorganic chemist who works essentially on low-valent germanium chemistry. He has been a faculty member at the Department of Chemistry, IIT Delhi, New Delhi, since 2008. Before this position, he was a JSPS and AvH post-doctoral fellow at the Tohoku University and the University of Göttingen. He obtained his Ph.D. from IIT Kanpur in 2002 by working under the supervision of Prof. V. Chandrasekhar. His other interests include organometallic chemistry and homogeneous catalysis.

Abstract: N-heterocyclic germylenes (NHGes) are the germanium analogs of N-heterocyclic carbenes (NHCs). The diverse applications of NHCs motivate the study of germylenes' utility. The catalytic applications of germylenes have recently garnered massive interest, especially for organic transformations, such as hydroboration, cyanosilylation, and hydrosilylation. The talk will highlight our contributions to this area using aminotroponiminate (ATI) stabilized germanium(II) compounds along with other applications we have developed.

SPEAKERS

FEATURED SPEAKER

Dr. Sanjit Konar
Department of Chemistry, IISER Bhopal

05 July | 4:30 PM - 4:50 PM

Spin-State Switching in Dynamic Molecules

Profile: Sanjit Konar received his Ph.D. from the IACS, Kolkata. He worked as a postdoctoral fellow at the University of Notre Dame, Texas A&M University, USA, and at the Universität Bielefeld, Germany as an Alexander von Humboldt Fellow. His research revolves around molecular magnetism, switchable magnetic materials, magnetic cages and polyoxometalates. He has published 160+ peer-reviewed journal articles, having ~6300 citations and an H-index of 46. He currently serves as the international editorial board member of the Wiley journal European Journal of Inorganic Chemistry, MDPI journal Magnetochemistry and an associate editor of ACS journal Crystal Growth and Design. He held a visiting professor position at the Kyushu University (2017) and Tohoku University (2022), Japan.

Abstract: The development of molecular materials that can be switched between two different spin states through the application of external stimuli is of great interest owing to their potential use in molecular devices and information technology. This switching behaviour can be triggered by different phenomena such as a charge/proton transfer, a change in the solid-state structure, or molecular orientation. When the cooperativity between spin centres is strong enough, a region of bistability might open, in which either of the two states can be found depending on the material's immediate past. This memory effect has been widely exploited in transition metal complexes. In the talk, some exciting recent discoveries of spin-state switching in the transition metal complexes in presence of external perturbation would be discussed in this presentation.

SPEAKERS

FEATURED SPEAKER

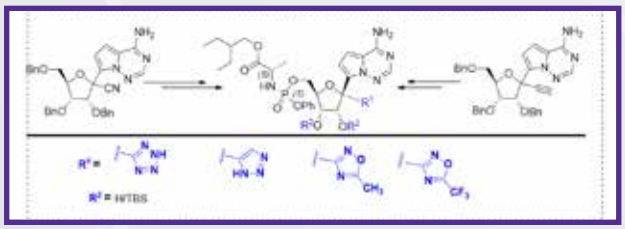
Prof. Vibha Tandon
Director, CSIR-IICB, Kolkata

05 July | 4:50 PM - 5:30 AM

Regio- and Stereoselective Synthesis of Functionalised N-Heterocycles and Carbocycles and Synthetic Diversification of Remdesivir

Profile: Prof.Vibha Tandon obtained her Ph.D. degree in 1991. She has published 93 papers in international journals, and have a few book chapters and patents to her credit. Prof. Tandon has mentored 25 Ph.D. students and around 70 students for six months' project. She has been teaching Masters and Ph.D. students from last 25 years. She has been recently awarded NASI fellow. She is an awardee of Royal Society Fellowship (2007-08) in MRC Cambridge, UK. She has been on DAAD fellowship (2010-2011) and INSA visiting fellowship (2011-12) to work in the Radiation Biology laboratory at Institute of Medical Radiation Biology at Essen, Germany; and Fulbright Senior Research fellowship (2012-13) to visit Department of Cell Biology, Georgia State University, Atlanta USA. Her group is largely involved in translational research. Professor Tandon have two strong leads (novel molecule) in pipeline to be developed as drugs; a) PPEF, an antibacterial agent against MDR Bacterial strains and b) DMA, a radio protector against radiation therapy in cancer patients. C) Identification of druggable targets in Head and Neck Cancer. Her group has been continuously working towards synthesis of pharmaceutically active small molecules. She is Associate editor of the Thieme publications and Journal of Biochemical and Molecular Toxicology.

Abstract: We investigated the regio- and stereoselective synthesis of N-containing heterocycles such as 1,2-dihydroisoquinoline, functionalized indenes, tetrahydroquinolines, and indole-2-carboxamides using novel methods. Michael-addition reactions were used to afford stereoselective indenes and cyclopentaquinolines from α,β-unsaturated ketones. Furthermore, we disclosed the protecting group-directed domino Michael addition-Mannich cyclization reaction to achieve diastereoselective tertrahydroquinolines. Moreover, we reported the regio- and enantioselective direct carboxamidation of 2-indolylmethanols with isonitriles at C2 position. In pursuance of getting potent antivirals, C1′β–CN in Remdesivir was substituted with tetrazoles, oxadiazoles, and triazoles to enhance killing of virions and better pharmacokinetic properties and successfully installed phosphoramidate group with Sp stereochemistry in good yields. The tetrazole, and oxadiazoles analogs displayed an IC_{90} of 14.1 μM each suggesting therapeutic efficacy of C1,1'-disubstituted C-nucleotides. Later, our group created novel 3,5,6-substituted triaryl 7-azaindoles and 2,3,5,6-substituted tetra aryl 7-azaindoles with potential of OLED's. The essential feature of this method is the stability of reaction to three sequential arylations, tolerating hetero-aryls and bulky substituents.



SPEAKERS

FEATURED SPEAKER

Prof. R Geetha Balakrishna

Centre for Nano and Material Sciences, Jain University

05 July | 5:30 PM - 5:50 PM

Surface and Interface Chemistry of Nanocrystals for optoelectronics

Profile: Prof Balakrishna is presently the Director of a research Centre CNMS, Jain University. Her research is on photochemistry and energy conversions in nanomaterials. She has published 208 research papers, 05 patents (03 granted) and guided 16 and 07 students leading to Doctoral and Post Doctoral degrees. She is also a founder of Greenchem Nano Pvt Ltd. She has been decorated by PM of UAE, also the Ruler of Dubai (The Mohammed bin Rashid Al Maktoum Global-Water-Award-2021), CM of Karnataka (Dr. Kalpana Chawla State Award). She is also the recipient of SERB Power Fellowship for outstanding women scientists, CRSI Medal, MRSI medal, CRS Silver Star Medal, and Fulbright Nehru award for Academic and Professional Excellence. She is a FRSC and member of Editorial Advisory Boards of 'ACS Energy Letters' and 'ACS Applied Engineering Materials'.

Abstract: Efficient utilization of the solar spectrum in tandem solar cells relies on selecting narrow bandgap and complementary wide bandgap (WBG) absorbers, with WBG solar cells primarily composed of bromine-iodine (Br-I) mixed-halide perovskite. However, their operational stability is hindered by halide segregation, a defect-driven process that initiate phase segregation (PS), propagating to grain boundaries, and causing performance degradation/hysteresis. We systematically address this challenge by passivating surface defects using appropriate zwitter ionic polymers that do not affect charge transport and can substantially suppress PS, and also contribute to higher thin film quality, chemical and photostability of WBG solar cells.

SPEAKERS

FEATURED SPEAKER

Dr. Anindita Das

Indian Association for the Cultivation of Science (IACS)

05 July | 5:50 PM - 6:10 PM

Polymer Crystallization-Driven Functional Two-Dimensional Assemblies

Profile: Anindita Das is an Associate Professor at the Indian Association for the Cultivation of Science (IACS). She works in the interdisciplinary area of polymer sciences and supramolecular chemistry. She received her Ph.D. degree in 2014 from IACS. Thereafter, she worked as an Alexander von Humboldt Postdoctoral Fellow at the University of Hamburg, Germany (2014–2016) and, subsequently, at the Eindhoven University of Technology, Netherlands (2016–2017). She started her independent research career at the IACS in 2017. She serves as the Editorial Board Member of the Journal of Macromolecular Science, Part A: Pure and Applied Chemistry, and as the Advisory and Early Career Advisory Board Members of RSC Applied Polymers and ChemNanoMat, respectively. As a recognition of her work, she has been awarded the Associate Fellowship of the INSA (2023) and the IASc (2022). She is the recipient of the ACES-CRSI Young Scientist Award (2024), SERB Women Excellence Research Grant (2024), and DAE-BRNS Young Scientist Research Award (2022). Her profile was featured in Angew. Chem. (2022).

Abstract: Dr. Das's group has demonstrated an unconventional strategy for programmed two-dimensional (2D) monolayered assemblies of different chromophore-conjugated poly(L-lactides) with predictable morphology and interesting photophysical properties by a solution-based polymer crystallization strategy. This enables enhanced π-stacking and electronic delocalization on the 2D surface, which opens up future scope for designing optoelectronic materials from purely organic biodegradable scaffolds. Further, her group demonstrated systematic structure-property effects on multi-chromophore assemblies on the 2D surface for cascade energy transfer, white-light emission, and biosensing, which will be the topic of this presentation.

SPEAKERS

FEATURED SPEAKER

Dr. Maheswaran Shanmugam
Indian Institute of Technology Bombay

05 July | 6:10 PM - 6:30 PM

Complexes for Efficient Catalysis and Sustainable Energy Harvesting

Profile: Born in Tamil Nadu, India, Maheswaran Shanmugam finished his Bachelor's degree in 2000 from Bishop Heber College, Trichy and Master's degree in 2002 in Bharathidasan University, Trichy. He earned his Ph.D. degree at the University of Manchester, UK under the supervision of Prof. Richard. E. P. Winpenny in 2006. In the following years he then joined as a postdoctoral fellow at University of California, Berkeley (P.I: Prof. Jeffrey R Long) and University of California, San Francisco (P. I: Prof. Stanley B Prusiner, Nobel Laureate in Medicine 1997) from 2006 to 2009, as well as University of California, Davis (P.I: Prof. Louise A Berben) from 2009 to 2011. He joined the department of Chemistry at the Indian Institute of Technology Bombay in 2011 and is currently working as a full time professor there. Among the numerous accolades, he is also a recipient of Bronze medal in Chemical Research Society of India for the year 2024, Indian National Science Academy Young Investigator Award (2015), IIT Bombay Research Publication Award (2019) etc.

Abstract: Amidst the soaring global energy demands propelled by population growth and industrial expansion, the quest for alternative, plentiful energy sources—like vibrational, thermal, solar, tidal—has gained momentum. On the other hand, increased reliance on nuclear power, fossil fuels, and carbon-intensive energy sources, growing urbanization, and exposure to air pollution are only a few of the reasons that have been associated with increases in global CO2 emissions. Our solution to these problems is to employ bio-compatible, flexible, cheaper and easier to synthesize molecular multiferroic complexes and coordinatively unsaturated molecular catalysts with enhanced thermal stability and catalytic activity. The multiferroic complexes, in the form of nanogenerator (NG) devices, can capture the different forms of energies and convert them into useful electricity, promising amplified power output for devices used in power plants and wearable electronics, whereas the catalysts designed by us can capture the CO2 and convert it into useful forms like methanol, to mitigate the global pollution

SPEAKERS

FEATURED SPEAKER

Dr. Tharamani C. Nagaiah
Indian Institute of Technology Ropar

06 July | 9:15 AM - 9:55 AM

Advanced energy materials for clean energy conversion

Profile: Tharamani is currently an Associate Professor and Head, Department of Chemistry at Indian Institute of Technology (IIT) Ropar, India. Her research interests include design and development of new materials with focus on energy conversion/storage and biosensing applications, in-depth fundamental analysis of the newly designed electrocatalysts by various electrochemical, spectroscopic, microscopic and scanning probe techniques.

She is a recipient of several prestigious fellowships like **Alexander von Humboldt Postdoctoral Fellowship, Germany** and **Ramanujan Fellowship** by Department of Science and Technology, Govt. of India. She is a **Fellow of Royal Society of Chemistry** admitted through "Leaders in the field" scheme and also an elected **Fellow of Indian Chemical Society.** She is a recipient of **CRSI-Bronze Medal 2023** from the Chemical Research Society of India and **Silver Medal of CRS 2023** from the Society Chirantan Rasayan Sanstha, **ECSI National Metrohm Award 2023** from Electrochemical Society of India and **A.V. Rama Rao prize for women 2024** from Chemical Research Society of India. She is an Associate Editor of Chemistry of Materials (ACS), an Editorial Board Member of Electrocatalysis (Springer Nature) and Sustainable Energy and Fuels (Royal Society of Chemistry).

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 systems which ought to be environmentally agreeable. Electrochemical energy conversion offers some most alluring aptitudes for providing clean energy. To name a few of these include fuel cells, rechargeable metal-air/oxygen batteries and HCl electrolysis and likewise. 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 thence to the melioration of the associated electrocatalysts. In the past decade research has depicted tremendous efforts towards ORR. But still an infinite pursuit towards the exploration of effective, sturdy and energy efficient catalysts continues. The hound for an equally or even more superior catalyst is en route for stinting and sustainable catalyst.

The talk addresses several strategies pursued to replace noble-metal free electrocatalysts towards ORR and oxygen depolarized cathode materials for HCl electrolysis and visualization of local electrocatalytic activity by SECM.

SPEAKERS

FEATURED SPEAKER

Dr. Sanjib Banerjee
Indian Institute of Technology, Bhilai

05 July | 9:55 AM - 10:15 AM

Sustainable Synthesis of Next Generation of Responsive Polymers

Profile: Dr. Sanjib Banerjee is a researcher in the area of chemical sciences and presently an Associate Professor and Head of the Department of Chemistry, IIT Bhilai. He leads the "Macromolecular Biomaterials Laboratory" at IIT Bhilai. His research group is working the development of innovative materials as key elements for healthcare, sustainability and energy applications.

Dr. Banerjee has published 64 research papers and 8 book chapters. He is also the (co)inventor of 4 patents. He is the recipient of numerous awards, including the SERB-Ramanujan Fellowship 2016, SERB-Early Career Research Award 2019, RSC-Molecular Systems Design & Engineering Outstanding Reviewer 2019, RSC-Polymer Chemistry Emerging Investigator-2020, Wiley-Next Generation of Polymer Researchers-2022 and Chemical Research Society of India (CRSI)-Bronze Medal for the year 2024, among others. Since Feb, 2024, he is serving as a Section Editor of Materials Today Communications journal (Synthetic Materials Chemistry and Polymer Chemistry Section).

Abstract: Since living things respond to stimuli by nature, researchers have developed stimuli-responsive smart polymeric materials as innovative materials for usage in energy, sustainability, and healthcare applications. When the environment's pH, temperature, electric/magnetic field, etc., changes, these polymeric materials alter physically, chemically, and configurationally. Compared to single or dual-stimuli responsive polymers, multi-stimuli responsive polymers offer more diversity, functionality, and control, making them the preferred material for the development of sensors and actuators for biomedical and engineering applications. But careful synthesis is required if these materials are to be employed in the future. This is made more difficult by (a) the need for stringent reaction conditions in multi-step synthesis methods and (b) the difficulty in modifying various material properties. We've created a sustainable synthesis protocol for the production of next generation of stimuli responsive polymers for applications as functional coating material with tunable wettability, self-healing sealant material, antifouling materials and nanocarrier for anti-cancer drug delivery.

SPEAKERS

FEATURED SPEAKER

Prof. G. Narahari Sastry
Department of Biotechnology, IIT, Hyderabad.

06 July | 10:15 AM - 10:45 AM

The Role and Relevance of Chemistry in the Industry 5.0 Driven Interdisciplinary Space

Profile: Dr. G. Narahari Sastry is a Professor in the Department of Biotechnology, IIT Hyderabad. Prior to joining IITH in 2024, Dr. Sastry was the Director of CSIR-North East Institute of Science and Technology (NEIST), Jorhat, Assam from February 2019. Before working at CSIR-NEIST, he was the chief scientist and head of the Canter for Molecular Modelling Division at CSIR-IICT, Hyderabad from 2002-2019. Prior to that Dr. Sastry has served as a Lecturer, Department of Chemistry, Pondicherry University, Pondicherry. Dr. Sastry has obtained his Postdoc studies from Israel and Switzerland (1994-1997) and Ph.D. degree from University of Hyderabad, Hyderabad.

Dr. Sastry is a well know researcher in the field of non-covalent interaction, Bucky bowl chemistry, aromaticity, pericyclic reaction. He has made a great contribution in open-source software development in the field of Computer Aided Drug Discovery, databases, web servers, all the resources developed by his group are freely accessible to the scientific community. He has published more than 330 research articles in reputed journals with an active average impact factor. Most of his papers are well cited with the citation score 12,877 an h-index of 54, and an i10-index of 239, as per the google scholar. Dr. Sastry and his group have mainly contributed and maintained various web-based platforms and databases like a) MPDS (for several diseases), b) CAD, c) A2ID, d) PLID e) NEI-MPDB, f) OSADHI.

Abstract: In this talk, I would like to trace the origins of modelling and data science in science and engineering, with a special reference to chemistry and how it impacted the areas like biology, medicine and material science. Illustrative examples taken from our and other groups will be provided to highlight the need for emergence of fifth paradigm. Modelling, structures, properties and molecular processes in macromolecular and biological systems have become rather indispensable to understand why the molecular systems and assemblies behave the way they behave. We delineate how significant insights can be obtained, through database analysis and quantum chemical calculations, on the structure and function of supramolecular assemblies. I specifically focus on two topics: a) recent advances in our understanding of non-covalent interactions and b) software development. Indigenous software, database, and webserver development activities of our group will be discussed. The importance of integrating the conventional modelling with that of more recent advancement in artificial intelligence, IoT and Industry 5.0 will be discussed, with the help of some initiatives started in the group.

SPEAKERS

FEATURED SPEAKER

Dr. E. Bhoje Gowd
CSIR-National Institute for Interdisciplinary Science and Technology Thiruvananthapuram

06 July | 10:45 AM - 11:05 AM

Hierarchical Structure Formation in Poly(lactides): Role of Polymer Chain Packing on the Emissive Properties of Chromophore Embedded Poly(Lactide)s

Profile: E. Bhoje Gowd received his M.Sc. (Tech) in Polymer Science and Technology from S. K. University, Anantapur and his Ph.D. from the University of Pune, Pune (work carried out at CSIR-NCL). He worked as a post-doctoral fellow at Toyota Technological Institute, Nagoya, Japan and as an Alexander von Humboldt Fellow at IPF, Dresden, Germany. After a short stay at the IISc, Bangalore as a Centenary post-doctoral fellow, he joined CSIR-NIIST, Thiruvananthapuram as a SERB Ramanujan Fellow. In 2011, he accepted the Senior Scientist position at CSIR-NIIST and was promoted to Senior Principal Scientist and Professor in 2018. He was awarded the IUSSTF research fellowship by IUSSTF in 2014 (Stony Brook University, NY, USA) and the Raman Research Fellowship by CSIR in 2018 (NTHU, Hsinchu, Taiwan). He was the recipient of the CRSI Bronze Medal in 2024, the MRSI Medal in 2016 and the Professor Kaushal Kishore Memorial Award of the SPSI in 2018. In 2020, he was elected as FRSC, London, UK. He was listed as one of the Pioneering Investigators of Polymer Chemistry in 2019 (RSC). He has authored more than 85 publications in peer-reviewed journals, edited a book, and contributed 5 book chapters.

Abstract: The structural ordering process plays a key role in controlling the nanostructured morphologies of multiphase systems for diverse applications. The covalent incorporation of chromophore molecules into polymers has several advantages such as processability, solubility, mechanical stability, and structural diversity. These materials have received increasing attention in various fields, such as cell imaging, fluorescent sensors, smart and intelligent packaging, and biological probes. In the first part, the crystallization behavior of enantiomeric polylactides will be discussed to elucidate insights into chain dispositions and develop crystalized structures through intra- and inter-chain chiral interactions. The stereocomplex formation and hierarchical structural changes during the heating of supramolecular gels obtained by polylactide racemic blends will be discussed. In the second part of my talk, the role of morphology and the polymer chain packing on the solid-state emission properties of the chromophore-embedded PLLAs will be discussed. In the last part of my talk, dual-color emissive hybrid materials based on PLLA and polyethylene glycol-modified layered double hydroxide quantum dots (PEG-LDHQDs) will be discussed.

SPEAKERS

FEATURED SPEAKER

Prof. Ruchi Anand
Department of Chemistry, IIT Bombay

06 July | 11:30 AM - 12:00 PM

Deciphering Methytransferase Mediated Mechanism of Antibiotic Resistance

Profile: Ruchi Anand completed her PhD in 2004 from the Department of Chemistry and Chemical Biology at Cornell University, USA. After conducting postdoctoral research at Sloan Kettering and the University of Pennsylvania she joined IIT-Bombay in 2008 as an Assistant Professor. Her laboratory employs a combination of X-ray Crystallography, Cryo-EM, biochemical and biophysical tools to understand molecular mechanisms with implications to human health. Her current research interests follow a multipronged approach where she has contributed to two major areas, antimicrobial resistance and biosensors development. She has been serving on the Editorial Advisory board for ACS Sensors, JPC(A/B/C), Asian JOC and JACS and serving as an Associate Editor of Biochemistry 2024. She is a fellow of all three National Academies of Sciences F FNASc, FNAAS FNA. She was awarded the National Women Bio-scientist Award, Department of Biotechnology, in 2018 and the CRSI bronze medal in 2020. She is also the recipient of the DBT-Wellcome Trust Alliance Senior Fellowship in 2020. She is also the recipient of Sun Pharma Award for year 2024.

Abstract: Antibiotic resistance is a silent epidemic which has risen to alarming proportions. It is projected that by 2050, drug resistance will result in more than 300 million deaths. Ribosomal methylation is a common modification adopted by bacteria to disrupt the binding site of several antibiotics, that bind the ribosome, thereby making these drugs ineffective. Here, we discuss the, specificity and targeting mechanism of N6 adenosine methylation by ribosomal methyltransferases (rMtases) that covalently modify ribosomes and thereby, do not allow antibiotics to bind. We specifically focus on the peptidyl exit tunnel where methylation at this site imparts resistance to macrolide, linconamide and streptogramin class of drugs. Thus here we embark on understanding the elements that impart specificity towards target recognition via a combination of X-ray crystallographic, biochemical and cryo- EM approaches. Overall, aim is to develop a broader insight into origins of antibiotic resistance to serve as a stepping stone towards development of drugs that can help in resisting resistance, thereby re-sensitizing the pathogens to existing antibiotics.

SPEAKERS

FEATURED SPEAKER

Prof. Ravi P Singh
Department of Chemistry, Indian Institute of Technology, Delhi

06 July | 12:00 PM - 12:20 PM

Vinylogy for Enantioselective Desymmetrization

Profile: Ravi P. Singh born in UP, India, is currently professor in chemistry department at the Indian Institute of Technology (IIT) Delhi, India. He obtained his Bachelor's degree in chemistry from U.P. College, Varanasi and Master's degree from Banaras Hindu University, Varanasi. Later, he moved to the Chemistry Department at IIT Kanpur, to pursue his Doctoral studies under the supervision of Prof. Vinod K. Singh. He gained his postdoctoral experience in U.S.A in the area of total synthesis and asymmetric catalysis. Dr. Singh spent two years (2005-2007) at Harvard University working with Nobel Laureate, Professor E. J. Corey and four years (2007-2011) at Brandeis University working with Professor Li Deng. He started his independent academic career at National Chemical Laboratory, Pune as a Senior Scientist in 2011 and later moved to the chemistry department at IIT-Delhi in 2013.

Dr. Singh has been recognized with ISCB Young Scientist Award-2017 In Chemical Sciences.

Abstract: Desymmetrization reactions have proven to be efficient in generating compounds bearing chiral quaternary carbon, a long standing challenge in synthetic chemistry. A successful example of this strategy is 1,4-addition of nucleophiles to 2,2-disubstituted 4-cyclopentene 1,3-dione, which typically gives corresponding products with stereogenic centers one by Michael addition and the other by an all-carbon quaternary center by desymmetrization.

In an attempt to explore the reactions further, we developed an asymmetric vinylogous Michael addition reaction between-3-cyano-4-methyl-cou-marins and biologically active male-imides, via non-covalentorgano-catalysis, enantios-elective desymmetric homolo-gation of cyclopentene-1,3-diones via domino process. In another optimization an asymmetric annulation of cyclopentane-1,3-dienones with cyano-methyl coumarin has been attempted. Further, alkylidene malononitrile with cyclopen-tane-1,3-dienones for (4+1) carbospiro annulation has been optimized. These newly realized reactions will be discussed in detail in the talk.

SPEAKERS

FEATURED SPEAKER

Prof. Satyendra Kumar Pandey
Department of Chemistry, Institute of Science, Banaras Hindu University,

06 July | 12:20 PM - 12:40 PM

Metal-Free Synthesis of Bioactive Molecules

Profile: Prof. Pandey received his Ph.D. in 2008 from the CSIR-National Chemical Laboratory, Pune, India, under the supervision of Dr. Pradeep Kumar. He then worked as a Postdoctoral Researcher at Purdue University, IN, USA, with Prof. Arun K. Ghosh. In 2010, he joined Aurigene Discovery Technologies Ltd. (Dr. Reddy's group) in Bangalore, India, as a Scientist. In 2012, he was appointed as an Assistant Professor in the School of Chemistry and Biochemistry at Thapar University, Patiala, Punjab, India, and was promoted to Associate Professor in 2017. That same year, he moved to the Department of Chemistry at the Institute of Science, Banaras Hindu University (BHU), Varanasi, where he has been a Professor of Organic Chemistry since 2020.

He was the recipient of Eli Lilly Asia outstanding thesis award in 2009, and the CRSI Bronze medal award in 2024. His broad research interests include the development of new synthetic methods, the total synthesis of biologically active natural products. He has published 58 papers and three patents till date. Furthermore, 9 students have received Ph.D. degree under his supervision. He has also guided 25 Master's students in their dissertation work.

Abstract: Metal catalyzed transformations of sulfoxonium ylides have gained prominence for the synthesis of a number of heterocyclic compounds, such as pyrrole, indole, furan, pyrimidine, and quinolone. However, their utility under metal free conditions is still under explored. In this context, we have demonstrated that the sulfoxonium ylides can be used as precursor for the synthesis of various bioactive molecules. These studies were expanded to include the diverse synthesis of several bioactive molecules such as Thiazolidine-2-thiones, Rhodanines, α-Ketothioamides, Thiazole-2-thiones, Quinoxalines, Thiazoles, α-Ketoamides, Dithiocarbamates and 2-Hydroxy-pyrrolones under mild, metal- and additive-free conditions. The talk will focus on some of the recent developments on the sulfoxonium ylides and asymmetric total synthesis of some bioactive compounds from our laboratory.

References:

1. S. K. Pandey et al. J. Org. Chem. 2024, 89, 5536.
2. S. K. Pandey et al. Org. Lett. 2023, 25, 5329.
3. S. K. Pandey et al. J. Org. Chem. 2023, 88, 6120.
4. K. Pandey et al. Org. Lett. 2022, 24, 8062.

SPEAKERS

FEATURED SPEAKER

Dr. Surya Prakash Singh
CSIR-IICT, Hyderabad

06 July | 12:40 PM - 1:00 PM

Synthesis of Functional π-Conjugated Small Molecules: From Structure to Function

Profile: Dr. Surya Prakash Singh is currently working as a Principal Scientist at Department of Polymers and Functional Materials, CSIR-Indian Institute of Chemical Technology, Hyderabad. Dr. Singh graduated with Ph.D. from University of Allahabad, India. After working at Nagoya Institute of Technology, Japan, as a postdoctoral fellow, he joined Osaka University, in 2008 as an Assistant Professor. He also worked as a researcher at Photovoltaic Materials Unit, National Institute for Materials Science (NIMS), Tsukuba, Japan before joining as a scientist at CSIR-IICT in 2011. He has published over 225 papers, reviews in peer-reviewed journals and patents, edited two books and authored one book chapter. BODIPY based dyes for mitochondrial tracking developed by Singh and colleagues has been licensed and commercialized by TCI (Japan). During his tenure at CSIR-IICT, he has been a recipient of several prestigious awards like CRSI-bronze medal (2024), NASI-young scientist platinum jubilee award (2012), AVRA young scientist award (2015). Dr. Singh is a Fellow of Telangana academy of sciences (2022) and Associate Fellow of Andhra Pradesh academy of sciences (2013) and Indian National Science Academy-INSA (2024).

Abstract: Energy is a crucial factor in driving social, economic, and industrial progress. Our daily energy consumption continues to rise gradually. In recent decades, rising energy demand has increased reliance on fossil fuels such as coal, petroleum and natural gas, releasing CO2 and contributing to global warming. Small organic molecules with suitable photophysical and electronic properties have garnered attention in advanced technology applications, especially in photonic devices such as dye-sensitized solar cells, organic solar cells, emissive displays like OLEDs; electronic materials such as organic semiconductors, and security printing. Organic photovoltaics are gaining popularity as a cost-effective, color-tunable, and mechanically flexible renewable energy technology. Numerous research endeavors aim to develop novel organic materials and enhance their efficiency and durability. Our research group is focusing on producing stable organic molecules for diverse applications. In the upcoming event, I will present our progress on developing hole-transport materials for perovskite solar cells. The presentation will commence with a brief introduction to solar cells, followed by an exploration of industrial applications and the commercialization potential of dye molecules.

POSTER TITLES

S No.	TITLE OF THE POSTER	Name of the Poster Presenter
1	Synthesis and Characterization of Stable Metal-Radical Complexes by EPR Spectroscopy	Subuhan Ahamed
2	Room temperature synthesis and low thermal conductivity of nanocrystalline Ag3CuS2	Anil Kumar B M
3	Synthesis, characterization, and catalytic evaluation of glucopyranosylamine-derived Mo(VI) complex toward organic sulfide oxidations	Anuvasita Parikh
4	Computational Investigation of Strong Ferromagnetic Coupling between Metal and Odd Electron (Anti)aromatic Radicals	Muskan Suranjan Shil
5	Chirality Generation in a Nickel(II) Square Planar Complex Supported by a Dipyrromethane-based Tetradentate Ligand	Tapas Guchhait
6	An Extended Rudolph Diagram: B3H5 and B3H6+ relate 3D-, 2D-boron allotropes and boranes	Prof. Jemmis E D
7	Structural Phase Transition and Interesting Magnetism of Ni Intercalated NbS2 ($0 \leq x \leq 0.5$)	Nunavath Ramakrishna
8	Exsolved Ni-Ru Alloy from Nickel-Ruthenium co-doped $SrFeO_{3-\delta}$ Perovskite: A Potential Hydrogenation Catalyst	M. Bhavisha
9	Self-Assembly of a Water-Soluble Pd16 Square Bicupola Architecture and its Use in Aerobic Oxidation in Aqueous Medium	Pranay Kumar Maitra
10	Silver Catalysed Direct Benzylic sp3 C-H Bond Oxidation: A facile Synthesis of Aldehyde	Zaheen Akhter
11	Synthesis, characterization and biological activity of acetophenone derived Schiff base and its Fe(III) complex	Mamta Ranka
12	Cavity-Shape Dependent Divergent Chemical Reaction Inside Aqueous Pd6L4 Cages	Debsena Chakraborty
13	Spectroscopic characterization, reactivity of a Cu(III) species supported by a proline-based pseudo peptide and effect of Lewis acid	Eerlapally Raju
14	Synthesis, Characterization, and Application Studies of Anionic Dithiolene Radical Ligand-based Metal Complexe	Sangita Mondal
15	Proton-assisted activation of a MnIII–OOH for aromatic C–H hydroxylation through a putative [MnV=O] species	Sikha Gupta

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17	Novel Heterogeneous Magnetic Pd-NHC Catalyst for Sustainable Nitroarene Reduction and Buchwald-Hartwig Amination	Dr. Sindhu Mathai
18	Functional models of ascorbate, amine, and catechol oxidases: Impressive catalytic promiscuity of monocopper(II) complexes	Selvaraj Shanmugavadivel
19	Group VIII Metal Decorated Inorganic Framework Materials: A Potential Catalysts for Hydrotreating of Biomass Model Components	N P Nimisha
20	Synthesis, characterization, antimicrobial and anticancerous studies of Mn(II) & Hg(II) bridging complexes	V K Srivastava
21	Functional Models of Ascorbate, Amine, and Catechol oxidases: Impressive Catalytic Promiscuity of Monocopper(II) Complexes	Selvaraj Shanmugavadivel
22	Low Platinum Loading ZnO/CQDs Bifunctional Electro-Catalyst Towards OER and ORR Impacting Zinc-Air Battery	Anup Kumar Pradhan
23	Synthesis, Characterization, and Catalytic Degradation of Methyl Orange with H2O2 by an Oxidovanadium(IV) Schiff Base Complex Derived from Glycine	Tanaya Medhi
24	“All-organic” Electrode Material Toward High-Performing Rigid to Flexible Supercapacitor Devices	Pradeep Sachan
25	Impact of surfactants in modulating the viscoelastic properties of Fmoc-Phe hydrogels	Dinesh Kumar Duraisamy
26	Know Your Insulin: Proposing A Self-Investigated Insulin	Shantanu Sen
27	Oxazine-based probe for the colorimetric detection of toxic mercuric ions	Keloth Sairam
28	Nitronaphthalimides Increase Nitric Oxide Bioavailability by Nitrite Donation: Potential Implications in Cardiovascular Complications	Shubham Sahu
29	A fluorescent benzothiazole dimer for sensing lead ions in an aqueous solution	Tanay Agarwal
30	pH-dependent Haloperoxidase-like Activity of Vanadium Pentoxide Nanostructures	Kiruthika

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32	From Solution to Microstructures in Minutes: Microdroplet-Derived Stand-alone TiO2 Surfaces for Simultaneous Water Harvesting and Treatment	Depanjan Sarkar
33	Metal Organic Frameworks-Carbon Dots Conjugates for Reach chemicals Recognition	Renuka M
34	Design, synthesis, and tunable self-assembly of a diamino diacid-based short cyclic peptide	Devki Nandan
35	Synthesis of C3N5 through Various Routes and development of C3N5 Composites for Improved Photocatalytic Dye Degradation Performance	Akanshi Gupta
36	Metal Organic Frameworks Based Triboelectric Nanogenerator	Rojalin Sahu
37	Molecular Versus Supramolecular: Chirality induction, inversion and amplification in 'Nano-size' Trizinc(II)porphyrin Trimers	D. Chandel
38	Multi-Functional Hydroxyquinoline-Derived Small Molecule Nano Dot for Alzheimer's Disease Detection and Treatment.	Priyam Ghosh
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40	An Electronic Device Incorporating Flexible Organic Single Crystals for Ultrasensitive Detection of NO2	Kiran Arora
41	Synthesis of Organic and Organic-inorganic Hybrid π-conjugated Semiconducting Materials for Optoelectronic Devices	Kamatham Narayanaswamy
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55	Facile synthesis of N-(α-furanyl) alkyl sulfoximines via gold catalyzed Michael addition/cyclization of enynones and sulfoximines	Antony Haritha Mercy
56	Synthesis of Quinazolinone Scaffolds via Zinc(II) Stabilized Amidyl Radical Promoted Deaminative Approach	Subarna Manna
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58	Direct Access to Trifluoromethylated Benzo[d]oxepines from o Alkynylaryl Aldehydes and Trifluorodiazoethane	Anamika Dhami
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65	Rh(III)-Catalyzed Controlled Amidation of Primary Amides Using Dioxazolones: En Route Synthesis of Ortho-Amidated Arylamides	Saksham Mishra
66	Visible light mediated selective synthesis of Allyl-Aryl Sulphoxides	Ballanki Trinadh
67	CsF-Mediated Reaction of Trifluorodiazoethane with 3 Nitroindoles Enables Access to Trifluoromethylpyrazolo[4,3 b]indoles.	Sandeep Kumar
68	New NNE Pincer Palladium (II) Complexes: Synthesis, Structure and Catalytic Application for Decarboxylative Heteroarylation of Coumarins	Prakash N. Swami
69	Photochemical Decarboxylative Formylation of Indoles with Aqueous Glyoxylic Acid Under Basic Condition	Aishwarya S
70	One-Pot Click Chemistry using Hydrazine as Azide Surrogate: Easy access to Triazole Functionalities	Muzamil Samad
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72	Visible-Light-Mediated Triplet Carbene Catalyzed Cis to Trans Isomerization	Maelle Thouzery
73	Silver-Catalyzed Asymmetric Double Desymmetrization via Vinylogous Michael Addition of Prochiral α,α-Dicyanoalkenes to Cyclopentendiones	Kavita Choudhary
74	Modular Access to Sulfur Substituted Analogues of Isocytosine via Photoredox Catalysis	Faheem Fayaz
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77	Synthesis, characterization and in silico molecular docking of some pyrimido-pyrazolo-phthalazine derivatives	Jayesh Sarvaiya
78	Base Catalysed Skeletal Rearrangements of Indole Guanidines that leads to 2,4-Disubstituted 4H-Imidazo[4,5,1-ij]quinoline Derivatives	Pragya Maheshwari
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80	One-pot synthesis of N-(α-aryl/ α-phosphonyl/O-silyl)alkyl sulfoximines/sulfonimidamides	K. Natarajan
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87	Investigation of Serotonin-Receptor Interactions, Stability, and Signal Transduction Pathways via Molecular Dynamics Simulations	Arunima Verma
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96	Stimuli-responsive release of active anionophore from RGD-peptide-linked proanionophore	Soumya Srimayee
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99	Functional Models of Ascorbate, Amine, and Catechol oxidases: Impressive Catalytic Promiscuity of Monocopper(II) Complexes	Selvaraj Shanmugavadivel
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104	Tailoring efficacious interventions against ER-positive cancer by targeting aromatase to constrain oestrogen production	Sheetal
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109	A metal-free amination of 1,2-diaza-1,3-dienes using hydrazine hydrate through N-N bond cleavage	A K Jaiswal
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