INTERDISCIPLINARY INITIATIVE IN CHEMICAL SCIENCES (IICS)

FORCE-IICS 2024

October 3-6, 2024

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Uday Backwater Resort
Alappuzha, Kerala

INTERDISCIPLINARY INITIATIVE IN CHEMICAL SCIENCES (IICS)

FORCE-IICS 2024

FORCE-IICS
Interdisciplinary Initiative in Chemical Sciences
2024

ABOUT THE SYMPOSIUM

The symposium includes invited lectures, special lectures, and brainstorming sessions by eminent chemists and scientists from the scientific community working in chemistry and allied areas. The FORCE-IICS is a platform for scientists to discuss the recent developments in chemical sciences across the sub-disciplines. In addition, FORCE-IICS creates opportunities to exchange ideas and build long-lasting collaborations in the frontier areas of chemistry and its allied disciplines. There will be 'Special Evening Lectures' in addition to 16 technical sessions covering 45 invited lectures and 50 poster presentations in the brainstorming session. The Royal Society of Chemistry (RSC) is an official partner of FORCE-IICS 2024.

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October 3-6, 2024
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Day 1: October 3, 2024 **| Thursday** (Day 1 Coordinator: **Ramesh Ramapanicker, IIT Kanpur**)	
REGISTRATION (17:30 – 18:00)	
INAUGURAL SESSION (18:00 – 18:05)	
18:00 – 18:05	Welcome by Convener, FORCE-IICS 2024
Session 1 (18:10 -19:40) Chairperson: **Prasanta K. Das, IACS Kolkata**	
18:10 – 18:40 (27 + 3)	**IL1**: G. Mugesh, IISc Bengaluru
18:40 – 19:00 (18 + 2)	**IL2**: Tapasya Srivastava, Delhi University
19:00 – 19:20 (18 + 2)	**IL3**: Shilpy Sharma, S.P. Pune University
19:20 – 19:40 (18 + 2)	**IL4**: Harinath Chakrapani, IISER Pune
DINNER (19:40 – 22:00)	
Day 2: October 4, 2024 **| Friday** (Day 2 Coordinator: **Alakesh Bisai, IISER Kolkata**)	
Session 2 (09:30 – 10:30) Chairperson: **K. Geetharani, IISc Bengaluru**	
09:30 – 10:00 (27 + 3)	**IL5**: Pradyut Ghosh, IACS Kolkata
10:00 – 10:20 (18 + 2)	**IL6**: Anindita Das, IACS Kolkata
10:20 – 10:40 (18 + 2)	**IL7**: Shaikh M. Mobin, IIT Indore
Session 3 (10:40 – 11:20) Chairperson: **Pallavi Debnath, IIT Roorkee**	
10:40 – 11:00 (18 + 2)	**IL8**: Amlan K. Roy, IISER Kolkata
11:00 – 11:20 (18 + 2)	**IL9**: Devendra Mani, IIT Kanpur
TEA/COFFEE BREAK (11:20 – 11:55)	
Session 4 (12:00 – 13:20) Chairperson: **Anuj Sharma, IIT Roorkee**	
12:00 – 12:20 (18 + 2)	**IL10**: Prasanta Ghorai, IISER Bhopal
12:20 – 12:40 (18 + 2)	**IL11**: R. Vijaya Anand, IISER Mohali
12:40 – 13:00 (18 + 2)	**IL12**: Syed Masood Hussain, CBMR Lucknow
13:00 – 13:20 (18 + 2)	**IL13**: Radhika Venkatesan, IISER Kolkata
LUNCH & NETWORKING (13:20 – 14:30)	
Session 5 (14:30 – 15:55) Chairperson: **Rambabu Chegondi, IICT Hyderabad**	
14:30 – 14:50 (18 + 2)	**IL14**: P. Anbarasan, IIT Madras
14:50 – 15:10 (18 + 2)	**IL15**: E. Balaraman, IISER Tirupati
15:10 – 15:35 (18 + 2)	**IL16**: R. Boomi Shankar, IISER Pune
15:35 – 15:55 (18 + 2)	**IL17**: Dharmaraja Allimuthu, IIT Kanpur

Session 6: Posters Presentations (15:55-17:10) Session coordinator: **Aparna Ganguly, Editorial Development Manager, RSC** **Poster Placement:** Oct. 4, 2024 during TEA/LUNCH BREAK; Posters can be collected after the brainstorming session. Poster numbers and details are given in the e-abstract book.	
GROUP PHOTO (17:10-17:30)	
Session 7 (17:30 – 18:30) Chairperson: **Satpal Singh Badsara, University of Rajasthan**	
17:30 – 17:50 (18 + 2)	**IL18**: Sureshkumar Devarajulu, IISER Kolkata
17:50 – 18:10 (18 + 2)	**IL19**: Ramakrishna G. Bhat, IISER Pune
18:10 – 18:30 (18 + 2)	**IL20**: D. P. Hari, IISc Bengaluru
Session 8: Evening Lecture (18:30 – 19:20) – ***EJOC Lecture*** **Nobel Laureate Prof. Robert J. Lefkowitz** **Chancellor's Distinguished Professor of Medicine, Duke University** Chairperson: **Sandeep Verma, IIT Kanpur**	
BANQUET DINNER (19:30 – 22:30)	
***Day 3: October 05, 2024* | Saturday** (Day 3 Coordinator: **G. Sekar, IIT Kanpur**)	
Boat Ride (6:45-8:00 AM)	
Session 9 (10:00 – 11:20) Chairperson: **Bhisma K. Patel, IIT Guwahati**	
10:00 – 10:20 (18 + 2)	**IL21**: A. T. Biju, IISc Bengaluru
10:20 – 10:40 (18 + 2)	**IL22**: Raji Reddy, IICT Hyderabad
10:40 – 11:00 (18 + 2)	**IL23**: Srinivas Dharavath, IIT Kanpur
11:00 – 11:20 (18 + 2)	**IL24**: Ashutosh Kumar Mishra, IIT Hyderabad
TEA/COFFEE BREAK (11:20 – 11:50)	
Session 10 (11:55 – 13:15) Chairperson: **Harinath Chakrapani, IISER Pune**	
11:55 – 12:15 (18 + 2)	**IL25**: Gouriprasanna Roy, IIT Tirupati
12:15 – 12:35 (18 + 2)	**IL26**: Debasis Das, IISc Bengaluru
12:35 – 12:55 (18 + 2)	**IL27**: Sunanda Chatterjee, IIT Guwahati
GROUP PHOTO (12:55-13:25)	
LUNCH & NETWORKING (13:25 – 14:30)	
Session 11 (14:30 – 15:30) Chairperson: **Vishal Rai, IISER Bhopal**	
14:30 – 14:50 (18 + 2)	**IL28**: Subi George, JNCASR
14:50 – 15:10 (18 + 2)	**IL29**: Ishu Saraogi, IISER Bhopal
15:10 – 15:30 (18 + 2)	**IL30**: Ahanjit Bhattacharya, IISER Bhopal

Session 12 (15:30 – 16:30) Chairperson: **Khushbu Kushwaha, Associate Editor, Wiley**	
15:30 – 15:50 (18 + 2)	**IL31**: Alexander Baker, Dalhousie University
15:50 – 16:10 (18 + 2)	**IL32**: Ganesh Venkataraman, IIT Kharagpur
16:10 – 16:30 (18 + 2)	**IL33**: Amit Kumar, IIT Patna
TEA/COFFEE BREAK (16:30-17:00)	
Session 13 (17:05 – 18:05) Chairperson: **Kiran Kumar Pulukuri, IISER Tirupati**	
17:05 – 17:25 (18 + 2)	**IL34**: K. Geetharani, IISc Bengaluru
17:25 – 17:45 (18 + 2)	**IL35**: Md. Mahiuddin Baidya, IIT Madras (AJOC Lecture)
17:45 – 18:05 (18 + 2)	**IL36**: Bhoopendra Tiwari, CBMR Lucknow
Session 14 (18:10 – 20:00) Chairperson: **Abhijit Patra, IISER Bhopal**	
18:10 – 18:20 (18 + 2)	**IL37**: Raju K. Gupta, IIT Kanpur
18:20 – 18:40 (18 + 2)	**IL38**: Mohd. Qureshi, IIT Guwahati
19:00 – 19:20 (18 + 2)	**IL39**: T.G. Gopakumar, IIT Kanpur
19:20 – 19:40 (18 + 2)	**IL40**: Sayan Bhattacharyya, IISER Kolkata
Vote of Thanks by Prof. Alakesh Bisai (19:40 – 19:45)	
CLOSING REMARKS by Prof. Sandeep Verma (19:45 – 19:50)	
SPECIAL DINNER (20:00 – 22:30)	
***Day 4: October 6, 2024* | Sunday**	
BREAKFAST & DEPARTURES (07:00 – 10:00)	

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Abstracts & Bio-Sketches – Evening Lectures

FORCE-IICS 2024 Conference
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Bio-sketch (Chairperson)

Profile

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Prof Sandeep Verma has been working at the Department of Chemistry and as an affiliated faculty at Center for Nanoscience and Mehta Family Center for Engineering in Medicine, Indian Institute of Technology Kanpur. He is also an Honorary Adjunct Professor at School of Science, Royal Melbourne Institute of Technology University, Melbourne, and School of Agriculture, Biomedicine and Environment, La Trobe University, Melbourne, Australia. Affiliated Faculty. His research interests include chemical neuroscience, new antibiotics, and microfluidic devices. With over 250 publications and several patents, his work has been recognized by Shanti Swarup Bhatnagar Prize, Distinguished Alumnus Award of Banaras Hindu University, Society of Materials Chemistry Gold Medal, CRSI Silver Medal, and Swarnajayanti Fellowship, to name a few. He is an elected Fellow of Indian National Science Academy, Indian Academy of Sciences, National Academy of Sciences, and Indian National Academy of Engineering. He is an Associate Editor of Chemical Communications (RSC, UK). He served as Secretary, Science and Engineering Research Board, Department of Science and Technology (2019-2022). At present, Prof. Verma is leading Gangwal School of Medical Sciences and Technology, at IIT Kanpur.

Representative Publications:

1. Synthesis of a highly thermostable insulin by phenylalanine conjugation at B29 Lysine. *Commun. Chem. 161*, (**2024**) (https://doi.org/10.1038/s42004-024-01241-z)
2. Membrane-targeting, ultrashort lipopeptide acts as an antibiotic adjuvant and sensitizes MDR Gram-negative pathogens toward narrow-spectrum antibiotics. *Biomed. Pharmacother. 176*, 116810 (**2024**) (https://doi.org/10.1016/j.biopha.2024.116810)
3. Amyloid mimicking assemblies formed by glutamine, glutamic acid, and aspartic acid. *ACS Chem. Neurosci.*, **2024**, *15*, 2253-2264.
4. Peptide-triggered IL-12 and IFN-γ mediated immune response in $CD4^+$ T-cells against *Leishmania donovani* infection. *Chem. Commun.*, **2024**, *60*, 4092-4095.
5. Anti-proliferative, -migratory and -clonogenic effects of long-lasting nitric oxide release in HepG2 cells. *Chem. Commun.*, **2024**, *60*, 3527-3530.
6. Machine learning approaches for antibiotic development and prediction of microbial resistance. *Chem. Asian J.* (**2024**) (https://doi.org/10.1002/asia.202400102) (Review).

G-protein Coupled Receptors

Prof. Robert J. Lefkowitz*
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Dr. Robert Lefkowitz, a physician-scientist, is an Investigator of the Howard Hughes Medical Institute, the Chancellor's Distinguished Professor of Medicine and Professor of Biochemistry and Chemistry at the Duke University Medical Center. He is an elected member of the National Academy of Sciences, National Academy of Medicine and the American Academy of Arts and Sciences. He has received numerous awards including the National Medal of Science, the Shaw Prize in Life Science and Medicine and the Canada Gairdner International award. In 2012 he and Brian Kobilka, a postdoctoral fellow in his laboratory in the 1980s, were awarded the Nobel Prize in Chemistry for their studies of G-protein coupled receptors.

Abstracts & Bio-Sketches – Invited Lectures

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Halogen Bonding in Cell Membrane Transport

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Small-molecule-based fluorescent probes have become important tools in biology for sensing and imaging applications. However, the biological applications of many of the fluorescent molecules are hampered by low cellular uptake and high toxicity. Recently, we showed for the first time that the introduction of halogen atoms enhances the cellular uptake of small molecules and proteins, and the nature of halogen atoms plays a crucial role in the plasma membrane transport in mammalian cells. The remarkably higher uptake of iodinated compounds as compared to that of their chloro or bromo analogues suggests that the strong halogen bonding ability of iodine atoms may play an important role in the membrane transport. This study provided a novel strategy for the transport of fluorescent molecules including proteins across the plasma membrane in living cells.

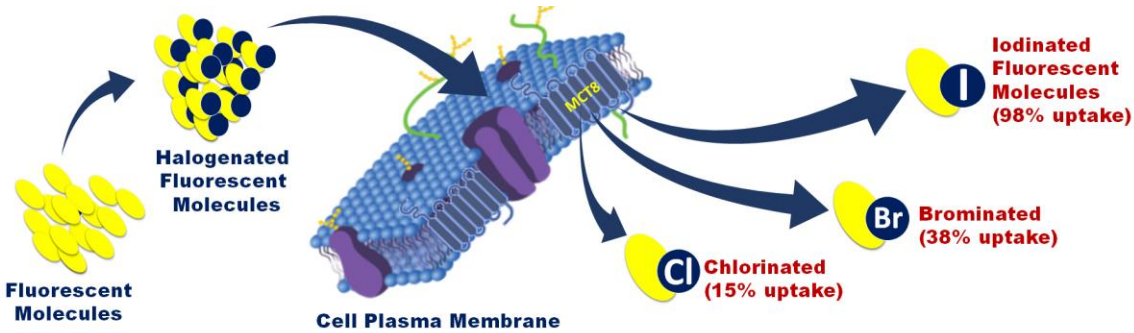

Figure 1: Halogen bond-assisted cellular uptake of fluorescent probes.

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1. H. Ungati, V. Govindaraj, G. Mugesh, The Remarkable Effect of Halogen Substitution on the Membrane Transport of Fluorescent Molecules in Living Cells. *Angew. Chem. Int. Ed.* **2018**, *57*, 8989.
2. H. Ungati, V. Govindaraj, C. R. Nair, G. Mugesh, Halogen-mediated Membrane Transport – An Efficient Strategy for the Enhancement of Cellular Uptake of Synthetic Molecules. *Chem. Eur. J.* **2019**, *25*, 3391.
3. S. R. Jakka, V. Govindaraj, G. Mugesh, A Single Atom Change Facilitates the Membrane Transport of Green Fluorescent Proteins in Mammalian Cells. *Angew. Chem. Int. Ed.* **2019**, *58*, 7713.
4. V. Govindaraj, H. Ungati, S. R. Jakka, S. Bose, G. Mugesh, Directing Traffic: Halogen Bond-mediated Membrane Transport. *Chem. Eur. J.* **2019**, *25*, 11180.
5. D. Giri, V. Govindaraj, S. Kumar, H. Ungati, G. Mugesh, G. A Highly Selective Fluorescent Probe for Monitoring the Thyroid Hormone Transporter Activity in Mammalian Cells. *Chem. Eur. J.* **2024**, *30*, e202401719.

Bio-sketch

Profile

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G. Mugesh received his B.Sc. (1990) and M.Sc. (1993) degrees from the University of Madras and Bharathidasan University, respectively. He obtained his Ph.D. (1998) at IIT, Bombay, under the supervision of Prof. H. B. Singh. In 2000, he moved to Germany as an Alexander von Humboldt Fellow at the Technical University, Braunschweig. He also worked with Prof. K. C. Nicolaou at the Scripps Research Institute, as a postdoctoral fellow. Mugesh's work ranges from artificial enzymes to novel cellular delivery strategies for biomedical applications.

Mugesh is recipient of Ignite Life Science Foundation Award (2023); IIT Bombay Distinguished Alumnus Award (2021); SASTRA-CNR Rao Award in Chemistry & Materials Science (2021); Infosys Prize in Physical Sciences (2019); CRSI Silver Medal (2019); National Prize for Research on Interfaces of Chemistry and Biology (2017); J. C. Bose National Fellowship (2015); Shanti Swarup Bhatnagar Prize (2012); AstraZeneca Excellence in Chemistry Award (2012); Swarnajayanti Fellowship (2006-07); Ramanna Fellowship, DST (2006). He is a fellow of the National Academy of Sciences, India (2012), Indian Academy of Sciences (2012) and Indian National Science Academy (2016).

Representative Publications:

1. Singh, N.; Sherin, G. R.; Mugesh, G. Antioxidant and Prooxidant Nanozymes: From Cellular Redox Regulation to Next-Generation Therapeutics. *Angew. Chem. Int. Ed.* **2023**, *62*, e202301232.
2. Geethika, M.; Singh, N.; Kumar, S.; Naveen Kumar, S. K.; Mugesh, G. A Redox Modulatory SOD Mimetic Nanozyme Prevents the Formation of Cytotoxic Peroxynitrite and Improves Nitric Oxide Bioavailability in Human Endothelial Cells. *Adv. Healthcare Mater.* **2023**, *12*, 202300621.
3. Ungati, H.; Govindaraj, V.; Narayanan, M.; Mugesh, G. Probing the formation of a Seleninic Acid in Living Cells by a Fluorescence Switching of a Glutathione Peroxidase Mimetic. *Angew. Chem. Int. Ed.* **2019**, *58*, 8156 - 8160.
4. Singh, N.; NaveenKumar, S. K.; Geethika, M.; Mugesh, G. Cerium vanadate nanozyme with specific superoxide dismutase activity regulates mitochondrial function and ATP synthesis in neuronal cells. *Angew. Chem. Int. Ed.* **2021**, *60*, 3121 - 3130.
5. Mondal, S.; Raja, K.; Schweizer, U.; Mugesh, G. Chemistry and Biology in the Biosynthesis and Action of Thyroid Hormones. *Angew. Chem. Int. Ed.* **2016**, *55*, 7606.

Nicotinamide Acetyl Choline Receptors (nAChR) in lung cancer: focus on never smokers and the tumour microenvironment

Tapasya Srivastava *
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Smoking and nicotine addiction are considered to be the strongest predisposing factors to lung cancer along with genetic predispositions and mutations. However, data suggests that a large number of lung adenocarcinoma cases are those of non-smokers. With the help of clinical data at AIIMS lung cancer clinic we determined that there was only a small difference in disease free progression and mortality between patients who were smokers and the never-smokers. We know that nicotinamide acetyl choline receptors (nAChR family; CHRNA1-11) are among the first ‘perceivers’ of nicotine therefore genetic alterations associated with these receptors can alter an individual’s response to nicotine. However, not much was known about the function of the CHRNA genes in patients who are never-smokers. Therefore we decided to evaluate– 1) previously undescribed genetic predisposition and association study of single nucleotide polymorphism of CHRNA5 in the Indian lung cancer patients vs controls. 2) molecular and mechanistic function of CHRNA7 in lung cancer progression in never-smokers. Our studies elucidate the importance of nAChR receptors in disease pathogenesis particularly in the hypoxic tumour microenvironment.

References and Notes:

1. Pandey N, Chongtham J, Pal S, Ali A, Lalwani S, Jain D, Mohan A, Srivastava T. When "No-Smoking" is not enough: Hypoxia and nicotine acetylcholine receptor signaling may drive lung adenocarcinoma progression in never-smokers. Biochim Biophys Acta Mol Cell Res. 2023 Feb;1870(2):119302. doi: 10.1016/j.bbamcr.2022.119302. PMID: 35649481.
2. Pandey N, Pal S, Sharma LK, Guleria R, Mohan A, Srivastava T. SNP rs16969968 as a Strong Predictor of Nicotine Dependence and Lung Cancer Risk in a North Indian Population. Asian Pac J Cancer Prev. 2017 Nov 26;18(11):3073-3079. doi: 10.22034/APJCP.2017.18.11.3073. PMID: 29172281; PMCID: PMC5773793.
3. Chongtham J, Pandey N, Sharma LK, Mohan A, Srivastava T. SNP rs9387478 at ROS1-DCBLD1 Locus is Significantly Associated with Lung Cancer Risk and Poor Survival in Indian Population. Asian Pac J Cancer Prev. 2022 Oct 1;23(10):3553-3561. doi: 10.31557/APJCP.2022.23.10.3553. PMID: 36308382; PMCID: PMC9924343.

Bio-sketch

Profile

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Prof Tapasya Srivastava was awarded her PhD in 2004. For her thesis she worked on genomic instability in astrocytic tumours. After a postdoctoral stint at AIIMS and appointment as a scientist in National Centre for Disease Control, she joined as an Assistant Professor at Department of Genetics, University of Delhi South Campus in 2009. She was awarded the INSA young scientist medal in 2010. She was also awarded the Indo-US Science and Technology Fellowship to pursue research at University of Minnesota. Her primary role at UDSC is of a teacher to post graduate students while pursuing her research on cancer biology in the department. Her lab works on the genetic basis, role of causal candidate genes, susceptibility, epigenetic controls and prognostic markers of cancers. The lab uses various NGS and molecular tools on primary tumours and cfDNA for early detection and prognosis. The lab frequently collaborates with clinicians and pathologists. Funding has come from various agencies- SERB, ICMR, DST and DBT. The Cancer Biology lab has published various international peer-review original papers with their work on lung, glioma and leukemia. The lab has produced 8 PhDs, 6 enrolled PhD and has trained many post-graduate and undergraduate students particularly from small universities. During the last 15 years in the University she has taken on various academic and administrative roles. She has served on various committees of ICMR and SERB. She has extensively served on Institutional Ethics Committee as Member secretary of UDSC and as a member in AYUSH. She has also served as member secretary of the Institutional Animal Ethics Committee of UDSC and as a member in Indraprastha University. She has also served as a member in the Institutional Stem Cell Research Committee in NII.

Representative Publications:

1. Prasad P, Chongtham J, Tripathi SC, Ganguly NK, Mittal SA, **Srivastava T.** Targeted inhibition of NRF2 reduces the invasive and metastatic ability of HIP1 depleted lung cancer cells. Biochem Biophys Res Commun. 2024 Sep 11;733:150676. doi: 10.1016/j.bbrc.2024.150676. Epub ahead of print. PMID: 39303527.

2. Gandhi S, Bhushan A, Shukla U, Pundir A, Singh S, **Srivastava T**. Downregulation of lncRNA SNHG1 in hypoxia and stem cells is associated with poor disease prognosis in gliomas. Cell Cycle. 2023 May;22(9):1135-1153. doi: 10.1080/15384101.2023.2191411.
3. Pandey N, Tyagi G, Kaur P, Pradhan S, Rajam MV, **Srivastava T**. Allicin Overcomes Hypoxia Mediated Cisplatin Resistance in Lung Cancer Cells through ROS Mediated Cell Death Pathway and by Suppressing Hypoxia Inducible Factors. Cell Physiol Biochem. 2020 Aug 19;54(4):748-766. doi: 10.33594/000000253. PMID: 32809300.
4. Shukla P, Deswal D, Pandit M, Latha N, Mahajan D, **Srivastava T**, Narula AK. Exploration of novel TOSMIC tethered imidazo[1,2-a]pyridine compounds for the development of potential antifungal drug candidate. Drug Dev Res. 2022 Apr;83(2):525-543. doi: 10.1002/ddr.21883. Epub 2021 Sep 27. PMID: 34569640.
5. Scouting for common genes in the heterogenous hypoxic tumor microenvironment and their validation in glioblastoma. 3 Biotech. 2021 Oct;11(10):451. doi: 10.1007/s13205-021-02987-2. Epub 2021 Sep 26. PMID: 34631352; PMCID: PMC8473528.
6. Prasad P, Mittal SA, Chongtham J, Mohanty S, **Srivastava T**. Hypoxia-Mediated Epigenetic Regulation of Stemness in Brain Tumor Cells. Stem Cells. 2017 Jun;35(6):1468-1478. doi: 10.1002/stem.2621. Epub 2017 Apr 24. PMID: 28376560.
7. Pradhan S, Mahajan D, Kaur P, Pandey N, Sharma C, **Srivastava T.** Scriptaid overcomes hypoxia-induced cisplatin resistance in both wild-type and mutant p53 lung cancer cells. Oncotarget. 2016 Nov 1;7(44):71841-71855. doi: 10.18632/oncotarget.12378. PMID: 27708247; PMCID: PMC5342127.
8. Pandey N, Dhiman S, **Srivastava T**, Majumder S. Transition metal oxide nanoparticles are effective in inhibiting lung cancer cell survival in the hypoxic tumor microenvironment. Chem Biol Interact. 2016 Jul 25;254:221-30. doi: 10.1016/j.cbi.2016.06.006. Epub 2016 Jun 4. PMID: 27270449.
9. Mittal S, Pradhan S, **Srivastava T**. Recent advances in targeted therapy for glioblastoma. Expert Rev Neurother. 2015;15(8):935-46. doi: 10.1586/14737175.2015.1061934. Epub 2015 Jun 28. PMID: 26118735.

Mapping metabolic perturbations using NMR spectroscopy as a tool for biomarker discovery

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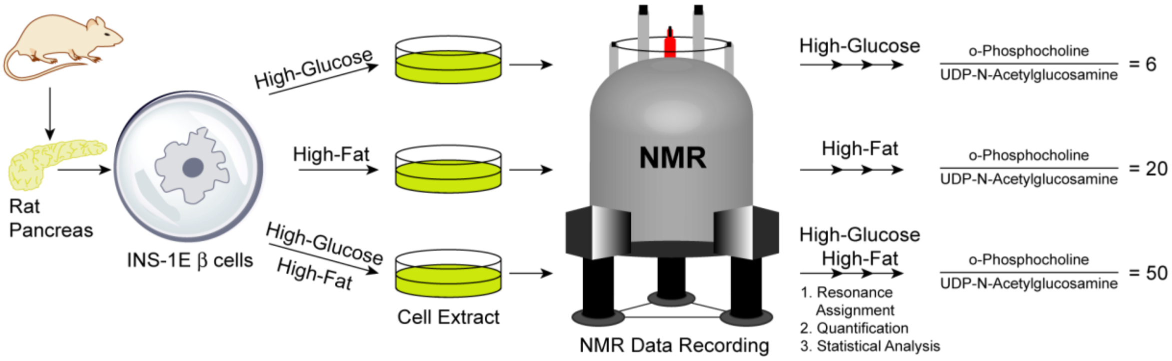
Abstract: The incidence of Type 2 Diabetes Mellitus (T2DM) is on the rise and has been attributed to changes in lifestyle, over-nutrition, stress, and lack of physical activity. It has been associated with β-cell dysfunction, defects in insulin secretion, and development of insulin resistance in the target tissues. The classical biomarkers and strategies currently used to diagnose T2DM, including plasma glucose levels and glycated haemoglobin, can help to know the disease state only after the metabolic syndrome has already been established in the body. Since diabetes detection by classical biomarkers is late, the current therapeutic options directed against T2DM only help to delay its progression and cannot reverse the condition. This brings up the need to identify early and novel biomarkers which will help predict the onset. Our lab has been making attempts in this direction to identify potential diagnostic biomarkers associated T2DM.

Metabolomics, the youngest omics platform after genomics, transcriptomics and proteomics, involves the detection of small molecular weight metabolites from body fluids, cells and their extracts, tissues, etc. These metabolites are the end products of different biochemical processes that are highly dynamic and get affected by both genetic and environmental changes. Hence, these can reveal the changes occurring in response to pathophysiological conditions, thereby serving as early and specific biomarkers for different diseases. Using INS-1E pancreatic beta-cells as a model system, we have used stressors including high glucose (glucotoxic) and saturated free fatty acids (lipotoxic) alone and in combination (glucoliopotoxic) to mimic T2DM-like conditions. This was associated with increased ROS levels, membrane damage, lipid accumulation, and DNA double-strand breaks and the induction of metabolic imbalance. Of the forty-nine abundant metabolites identified and quantified using ^{1}H-NMR spectroscopy, UDP-N-acetylglucosamine and o-phosphocholine were identified as the commonly perturbed metabolites in the three nutrient overload conditions. The supplementation of o-phosphocholine in glucolipotoxic conditions was associated with the restoration of function and viability of the β-cells. Follow-up studies in a well characterized human cohort also hinted at identification of o-phosphocholine as the major metabolite, which

was altered in the pre-diabetic and diabetic subjects. The results from these investigations will be elaborated.

Figure/Scheme (if any):



References and Notes:

1. Yousf S, Batra HS, Jha RM, Sardesai DM, Ananthamohan K, Chugh J,[$] **Sharma S[$].** *Identification of potential serum biomarkers associated with HbA1c levels in Indian type 2 diabetic subjects using NMR-based metabolomics.* **Clin Chim Acta. 2024 Apr 15;557:117857. doi: 10.1016/j.cca.2024.117857.**
2. Yousf S, Sardesai DM, Mathew AB, Khandelwal R, Acharya JD, **Sharma S[$]**, Chugh J[$]. *Metabolic signatures suggest o-phosphocholine to UDP-N-acetylglucosamine ratio as a potential biomarker for high-glucose and/or palmitate exposure in pancreatic β-cells.* **Metabolomics. 2019 Mar 29;15(4):55.**

Bio-sketch

Profile

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Dr. Shilpy Sharma is an Assistant Professor working at the Department of Biotechnology, Savitribai Phule Pune University, Pune, India since 2018. She joined the same Department in June 2013 as a DBT-Ramalingaswami Fellow. She is also serving as an adjunct faculty in Kasturba Medical College, Manipal academy of higher education since 2018. Dr. Sharma obtained her PhD from CSIR-IGIB, New Delhi, where she studied the genetic variants associated with asthma in the Indian population. Before moving to Pune, she worked as a post-doc fellow in The University of Michigan, The University of Chicago, and at TIFR, Mumbai. During her tenure in the US, she focused on studying DNA damage and repair and immunological defects that occur in non-communicable diseases. She has several publications in journals of high impact and repute, has guest edited a book 'prognostic epigenetics', and has contributed to 5 book chapters. She has received several awards, including Dr. GP Talwar young scientist award, the AAAAI Star award, and Dr. Dipti Kapoor Endowment award. Currently, her group at DBT, Savitribai Phule Pune University, is trying to understand the pathophysiology of type 2 diabetes, wherein attempts are being made to identify novel biomarkers for identifying individuals at risk. Her lab is also trying to gain mechanistic insights into the development of insulin resistance, and how natural compounds and ayurvedic medicines mediate their anti-diabetic activity using in vitro 2D and 3D cell culture models, and animal models.

Representative Publications:

1. Naik AR, Save SN, Sahoo SS, Yadav SS, Kumar A, Chugh J, **Sharma S.**[$] *Metabolic Perturbations associated with hIAPP-induced insulin resistance in Skeletal Muscles: Implications to the Development of Type 2 Diabetes*. **Int J Biochem Cell Biol. 2024; In press.**
2. Yousf S, Batra HS, Jha RM, Sardesai DM, Ananthamohan K, Chugh J,[$] **Sharma S**[$]**.** *Identification of potential serum biomarkers associated with HbA1c levels in Indian type 2 diabetic subjects using NMR-based metabolomics.* **Clin Chim Acta. 2024 Apr 15;557:117857. doi: 10.1016/j.cca.2024.117857.**
3. Yousf S, Malla JA, Sardesai DM, **Sharma S**, Talukdar P, Chugh J[$]. *Mapping metabolic perturbations induced by glutathione activatable synthetic ion channels in human breast cancer cells.* **J Pharm Biomed Anal. 2023 Oct 25;235:115605. doi: 10.1016/j.jpba.2023.115605.**

Bio-sketch

4. Malla JA, Umesh RM, Yousf S, Mane S, **Sharma S**, Lahiri M, Talukdar P[$]. *A Glutathione Activatable Ion Channel Induces Apoptosis in Cancer Cells by Depleting Intracellular Glutathione Levels.* **Angew Chem Int Ed Engl. 2020 2020 May 11;59(20):7944-7952.**
5. Yousf S, Sardesai DM, Mathew AB, Khandelwal R, Acharya JD, **Sharma S[$]**, Chugh J[$]. *Metabolic signatures suggest o-phosphocholine to UDP-N-acetylglucosamine ratio as a potential biomarker for high-glucose and/or palmitate exposure in pancreatic β-cells.* **Metabolomics. 2019 Mar 29;15(4):55.**

Modulating Biocatalysis to Promote Antioxidant Response

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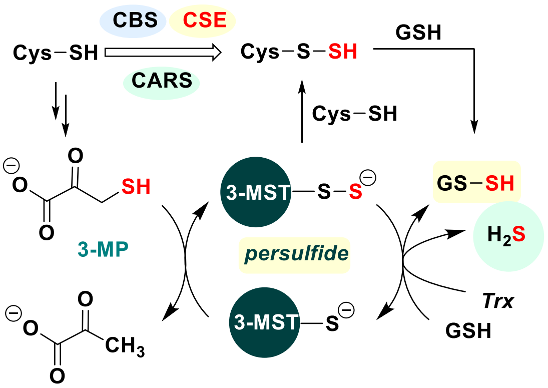
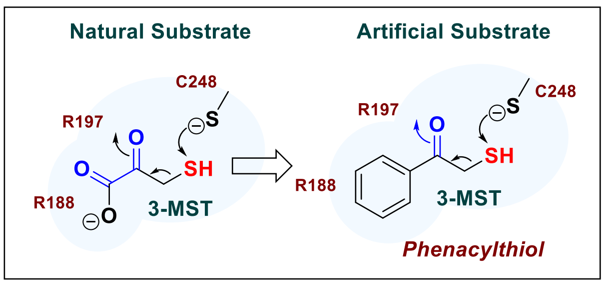
Abstract: Hydrogen sulfide (H_2S), persulfides (RS-SH), and related sulfur species are produced in nearly all cells and have diverse roles including as antioxidants.[1] Cysteine is the primary source of such sulfur species in cells, and enzymes that generate H_2S include cystathionine β-synthase (CBS), cystathionine γ-lyase (CSE), cysteinyl-tRNA synthetase (CARS) as well as 3-mercaptopyruvate sulfurtransferase (3-MST).[2] In an attempt to promote endogenous antioxidant response, our lab designed and developed artificial substrates for 3-MST, an enzyme whose natural substrate is 3-mercaptopyruvate (3-MP), and produces a persulfide, which is cleaved by thioredoxin (Trx) to generate H_2S. The first generation of artificial substrates showed excellent antioxidant and anti-inflammatory properties in both cellular and animal models.[3] Using a computational structure-guided approach, we designed and developed a new series of artificial substrates for 3-MST. These compounds were found to enhance endogenous persulfides, and protect cells from oxidative stress-induced cell death. Together, we provide evidence that underscores a new therapeutic paradigm of using small molecules to promote cells' own antioxidant response.





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2. Pedre, B.; Talwar, D.; Barayeu, U.; Schilling, D.; Luzarowski, M.; Sokolowski, M.; Glatt, S.; Dick, T. P. *Nat. Chem. Biol.* **2023**, *19* (4), 507–517.
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Bio-sketch

Profile

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Harinath Chakrapani completed his undergraduate and post-graduate studies in Chemistry from Loyola College (1994-97) and Indian Institute of Technology Madras (1997-99), respectively. In the fall of 1999, he moved to Duke University, USA to pursue his doctoral studies, which he completed in Dec. 2005. After a brief stint as a postdoctoral research associate at Wake Forest University, USA, he moved to the Center for Cancer Research, National Cancer Institute USA as a Visiting Fellow in Aug 2006. He joined Indian Institute of Science Education and Research Pune in July 2009 and is currently Professor. His primary research interests are in the area of physical and mechanistic organic chemistry, with applications in understanding biological responses to stress, circumventing mechanisms of antimicrobial resistance, and prodrug design and delivery.

Recent Publications

1. Manna, S.; Agrawal, R.; Yadav, T. Anand Kumar, T.; Kumari, P. Dalai, A.; Kanade, S. Balasubramanian, N. Singh, A.; **Chakrapani, H.** "Orthogonal Persulfide Generation through Precision Tools Provides Insights into Mitochondrial Sulfane Sulfur" *Angewandte Chemie International Edition* **2024**, in press https://doi.org/10.1002/anie.202411133
2. Chaudhary, B.S.; Anand Kumar, T.; Vashishta, A.; Tejasri, S.; Kumar, A. S.; Agarwal, R.; **Chakrapani, H.** "An Esterase-Cleavable Persulfide Donor with No Electrophilic Byproducts and a Fluorescence Reporter" *Chemical Communications*, **2024**, 60, 1727-1730.
3. Sawase, L.; Anand Kumar, T.; Mathew, A. B.; Khodade, V. S.; Toscano, J. P.; Saini, D. K.; **Chakrapani, H "**β-Galactosidase-activated nitroxyl (HNO) donors provide insights into redox cross-talk in senescent cells" *Chemical Communications*, **2023**, *59*, 12751-12754.
4. Sawase, L.; Jishnu, C.V.; Manna, S..; **Chakrapani, H.** "A modular scaffold for triggerable and tunable nitroxyl (HNO) generation with a fluorescence reporter" *Chemical Communications*, **2023**, *59*, 3415-3418.
5. Bora, P.; Sathian, M.B.; **Chakrapani, H.** "Enhancing Cellular Sulfane Sulfur Through β-glycosidase-Activated Persulfide Donors: Mechanistic Insights and Oxidative Stress Mitigation" *Chemical Communications*, **2022**, *58*, 2987–2990.
6. Bora, P.; Manna, S.; Nair, M.; Sathe, R.M.S.; Singh, S.; Adury, V.S.S.; Gupta, K.; Mukherjee, A.; Saini, D. K.; Kamat, S.S.; Hazra, A. B.; **Chakrapani, H.** "Leveraging an Enzyme/ Artificial Substrate System to Enhance Cellular Persulfides and Mitigate Neuroinflammation" *Chemical Science*, **2021**, *12*, 12939-12949.

Anion Recognition through σ-hole Interactions

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Abstract: Selective recognition, sensing and efficient extraction of inorganic anions from aqueous medium is of great importance for promising analytical, industrial and environmental applications. In this direction, in recent years, significant advances have been made in the design of superior supramolecular anion receptors having Sigma-hole (σ-hole) interactions, in particular halogen bonding (XB) and chalcogen bonding (ChB) where a positively charged region on a polarised, electron deficient halogen or chalcogen atom (the σ-hole) interacts with the Lewis base (anion). In this talk, I will discuss on our recent development in the area of anion recognition chemistry, which particularly deals with the XB/ ChB based receptors for (i) selective removal of bromide and iodide,[1-3] (ii) selective sensing of phosphates[4-7] and (iii) selective extraction of perrhenate.[8-9]

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2. S. Chakraborty, S. Maji, R. Ghosh, R. Jana, A. Datta, P. Ghosh, ***Chem. Commun.*** 2019, *55*, 1506-1509.
3. A. S. M. Islam, S. Pramanik, S. Mondal, R. Ghosh, P. Ghosh, ***iScience*** 2024, *27*(2),108917 (1-15).
4. B. Chowdhury, S. Sinha and P. Ghosh, ***Chem. Eur. J***., 2016, 22, 18051-18059.
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8. R. Ghosh, T. K. Ghosh, S. Pramanik, A.S.M. Islam, and P. Ghosh, ***ACS Appl. Mater. Interfaces*** 2023, *15*, 25184-25192.
9. S. Pramanik, A. S. M. Islam, I. Ghosh and P. Ghosh, ***Chem. Eur. J.*** 2024, e202402153.

Bio-sketch

Profile

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Dr. Pradyut Ghosh obtained his Ph. D. in Chemistry from Indian Institute of Technology, Kanpur for his research on Heteroditopic Cryptands under the supervision of Professor Parimal K. Bharadwaj in 1998. He spent two years as a Post-doctoral Research Associate at Texas A&M University, USA with Professor Richard M. Crooks where he worked on Surface Chemistry and Soft Lithography, and one year as an Alexander von Humboldt Fellow at University of Bonn, Germany in Professor Fritz Vögtle's group in the area of Rotaxane Chemistry and Molecular Machines. Upon his return to India in 2000 he joined in Central Salt & Marine Chemicals Research Institute (CSMCRI), Bhavnagar. In April 2007, he moved to Indian Association for the Cultivation of Science (IACS), Kolkata, as an Associate Professor and then he was promoted to the post of Professor in April, 2011. Since April 2016 he is serving as a Senior Professor in the department and presently in the School of Chemical Sciences at IACS. In 2014 Professor Ghosh also spent three months in Professor Christoph A. Schalley's group for a collaborative research work on Mass spectrometry in Free University of Berlin, Germany. His current research interest includes chemical sensing of ions, recognition and extraction of anions of environmental and biological relevance and catalysis. His contributions on interlocked molecules, water clusters and self-assembly are noteworthy. His work has produced 165 publications in peer-reviewed international journals and international patents. For his research accomplishments he has been awarded Indian Science Congress Association (ISCA) Young Scientist Award (1998), Alexander von Humboldt (AvH) Fellowship (2000), CSIR Young Scientist Award in Chemical Sciences (2004), Swarnajayanti Fellowship in Chemical Sciences (2009), B. M. Birla Prize in Chemical Science (2009) and CRSI Bronze medal (2012). He has been awarded the prestigious Shanti Swarup Bhatnagar (SSB) Prize in Chemical Sciences (2015), has been elected as Fellow of Indian Academy of Science (FASc), Bangalore (2016). More recently, he has been awarded Professor Priyadaranjan Ray Memorial Award 2020 (Indian Chemical Society), has been elected as Fellow Indian National Science Academy (FNA), New Delhi (2020) and has been awarded the J C Bose National Fellowship (2022).

Representative Publications:

1. A. S. M. Islam, S. Pramanik, S. Mondal, R. Ghosh, P. Ghosh, ***iScience*** 2024, *27*(2),108917 (1-15).
2. S. Mondal, S. Mandal, S. Mondal, S. P. Midya, P. Ghosh, ***Chem. Commun.*** 2024, *60*, 9645-9658.
3. S. Pramanik, A. S. M. Islam, I. Ghosh, P. Ghosh, ***Chem. Sci.*** 2024, *15*, 7824-7847.
4. R. Ghosh, T. K. Ghosh, S. Pramanik, A.S.M. Islam, P. Ghosh, ***ACS Appl. Mater. Interfaces*** 2023, *15*, 25184-25192.
5. M, Nandi, S. Bej, T. Jana, P. Ghosh, ***Chem. Commun.*** 2023, *59*, 14776-14790.

Title: A Versatile Step-Growth Polymerization Route to Enzymatically Degradable Functional Polyesters and Their Biomedical Implications

Name: Dr. Anindita Das
Institution: Indian Association for the Cultivation of Science (IACS), Kolkata, India
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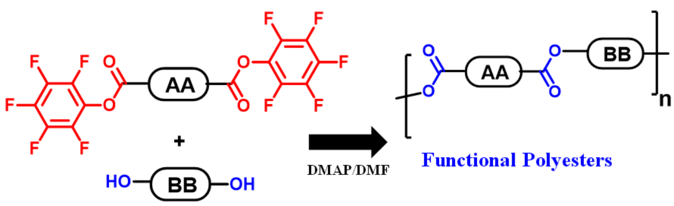
Abstract: Our work describes a versatile and efficient step-growth polymerization route to functional aliphatic polyesters through an organo-catalyzed transesterification reaction between an activated pentafluorophenyl-diester of adipic acid (AA) and various structurally different diols (BB) (Scheme 1).[1] The use of an activated diester enables us to obtain a near quantitative reaction under mild conditions with no requirement of by-product (pentafluorophenol) removal, which remains a major drawback in the conventional polyester synthesis with non-activated diesters. Enzymatic degradation of the resultant polyesters has been demonstrated, which can be tuned by playing with the hydrophobicity of the polyester backbone. Following the same synthetic strategy, water dispersible amphiphilic, cationic polyesters with pendant naphthalene monoimide (NMI) derivatives were prepared by pre-quaternization of the fluorescent monomers with different alkyl chain ends in order to design polyesters with positively charged hydrophobic pendant moieties. These amphiphilic polyesters produced fluorescent nanoparticles in water, which exhibit broad-spectrum antibiotic properties against both gram-positive and gram-negative bacteria depending upon the nature of the cationic side chains.[2] The intrinsic fluorescent nature of the nanoparticles enabled us to study their interactions with bacterial cells by fluorescence live-dead assay, which provided us insights of bacterial disruption by membrane perturbation similar to the mechanism followed by host defense peptides. The facile synthetic methodology enables us to investigate systematic structure-activity relationships in such rarely reported dye-conjugated polyester backbones, which suggests the dual role of the aliphatic chain and the aromatic dyes in conferring biocidal activity, selectively against the bacterial cells. Some of these cationic polyesters exhibit remarkably high cellular uptake by the endocytic pathway and mitochondrial targeting ability following lysosomal escape.[3] Further, this methodology enables us to design and prepare biotin-functionalized polyesters that exhibit selective uptake in cancer cells, thus showing their potential for targeted drug delivery applications. This presentation will showcase multiple aspects of our newly established synthetic methodology for functional polyesters and their biomedical implications.



Scheme 1. Synthetic scheme for functional polyesters from activated pentafluorophenyl ester of adipic acid and structurally different diols.

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1. S. Biswas, A. Das, *Chem. Eur. J.* **2023**, 29, e202203849
2. S. Biswas, R. Barman, M. Biswas, A. Banerjee, A. Das, *Polym. Chem.* **2024**, 15, 2753
3. S. Biswas, P. Rajdev, A. Banerjee, A. Das (manuscript under preparation)

Bio-sketch

Profile

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Biosketch: 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, The Netherlands (2016–2017). She started her independent research career at the IACS in 2017. Her research interests include supramolecular polymerization of functional π-systems and macromolecules by directional non-covalent interactions, crystallization-driven macromolecular assemblies, and functional degradable polymers.

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).

Representative Publications:

1) Chakraborty, C.; Rajak, A.; Das, A. *Nanoscale* **2024**, *16*, 13019-13028
2) Biswas, S.;ǂ Barman, R.;ǂ Biswas, M.; Banerjee, A.; Das, A. *Polym. Chem.* **2024,** *15*, 2753-2762 (ǂ equal contribution)
3) Khanra, P.; Rajdev, P.; Das, A. *Angew. Chem. Int. Ed.* **2024**, *63*, *e20240048* (VIP)
4) Rajak, A.; Das, A. *Angew. Chem. Int. Ed.* **2023**, *62*, e202314290
5) Khanra, P.; Singh, A. K.; Roy, L; Das, A. *J. Am. Chem. Soc.* **2023**, *145*, 5270

6) Biswas, S.; Das, A. *Chem. Eur. J*. **2023**. *29*, e202203849
7) Rajak, A.; Das, A. *Angew. Chem. Int. Ed.* **2022**, *61*, e202116572 (Hot Paper)
8) Jamadar, A; Singh, A. K.; Roy, L*; Das, A. *J. Mater. Chem. C* **2021**, *9*, 11893

Water Crisis Management: Lignin-derived Carbon Dots Upgraded Bacterial Cellulose Membrane as All-in-one Interfacial Evaporator for Solar-driven Water Purification

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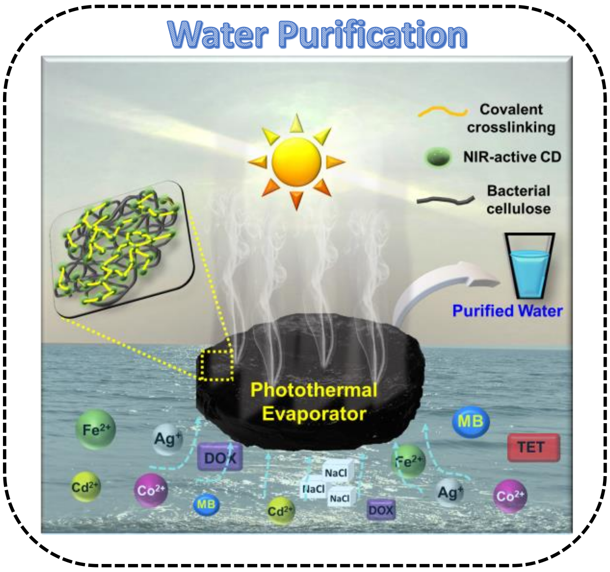
Abstract:
New trends demand adaptive technology to develop photothermal membranes with multifunctional features to address water crisis. Herein, report a robust multi-purpose near infrared (NIR)-active hydrogel composite (*c*-BC@N-LCDs) from broad-spectrum active nitrogen-doped lignin-derived carbon dots (N-LCDs) by covalently cross-linked with bacterial cellulose (BC) matrix. Adopting such cross-linking strategy to append quantum size particles with porous polymeric matrices would bear the benefits of multiple reuses of nanoparticles while preventing their elution into the environment. Owing to highly entangled nanofibrous network structure, BC provides adequate porosity, hydrophilicity required for the easy water transport, while effectively managing heat loss. As-fabricated *c*-BC@N-LCDs achieves a commendable evaporation rate of 2.2 kg m^{-2} h^{-1} under one sun (1 kW m^{-2}). Furthermore, the developed hydrogel system also found efficient for desalination (~2.1 kg m^{-2} h^{-1}) and for remediating various pollutants (heavy metal ions, dyes, and pharmaceuticals) from feed water on account of the photocatalytic activities and complex forming properties of CDs. The efficacy of the membrane is not much affected by different grade of water and hence can be adoptable for economically stressed communities living in water polluted regions as well as those residing in coastal area.



Keywords: Carbon dots, Hydrogels, Photothermal membrane, Solar water evaporation, Water purification.

References:
(1) Mate, N.; Nabeela, K.; Preethikumar, G.; Pillai, S.; Mobin, S. M. *Materials Horizons* **2024**.
(2) Mate, N.; Khandelwal, D.; Nabeela, K.; Mobin, S. M. *J. Mater. Chem. C* **2023**, *11*, 16201–16213.

Bio-sketch

Profile

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Biosketch:

Dr. Shaikh currently working as Professor in Department of Chemistry at IIT Indore. He had developed his research group working in wide area of multi-disciplinary research with focus on Inorganic Materials Chemistry which includes Solid-state structural reactivity, MOFs / COFs based supercapacitors for energy storage, catalysis, sensing and bio-medical applications. Metal oxide nanomaterials derived by employing metal complexes / MOFs as single atom catalysts for various organic transformation and electrocatalysts for energy conversion. Design and synthesis of greener c-dots and their wide range of bioimaging viz cellular organelles target and cell imaging and biosensing applications and Lead-Free solar cells for cleaner energy harvesting are major area of focus by the group.

Achievements:

- Elected council member of the Dalton Transaction Community, Royal Society of Chemistry.
- Fellow of Royal Society of Chemistry (FRSC) 2021.
- Recipient of Material Research Society of India (MRSI) Medal 2021.
- Fellow of Maharashtra Academy of Sciences (FMASc) 2020.
- Dr Shaikh has been named as ***Golden Author*** by *Dalton Transaction*, Royal Society of Chemistry on occasion of 50th Volumes of Dalton Trans.
- Dr. Shaikh has been recognised as the Outstanding Reviewers for *Dalton Transactions* in 2018 (*Dalton Trans.*, 2019, ***48***, 4758-4758).

Representative Publications:

1. Mate, N., Kallayi, N., Preethikumar, G., Pillai, S., and **Shaikh M. Mobin**. (2024): Lignin-derived Carbon Dots Upgraded Bacterial Cellulose Membrane as All-in-one Interfacial Evaporator for Solar-driven Water Purification. *Mater. Horizon*, *000*,Accepted.
2. Kumar, P., Kaur, N., Tiwari, P., Gupta, A., and **Shaikh M. Mobin**. (2023): Gelatin-coated Copper based Metal-Organic Framework for Controlled Insulin Delivery: Possibility towards oral delivery system. *ACS Mat Lett.*, *5*, *4*, 1100-1108.
3. Abbas, Z., Hussain, N., and **Shaikh M. Mobin**, (2024): Crumpled Fibrous 2D-Graphdiyne Network Decorated Metal-Organic Framework: A Promising Heterostructure for Improved Energy Storage Performance. *J. Mater. Chem. A*, *12*, 20170-20178.

A helium nanodroplet spectrometer to study molecular aggregation at ultracold temperatures

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Abstract: Helium droplets are clusters of helium atoms formed by the supersonic expansion of precooled helium gas (at temperatures of 4–25 K and backing pressures of 10–80 bar) through a 5-micron diameter nozzle.[1-2] These droplets achieve an equilibrium temperature of approximately 0.4 K and exist in a superfluid state. Molecules of interest can be easily embedded within the droplets, allowing the study of molecular aggregation using mass spectrometry and infrared spectroscopy.[1-4] Due to the weak interaction between the doped molecules and the helium droplets, the resulting infrared spectra closely resemble gas-phase spectra, providing valuable insights into isolated molecular behaviour.

We have recently constructed a helium nanodroplet spectrometer in our laboratory at IIT Kanpur. In this presentation, I will demonstrate the performance of the spectrometer by showcasing our results from the mass-spectrometric analysis of acetonitrile clusters. Additionally, I will discuss our plans to integrate the spectrometer with a high-resolution infrared laser, which will enable us to perform mass-selective infrared spectroscopy of molecular processes relevant to fundamental and interstellar chemistry.

References and Notes:

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2. Yang, S.; Ellis, A. M. *Helium Droplets: A Chemistry Perspective.* Chem. Soc. Rev. 2013, 42 (2), 472–484.
3. Schwan, R.; Qu, C.; Mani, D.; Pal, N.; Schwaab, G.; Bowman, J. M.; Tschumper, G. S.; Havenith, M. *Observation of the Low-Frequency Spectrum of the Water Trimer as a Sensitive Test of the Water-Trimer Potential and the Dipole-Moment Surface.* Angew. Chem. Int. Ed. 2020, 132, 11496–11504.
4. Mani, D.; De Tudela, R. P.; Schwan, R.; Pal, N.; Körning, S.; Forbert, H.; Redlich, B.; Van Der Meer, A. F. G.; Schwaab, G.; Marx, D.; Havenith, M. *Acid Solvation versus Dissociation at "Stardust Conditions": Reaction Sequence Matters.* Sci. Adv. 2019, 5 (6).

Bio-sketch

Profile

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Biosketch: Devendra Mani earned his Ph.D. in 2014 from the Indian Institute of Science (IISc) Bangalore, specializing in microwave spectroscopy of weakly bound molecular clusters. He then pursued postdoctoral research at Ruhr University Bochum, Germany, where he focused on infrared spectroscopy in helium nanodroplets. In 2020, he joined the Department of Chemistry at IIT Kanpur as an assistant professor, where he is currently working. His research group has built the first helium nanodroplets spectrometer in India. His research interests span high-resolution gas-phase spectroscopy, particularly emphasizing the use of helium nanodroplets to investigate molecular aggregation and chemical reactions at ultracold temperatures.

Representative Publications:

1. R. Gupta, S. Singha and D. Mani, Cooperativity between Intermolecular Hydrogen and Carbon Bonds in ZY···CH_3CN/CH_3NC···HX Trimers (ZY = H_2O, H_2S, HF, HCl, HBr, NH_3, and H_2CO; HX = HF, HCl, and HBr), J. Phys. Chem. A, 128, 4605-4622 (2024).

2. D. Mani, T. K. Roy, J. Khatri, G. Schwaab, S. Blach, C. Hölzl, H. Forbert, D. Marx, M. Havenith, Internal Electric Field-Induced Formation of Exotic Linear-Acetonitrile Chains, J. Phys. Chem. Lett. 13 (29), 6852–6858 (2022).

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Organocatalysis by Cyclopropenium-based Small Molecules

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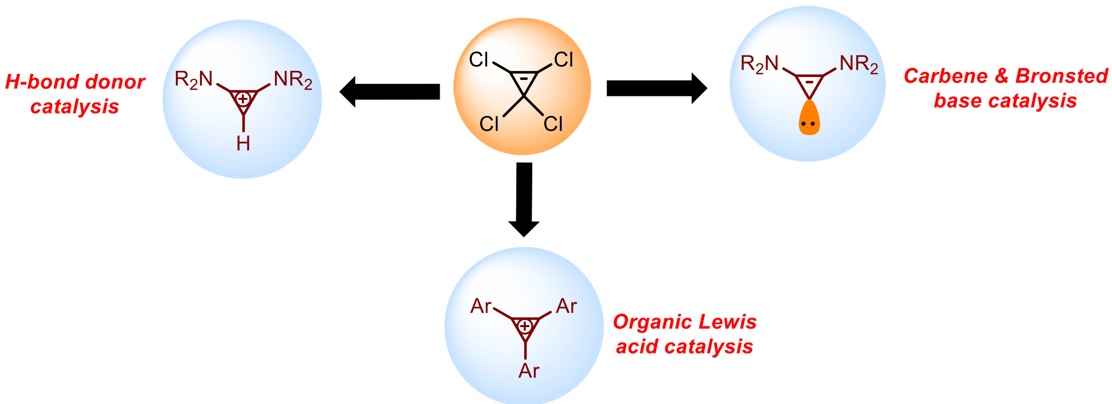
Abstract:

The development of novel small molecules-based catalysts for organic transformations has increased noticeably in the last two decades. A very recent addition to this research area is cyclopropenium-based catalysts.[1,2] While working on the synthetic transformations of *p*-quinone methides (*p*-QMs),[3] we have developed bis(amino)cyclopropenium-derived carbene catalyzed 1,6-conjugate addition of aromatic aldehydes (vinylogous Stetter type reaction) and enones (Rauhut-Currier reaction) to *p*-QMs.[4] A few year ago, we have utilized bis(amino)cyclopropenium salt as a hydrogen-bond donor catalyst[5] in 1,6-conjugate addition of indoles to *p*-QMs.[6] The results will be discussed in the talk.



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Dr. Ramasamy Vijaya Anand obtained Ph.D. in synthetic organic chemistry from the Indian Institute of Technology (IIT) Kanpur in 2003. Subsequently, he moved to Glasgow, UK to take up a postdoctoral position at the University of Strathclyde, where he worked for two years. He held another postdoctoral stint at the Texas A&M University, College Station, USA prior to joining Dr. Reddy's Laboratories at Hyderabad, India in 2006. In 2010, he moved to IISER Mohali, where he is currently working as a Professor at the Department of Chemical Sciences. He also served as the Dean of Research & Development at IISER Mohali during 2021-24. His research group is interested in developing cyclopropenium salt-catalyzed organic transformations, and in the synthesis of natural and unnatural biologically active compounds from *p*-QMs.

Title: Stereodivergent Syntheses to Natural Products Preparations Using Enzymes

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Abstract:

Enzymes are exquisite catalysts that are capable of providing unparalleled levels of chemo-, regio-, diastereo- and enantioselectivity. We have leveraged these properties of enzymes to establish biocatalytic methods and one-pot multienzyme cascades for the stereodivergent synthesis of six and seven-membered N-heterocycles such as tetrahydroquinolines, and tetrahydro-1,2, & 3-bezazepines with therapeutic potential.[1-2] Furthermore, the challenge of building complex natural products in a lab using existing chemistry is overcome by taking inspiration from the biosynthetic pathways that are perfected to synthesize such molecules with ease. We have made an elegant selection of putative biosynthetic enzymes to establish one-pot multienzyme cascades containing ene- and naphthol reductases to synthesize (+)-isoshinanolone and other related natural naphthalenones.[3] In another work, modified bisanthraquinones containing eight chiral centers were synthesized by using just a single enzyme in a biomimetic manner. The strategy relies on the use of putative anthrol reductases from fungi in a three-step chemoenzymatic synthesis of (–)-rugulosin, (–)-luteoskyrin, and (–)-deoxyluteoskyrin starting from anthraquinones.[4-7] These biocatalytic methods give facile access to biologically active complex molecules as well as pharmaceutically relevant N-heterocycles.

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3. A. De, N. Saha, T. Manna, V. Singh, S. M. Husain *ACS Catalysis* **2022**, *12*, 12179–12185.
4. N. Saha, A. Mondal, K. Witte, S. K. Singh, M. Müller, S. M. Husain *Chem. Eur. J.* **2018**, *24*, 1283–1286.
5. A. Mondal, S. K. Singh, T. Manna, S. M. Husain *Chem Commun.* **2020**, *56*, 3337–3340.
6. A. Mondal, N. Saha, S. M. Husain *Tetrahedron Chem.* **2022**, *3*, 100030.
7. A. Rajput, T. Manna, S. M. Husain *Natural Product Reports* **2023**, *40*, 1672–1686.

Bio-sketch

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Bio-sketch:
Dr Husain obtained his B.Sc. degree from the University of Delhi and M.Sc. degree from the Indian Institute of Technology Bombay. In 2005, he joined the group of Prof. Bernhard Wünsch at the University of Münster, Germany for his Ph.D. and worked on the asymmetric synthesis of NMDA and sigma receptor antagonists. From 2009 to 2012, he worked with Prof. Michael Müller at the University of Freiburg, Germany as a postdoctoral researcher and gained experience in the field of enzyme catalysis and elucidation of biosynthetic pathways of natural products. After returning to India, he worked with Prof. Yamuna Krishnan at the National Centre for Biological Sciences, Bangalore in the area of DNA nanotechnology. Dr. Husain's laboratory is working on different aspects of enzymes that include the discovery of new enzymes, the development of biocatalytic methods and one-pot multienzyme cascade reactions, chemoenzymatic synthesis of complex natural products, enzyme engineering, and enzyme-based biosensors. In the last ten years, his group has made tremendous contribution in the area of biocatalysis, with work on chemoenzymatic synthesis of bisanthraquinones,[1-5] methods for the stereodivergent synthesis of six and seven-membered N-heterocycles,[6,8] and development of multienzyme cascades.[7,8]

Representative Publications:
1. N. Saha, A. Mondal, K. Witte, S. K. Singh, M. Müller, S. M. Husain *Chem. Eur. J.* **2018**, *24*, 1283–1286.
2. S. K. Singh, A. Mondal, N. Saha, S. M. Husain *Green Chem.* **2019**, *21*, 6954–6959.
3. A. Mondal, S. K. Singh, T. Manna, S. M. Husain *Chem Commun.* **2020**, *56*, 3337–3340.
4. A. Mondal, A. De, S. M. Husain *Org. Lett.* **2020**, *21*, 8511–8515.
5. A. Rajput, T. Manna, S. M. Husain* *Natural Product Reports* **2023**, *40*, 1672–1686.
6. A. Rajput, T. Manna, A. Mondal, A. De, J. Mondal, S. M. Husain *ACS Catalysis* **2023**, *13*, 6185–6194.
7. A. De, N. Saha, T. Manna, V. Singh, S. M. Husain *ACS Catalysis* **2022**, *12*, 12179–12185.
8. A. De, A. Shukla S. M. Husain* *Angew Chem. Inter. Ed.* **2024**, e202411561.

Title: From Ecology to Medicine: Harnessing Plant Chemicals for Pest Management and Human Health

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Abstract: Chemical ecology is a rapidly growing field that bridges chemistry and ecology by examining the chemically mediated interactions between organisms. Plants, in particular, produce a wide array of chemicals to defend against both biotic and abiotic stressors. My lab focuses on understanding how these chemicals shape ecological interactions and their potential applications.

In the first part of my talk, I will discuss our research on impact of plant chemicals on insect egg-laying decisions and how this can applied for pest management. Our findings demonstrate that insect immune responses vary based on host plant chemistry that in turn impacts interactions with third trophic organisms. This part of the presentation underscores the crucial role of plant chemicals in tri-trophic interactions. The second part of my talk will shift focus to non-volatile plant chemicals with promising applications in human health. Specifically, I will highlight our study on the therapeutic potential of cysteine-rich, ultra-stable cyclic peptides extracted from *Clitoria ternatea*, a plant used widely in traditional medicine. Alzheimer's disease is a progressive neurodegenerative disorder marked by the accumulation of beta-amyloid peptide (Aβ) plaques and neurofibrillary tangles in the brain. Using *Caenorhabditis elegans* as a model system, our work shows that these cyclic peptides can significantly mitigate the detrimental effects of Aβ aggregation. Overall, our work suggests that these unique peptides could serve as novel pharmacophores for developing treatments against neurodegenerative diseases.

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- Ghosh E, Varshney R, Venkatesan R*. Performance of larval parasitoid, *Bracon brevicornis* on two *Spodoptera* hosts: implication in bio-control of *Spodoptera frugiperda*. *J Pest Sci*. 2022, 95, 435-446.
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- Kalmankar N, Hari H, Sowdhamini R, Venkatesan R*. Disulfide-Rich Cyclic Peptides from *Clitoria ternatea* Protect against β-Amyloid Toxicity and Oxidative Stress in Transgenic *Caenorhabditis elegans*. *J Med Chem*. 2021, 64(11): 7422-7433. (Featured on cover page)

Bio-sketch

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Biosketch: Dr. Radhika Venkatesan obtained her PhD working with Prof. Boland at the Bioorganic Chemistry Department, Max Planck Institute for Chemical Ecology, Jena, Germany. Her PhD work unraveled the role of light in jasmonate-mediated regulation of extrafloral nectar secretion, an indirect plant defence. She has also published other important findings in the field of chemical ecology in her PhD such as jasmonate control of floral nectar and differential regulation of volatiles and herbivory in ancient fern. Her postdoctoral work uncovered novel cytokinin-mimics from a plant pathogen that helped understand a long-standing question in plant pathogenesis by *Rhodococcus fascians*. Since moving to India, her lab has reported immune responses of important pest insect, *Spodoptera litura* and for the first time, showed that specific plant volatiles modulate insect innate immunity. Her lab has also done practical field trials using wasps to control pest population. Their project on plant cyclic peptides has also been successful as these peptides were shown to protect against beta amyloid toxicity and oxidative stress. Dr. Radhika Venkatesan has been instrumental in establishing and popularizing chemical ecology as a research topic in India by organizing workshops, seminars and teaching courses. She holds a patent for application of chemical ecological principles in pest management and her start up incubation is under progress. She has been awarded with the prestigious Ramanujan Fellowship and has also been the recipient of Early Career Award and POWER grant. She has also been heading Max Planck – India Partner group program in chemical ecology from 2016-2022. Recently she has been awarded Alexander von Humboldt fellowship for experienced researchers. She was elected as the Fellow of the Royal Entomological Society, London for her contributions in 2022. She is featured in the book "She is – 75 Women in Chemistry", that highlights the contribution of 75 women in the field of Chemistry, a project where Beyond Black collaborates with the Royal Society of Chemistry and The Office of the Principal Scientific Adviser to the Government of India.

Representative Publications:

1. Theenoor R, Ghosh A, Venkatesan R* (2024) Harmonising control: understanding the complex impact of pesticides on parasitoid wasps for enhanced pest management, Current Opinion in Insect Science, 65, 101236.
2. Sasidharan, A, Ghosh E, Venkatesan, R* (2024) Making a healthy choice: Tactical host selection behaviour of a parasitoid wasp. *Ecological Entomology*, 1–10.

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5. Ghosh E, Varshney R, Venkatesan R* (2022) Performance of larval parasitoid, *Bracon brevicornis* on two *Spodoptera* hosts: implication in bio-control of *Spodoptera frugiperda*. Journal of Pest Science. 95, 435-446.
6. Kalmankar N, Balaram P*, Venkatesan R* (2021) Mass spectrometric analysis of cyclotides from *Clitoria ternatea*: Xxx-Pro bond fragmentation as convenient diagnostic of Pro residue postioning. Chemistry Asian Journal. 16: 2920. (Featured on Cover Page)
7. Kalmankar N, Hari H, Sowdhamini R, Venkatesan R* (2021) Disulfide-Rich Cyclic Peptides from *Clitoria ternatea* Protect against β-Amyloid Toxicity and Oxidative Stress in Transgenic *Caenorhabditis elegans*. Journal of Medicinal Chemistry. 64(11): 7422-7433. (Featured on Cover Page)

Ligand Substitution Controlled Stereodivergent Functionalization of C-H bonds with Cyclopropenes

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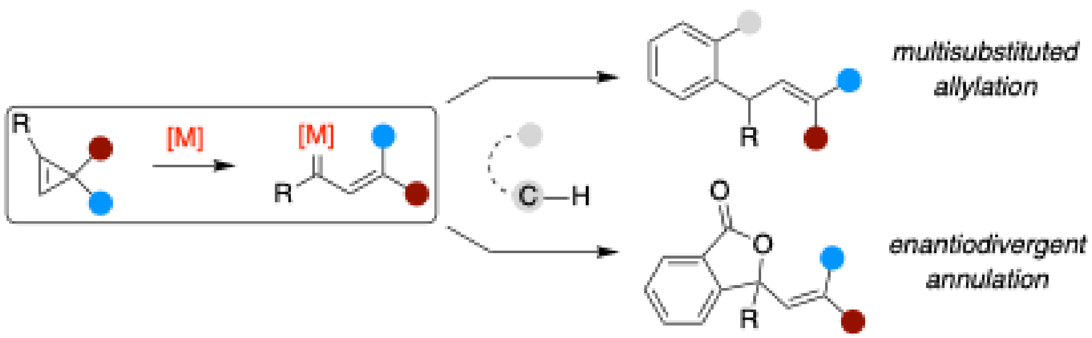
Abstract:

Metallocarbenes show versatile reactivity in organic synthesis and offers access to diverse complex frameworks in single step. Most often these metallocarbenes are generated from reactive α-diazocarbonyl compounds in the presence of suitable transition metal.[1] In the quest of finding suitable alternative, cyclopropenes have emerged as unique surrogates and offers structurally different metallocarbenes, viz. metallovinylcarbenes, which possess distinct reactivity.[2] The unique reactivity of these metallocarbene precursor have been efficiently integrated with the C-H bond functionalizations for the multisubstituted allylation of arenes and enantiodivergent annulation reactions.[3] In this presentation, our efforts on the catalytic functionalization of C-H bonds with cyclopropenes and their asymmetric version will be discussed.



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Bio-sketch

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Anbarasan obtained PhD on the enantioselective total synthesis of natural product from Indian Institute of Science, Bangalore with Prof. Kavirayani R. Prasad, in 2007. Subsequently, he held postdoctoral position at Leibniz Institute for Catalysis, Germany as Alexander von Humboldt fellow with Prof. Matthias Beller and University of California, Berkeley, USA with Prof. Dean Toste. He joined the Department of Chemistry, Indian Institute of Technology Madras (IITM) in Dec-2011, where currently he is a Professor of Chemistry.

Research Interest:

- Design and development of asymmetric transformations
- Stereoselective functionalization of metallocarbenes
- Trifluoromethylation and trifluoromethylthiolation
- Synthesis of therapeutically important natural products
- Conversion of biomass and carbon dioxide to chemicals and fuels

Awards and Recognitions:

AVRA Young Scientist Award, 2021 – SwarnaJayanti Fellowship, 2019-20 – CRSI-Bronze Medal, 2020 – Young Scientist Award of the Academy of Sciences, Chennai, 2020 – CRSI-Young Scientist Award, 2019 – ISCB Young Scientist Award, 2017 − NASI-Young Scientist Platinum Jubilee Award, 2016 − Institute Research & Development Award (IRDA) of IIT Madras, 2015-2016 − Young Scientist Medal of the Indian National Science Academy (INSA), 2015 − Associate Member of the Indian Academy of Sciences, Bangalore (2015-2018) − DAE-Young Scientist Research Award − Thieme Chemistry Journals Award-2013 − Alexander-*von*-Humboldt fellowship

Dehydrogenative coupling of alcohols with internal alkynes: An access to β-deuterated branched ketones

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In the realm of synthetic organic chemistry, the pursuit of novel methods for complex chemical synthesis presents both intriguing opportunities and formidable challenges. Traditionally, alcohols serve as alkylating agents in forming C-C and C-N bonds through a dehydrogenative borrowing hydrogen approach in transition-metal catalysis. However, their use as acylating agents in C-C bond formation is notably difficult and infrequently documented. This study introduces the dehydrogenative coupling of benzylic alcohols with internal alkynes under nickel(II) catalysis, employing alcohols as acylating agents. The process yields an array of α-branched aryl ketone derivatives, achieving zero waste via an umpolung borrowing hydrogen technique. Additionally, the study showcases the versatile applications of the resulting α-di-substituted ketones as precursors for other valuable compounds, including the large-scale production of β-deuterated branched ketones. To shed light on the underlying reaction mechanism, a series of spectroscopic analyses, the identification of intermediates, and density functional theory calculations were conducted.

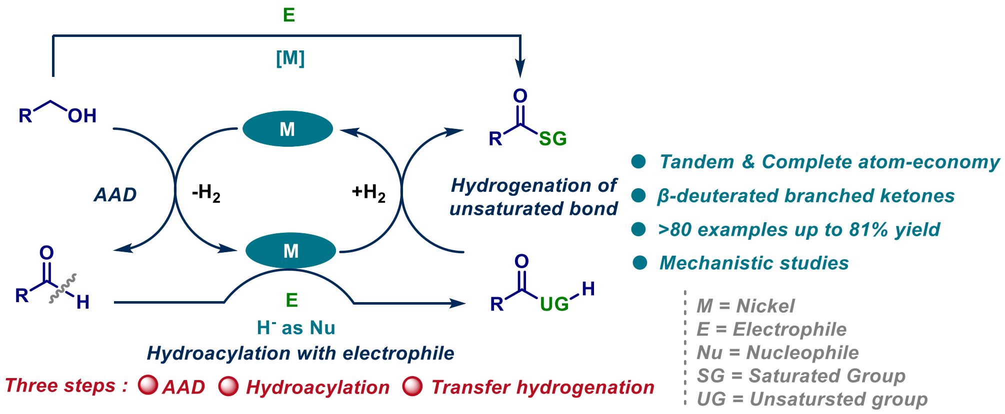

Figure 1. Nickel-catalyzed dehydrogenative coupling of alcohols with internal alkynes.

Reference: M. Subaramanian, C. Gouda, Triptesh K. Roy, G. Sivakumar, S. Banerjee, K. Vanka, E. Balaraman*. Dehydrogenative Coupling of Alcohols with Internal Alkynes under Nickel Catalysis: An access to β-deuterated branched ketones. *ACS Catal.* **2024**, *11*, 8294-8309.

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Dr. Ekambaram Balaraman received his M.Sc in Chemistry from R.K.M. Vivekananda College, Chennai (2002), and Ph.D from the Central University of Hyderabad (2008). Subsequently, he has been an FGS-Post Doctoral Fellow at the Weizmann Institute of Science (2008-2012). In July 2013, he started his independent career as a senior scientist at the CSIR-National Chemical Laboratory. In Dec'2018, he moved to the IISER-Tirupati as a faculty in chemistry. He is the recipient of the MRSI Medal (2021), SwarnaJayanti Fellowship (2020), CRSI-Bronze Medal (2020), The Asian and Oceanian Photochemistry Association (APA) for Young Scientist (2019), Fellow of Royal Society of Chemistry (2019), AV Rama Rao (AVRA) Young Scientist Award (2018). He is a member of the Indian National Young Academy of Science (INYAS), INSA (2018).
Dr. Balaraman's research primarily focuses on generating resources for green energy and recycling atmospheric waste. Specifically, he works on the design and development of catalytic materials for hydrogen generation from feedstocks, sustainable chemical synthesis, and conversion of CO_2 to value-added products. He is also interested in the development of electron donors for heterogeneous Ziegler catalysts used in the manufacture of isotactic polypropylene.

Molecular Ferroelectrics Derived from Ammonium and Phosphonium Cations

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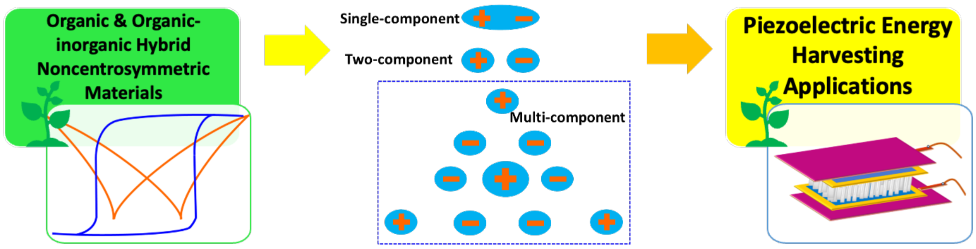
Abstract: Materials that display ferro- and piezoelectric are attractive for technology applications in the area of non-volatile memory devices, electronic sensors, electro-optical systems and as piezoelectric energy harvesters, which are popularly denoted as piezoelectric nanogenerators. Small molecules with organic and hybrid organic-inorganic backbones exhibiting ferroelectric and piezoelectric properties are of major attention as alternatives for ceramic materials for their ease of synthesis and in the preparation of flexible devices based on them.[1] Our group focuses on the development of ferro- and piezoelectric materials supported by phosphorus and nitrogen-centric scaffolds. Ammonium and phosphonium cations with heteroleptic and chiral substituents were employed in particular for the development of single and multi-component organic and hybrid ferroelectrics. Some recent significant results from our group are covered in this presentation.[2-7]

Figure/Scheme (if any):



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Biosketch: **Ramamoorthy Boomishankar** obtained his Ph.D. in Chemistry in 2004 from the Indian Institute of Technology (IIT), Kanpur, India. He then took up postdoctoral stints at the University of Illinois at Urbana-Champaign, USA, and the University of Liverpool, UK. He joined IIT, Guwahati as an assistant professor in April 2008. He moved to the Indian Institute of Science Education and Research (IISER), Pune, in 2010 and became a professor in December 2019. His research is focused on the development of polyhedral metal-ligand cages for host-guest studies and chiral separations and on molecular ferro- and piezoelectrics for energy and electronic applications. He is a recipient of the Bronze medal of the Chemical Research Society of India (CRSI) in 2022 and the Science and Technology Award for Research (STAR) from the Science and Engineering Research Board (SERB) in 2021. He is fellow of the India Chemical Society and Recipient of the 2024 Annual Alumni Materials Lecture Award of the Chemistry and Physics of Materials Unit (CPMU) at the JNCASR. Currently, he is an Editorial Board Member of the ACS-Inorganic Chemistry.

Representative Publications:

1. *Angew. Chem.Int. Ed.*, **2024**, *63,* e202406358.
2. *Angew. Chem.Int. Ed.*, **2024**, *63*, e202400366.
3. *Angew. Chem.Int. Ed.*, **2023**, *62*, e2022149.
4. *Angew. Chem. Int. Ed.,* **2021**, *60*, 4023 – 4027.
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Title: Redox modulator iron complexes trigger intrinsic apoptosis pathway in cancer cells

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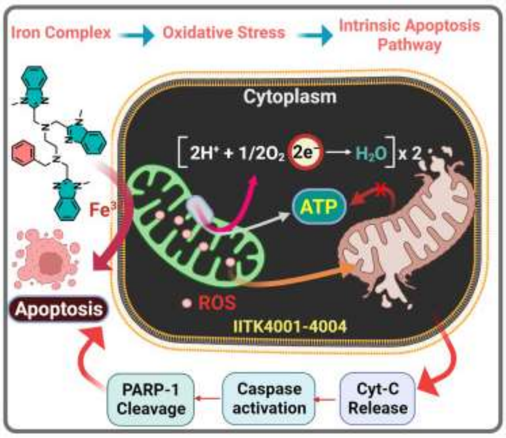
Abstract:
The emergence of multidrug resistance in cancer cells necessitates the development of new therapeutic modalities. One way cancer cells orchestrate energy metabolism and redox homeostasis is through overloaded iron pools directed by iron regulatory proteins, including transferrin. Here, we demonstrate that targeting redox homeostasis using nitrogen-based heterocyclic iron chelators and their iron complexes efficiently prevents the proliferation of liver cancer cells (EC50: 340 nM for IITK4003) and liver cancer 3D spheroids. These iron complexes generate highly reactive Fe(IV)=O species and accumulate lipid peroxides to promote oxidative stress in cells that impair mitochondrial function. Subsequent leakage of mitochondrial cytochrome c activates the caspase cascade to trigger the intrinsic apoptosis pathway in cancer cells. This strategy could be applied to leverage the inherent iron overload in cancer cells to selectively promote intrinsic cellular apoptosis for the development of unique iron-complex-based anticancer therapeutics.

Figure/Scheme (if any):



References and Notes:
Sai Kumari Vechalapu, Rakesh Kumar, Niranjan Chatterjee, Sikha Gupta, Shweta Khanna, Pooja Yedehalli Thimmappa, Sathyapriya Senthil, Raju Eerlapally, Manjunath B Joshi, Santosh K Misra*, Apparao Draksharapu*, Dharmaraja Allimuthu*, Redox Modulator Iron Complexes Trigger Intrinsic Apoptosis Pathway in Cancer Cells. iScience (2024, 29, e202301506)

Bio-sketch

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Representative Publications:

1. Sona Tiwari, Sathyapriya Senthil, Shweta Khanna, Santhosh Duraisamy, Sai Kumari Vechalapu, Sharath Chandra Mallojjala, Dharmaraja Allimuthu*, *Cell Rep. Phys. Sci*. (**2024**, *Accepted*)
2. Sai Kumari Vechalapu, Rakesh Kumar, Sharad Sachan, Kanchan Shaikh, Amarjyoti Mahapatra, Apparao Draksharapu,* Dharmaraja Allimuthu*. *ACS. Appl. Bio Mat.* (*2024*, *Accepted*)
3. Sai Kumari Vechalapu, Rakesh Kumar, Niranjan Chatterjee, Sikha Gupta, Shweta Khanna, Pooja Yedehalli Thimmappa, Sathyapriya Senthil, Raju Eerlapally, Manjunath B Joshi, Santosh K Misra*, Apparao Draksharapu*, Dharmaraja Allimuthu*, *iScience*., (**2024**, *29*, e202301506)
4. Dharmendra K Yadav, Sona Tiwari, Sathyapriya Senthil, Sai Kumari Vechalapu, Santhosh Duraisamy, Viral Rawat, Mohammed Isfahur Rahman, Shweta Khanna, Dharmaraja Allimuthu*, *Chem. Comm* (**2024**, *60*, 1928-1931)
5. 9. Viral Rawat, Sona Tiwari, Shweta Khanna, Umang Gupta, S. N. C. Sridhar, Dharmendra Yadav, Grace Kaul, Abdul Akhir, Deepanshi Saxena, Saravanan Matheshwaran, Sidharth Chopra, Dharmaraja Allimuthu*. *Chem. Comm.* (**2022**, *58*, 11669 - 11672)

Photocatalyzed Functionalization of [1.1.1]Propellane

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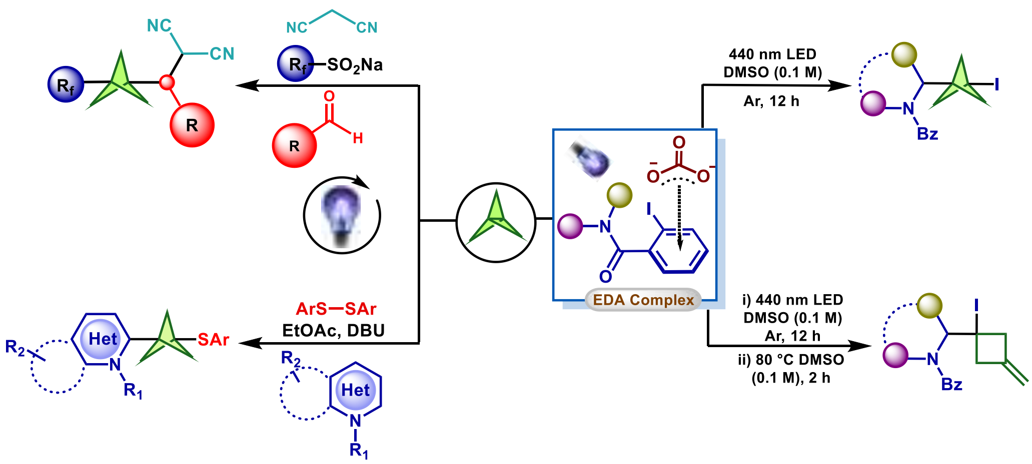
Abstract: [1.1.1]Propellane, a highly strained molecular system, has attracted significant interest from synthetic chemists due to its role as a precursor to bicyclo[1.1.1]pentanes (BCPs). We have developed methodologies to introduce diverse functional groups on propellane, enabling the synthesis of 1,3-functionalized BCP derivatives.

Among these derivatives, trifluoromethyl-substituted BCPs have garnered particular interest within the scientific and pharmaceutical communities for their favorable physicochemical properties as arene bioisosteres. We have devised a four-component strategy that initiates with photoredox perfluoroalkylation of [1.1.1]propellane, triggering a tandem reaction. This process forms a perfluoroalkyl BCP radical, which undergoes Giese addition to an electron-deficient alkene generated in situ via Knoevenagel condensation, forming 1,3-functionalized BCPs. This approach provides convenient access to various perfluoroalkyl BCP derivatives, with the nitrile group offering a versatile handle for further transformations.

Additionally, we developed a metal- and photocatalyst-free methodology that employs visible light-induced radical cascades to synthesize essential thio-BCP derivatives. These serve as valuable precursors for sulfoxides, sulfones, and sulfoximines. Finally, recognizing the importance of amines, we established an EDA-complex-assisted divergent synthesis, enabling access to α-amino bicyclo[1.1.1]pentyl iodides or cyclobutanes.



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2. V. Srinivasu, D. Das, P. Chandu, K. G. Ghosh, and D. Sureshkumar; *Org. Lett.*, **2023**, *25*, 5308.
3. V. Srinivasu, S. Gupta, and D. Sureshkumar; *Org. Biomol. Chem.*, **2023**, *21*, 8136.
4. V. Srinivasu, and D. Sureshkumar; *Manuscript in preparation*.

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Career Profile:

Devarajulu Sureshkumar completed his B. Sc. in Chemistry and M. Sc. in Organic Chemistry at the University of Madras. He earned his Ph.D. in 2007 under the supervision of Prof. S. Chandrasekaran, Department of Organic Chemistry, IISc Bangalore. From 2008 to 2010, he was an AvH postdoctoral fellow, working with Dr. Martin Klussman in Prof. Benjamin List's group at the Max-Planck-Institute for Kohlenforschung, Germany. He then undertook a short postdoctoral associate position with Prof. Wilhelm Boland at the Max-Planck-Institute for Chemical Ecology in Jena, Germany, before moving to Japan as a JSPS fellow. There, he worked with Prof. Masakatsu Shibasaki at the Institute of Microbial Chemistry in Tokyo (2010-2015). He joined the IISER Kolkata as a faculty in the Department of Chemical Sciences in February 2015. Currently, his research focuses on visible-light-mediated photocatalysis for C–C bond-breaking and forming and fluorination reactions through C(sp^3)–H functionalization.

Significant Awards/Achievements:

Early Carrier Research Award-2017 from SERB, Government of India.
Ramanujan Fellowship-2016 from SERB/DST, Government of India.
JSPS Fellowship-201 for Foreign Researchers (Pathway to University Positions in Japan).
JSPS Fellowship-2011 at Institute of Microbial Chemistry, Tokyo, Japan.
AvH Fellowship-2008 at Max-Planck Institute for Khölenforschung, Germany.

Representative Publications:

1. Visible-Light Driven Synthesis of Vinyl Amines without Photocatalyst. Pal, K.; Das, D.; Ghosh, K. G.; Sureshkumar. D. *J. Org. Chem.* **2024**, *Accepted*.
2. Photocatalyzed Direct C(sp^3)–H Alkenylation of Unactivated Alkanes *via* Tandem C–C Activation of Cyclopropenes. Biswas. S.; Das, D.; Pal, K.; Chandu, P.; Sureshkumar. D. *J. Org. Chem.* **2024**, *89*, 12421-12431.
3. Photoredox Cross Dehydrogenative C(sp^2)–C(sp^3) Coupling of Heteroarenes with Secondary Amines through 1,5-HAT. Srinivasu, V.; Patanaik, S.; Sureshkumar, D. *Chem. Commun*. **2024**, *60*, 9757-9760.
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6. Organophotocatalyzed Alkyl/Arylsulfonylation of Vinylcyclopropanes. Chandu, P.; Mallick, M.; Srinivasu, V.; **Sureshkumar**, **D***. *Chem. Eur. J.* **2024**, *30*, e202303187.
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9. Diastereoselective Organophotocatalytic Hydrosulfonylation of Cyclopropenes. Chandu, P.; Biswas, B.; Garai, S.; **Sureshkumar**, *****. *Green Chem.* **2023**, *25*, 9086-9091.
10. Palladium-catalyzed Direct C(sp^2)–H Cyanomethylation of Arylamides using Chloroacetonitrile. Garai, G.; **Sureshkumar**, **D***. *J. Org. Chem.* **2023**, *88*, 12755-12764.
11. Visible-Metal-Free Photoredox Four-Component Strategy to 1,3-Functionalized BCP Derivatives. Srinivasu, V.; Das, D.; Chandu, P.; Ghosh, K. G.; **Sureshkumar**, **D***. *Org. Lett.* **2023**, *25*, 5308-5313.
12. Photoinduced Cascade Difluoroalkylative Ring-Opening of Vinyl Cyclopropanes. Chandu, P.; Das, D.; Ghosh, K. G.; **Sureshkumar**, **D***. *Org. Lett.* **2023**, *25*, 2857-2862.
13. Diastereoselective Palladium-Catalyzed C(sp^3)–H Cyanomethylation of Amino Acid and Carboxylic Acid Derivatives. Garai, S.; Ghosh, K. G.; Biswas, A.; Chowdhury, S.; Sureshkumar, D. *Chem. Commun*. **2022**, *58*, 7793-7796.
14. Visible-Light-Driven Organophotocatalyzed Multi-component Approach for Tandem C(sp^3)−H Activation and Alkylation Followed by TrifluoromethylthiolationMondal, Ghosh, K. G.; Ghosh, K. G.; Das, D.; Garai, G.; Chandu, P.; **Sureshkumar**, **D***. *J. Org. Chem.* **2022**, *87*, 8611-8622.
15. Visible-Light Photoredox Catalyzed Decarboxylative Alkylation of Vinylcyclopropanes Chandu, P.; Das, D.; Ghosh, K. G.; **Sureshkumar**, **D***. *Adv. Synth. Catal.* **2022**, *364*, 2340-2345. Selected as a "***VIP* Article**".

Versatile Reactivity of Diazo Carbonyl Compounds Towards Metal Catalysts and Visible Light

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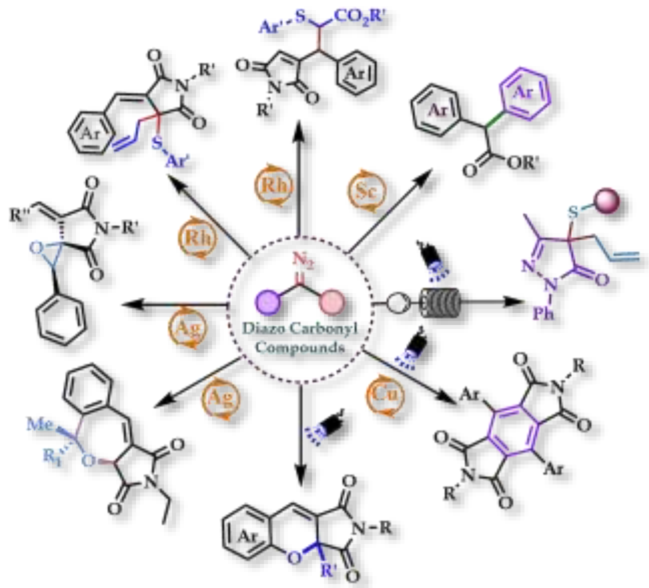
Abstract: Diazo carbonyl compounds have broad and tuneable reactivity.[1a] Owing to their versatile reactivity, diazo compounds have been utilized in diverse transformations in organic synthesis as well as in interdisciplinary fields.[1b] Developing catalytic methods for the chemo- and regio-selective C-H bond functionalization is highly desirable as well as challenging. Over the years, we have been exploring the reactivity of diazo carbonyl compounds both under metal and visible light catalysis. We have developed a robust propargyl α-aryl-α-diazoacetate as a new class of reagent for the effective C-H bond functionalization of unactivated arenes, 1,3 diketones & β-keto acids via scandium catalysis to access useful functionalized compounds.[2] Likewise, we have been exploring the diverse reactivity of diazo arylidene succinimides (DASs) under metal as well visible light catalysis to access useful compounds like 2*H*-chormenes, PMDI etc.[3] This presentation will provide an overview of some of the recent advancements from our research group.



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3. a) *Laha, D.;* Bhat, R. G. *Asian J. Org. Chem.* **2020**, *9*, 918-921 b) Bankar, O. S.; Laha, D.; Meher, K. B.; Bhat, R. G. *Chem Asian J.* **2023**, *e202300774. c) Laha, D.; Meher, K. B.; Bankar, O. S.;* Bhat, R. G. *Asian J. Org. Chem.* **2022**, e202200062 d) Bankar, O. S.; Pal, C.; Laha, D.; Abhijeet S. Sabale, Bhat, R. G. *Organic Lett.*, ***2024*** *Minor revision e) Laha, D.;* Bankar, O. S.; Navale, B. S.; Santra, S.; Gosh, D.; Bhat, R. G. *Organic Lett.* **2024** *Minor revision f) Meher, K. B. Laha, D. Dharpure, P. D.; Bhat, R.G. https://doi.org/10.26434/chemrxiv-2023-5jd6t and Under Review*

Bio-sketch

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Professor Ramakrishna G. Bhat (RGB) obtained his PhD degree (2004) from the Department of Organic Chemistry, Indian Institute of Science (IISc) Bengaluru under the supervision of Prof. Srinivasan Chandrasekaran. Subsequently, he joined Prof. Brian M. Pinto's research group as a postdoctoral fellow at the Simon Fraser University, British Columbia, Canada. Later in the year 2006, he began his independent career at the Indian Institute of Science Education and Research (IISER) Pune and he was promoted to Full Professor in 2019. His research focusses on 'Organic Synthesis and Catalysis' encompassing the broad research areas on Photoredox catalysis, Photoinduced as well as metal catalyzed Carbene transfer reactions, C-H bond functionalization and Organocatalysis. He has been actively involved in the outreach educational activities and Teachers' training programs extensively. IISER Pune has conferred on him the very first 'Excellence in Teaching and Contributions to Teaching' award in 2022, the commencement year of the Teaching Award. He is also a member of Early Career Editorial Board in the *Tetrahedron Letters and Tetrahedron*.

Representative Publications:

1. Bankar, O. S.; Laha, D.; Meher, K. B. and Bhat, R. G. *Chem Asian J.* **2023**, *e202300774*. (*Invited Article*)
2. Bhowmick, A.; Chatterjee, A.; Pathak, S. S.; Bhat, R. G. *Chem. Commun.*, **2023**, *59*,11875-11878
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4. Shaikh, J. Y.; Bhowmick, A.; Chatterjee, A.; Thombare, N. A.; Bhat, R. G. *Adv. Synth. Catal.* **2023**, *365*, 2922-2928.
5. Navale, B. S.; Laha, D.; Banerjee, S.; Vanka, K.; Bhat, R. G. *J. Org. Chem.* **2022**, *87*, 13583–13597
6. Bhowmick, A.; Warghude, P. K.; Dharpure, P. D.; Bhat, R. G. *Org. Chem. Front.* **2021**, *8*, 4777
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Organic Stress: A Tool for Chemical Synthesis

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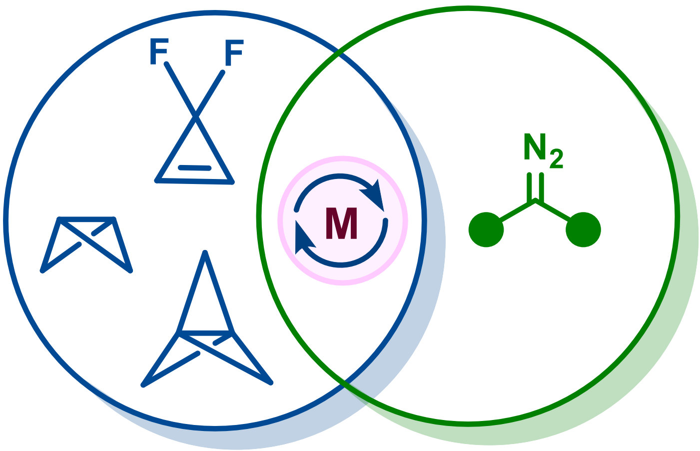
Ring-strain in organic molecules is a powerful driving force that promotes reactivity through strain-release, allowing the facile construction of a myriad of useful scaffolds via ring-opening or ring-expansion reactions. Carbene chemistry has been widely studied, and numerous applications in organic synthesis such as X–H (X = C, Si, N, O, etc.) insertions, cyclopropanations, ylide formations, and 1,2-migrations. Due to their high reactivity, carbenes are also ideal for initiating a cascade sequence, leading to rapid generation of structural complexity. We merged strain-release and metal-carbene chemistry to unlock new strategies for organic synthesis. In this lecture, I will first discuss a copper-catalyzed highly diastereoselective strain-release [2,3]-sigmatropic rearrangement.[1] Then, I will present how we utilized the ring strain in [1.1.1]propellane to access copper-carbenes for [2,3]-sigmatropic rearrangement.[2] At the end, I will focus on rhodium-catalyzed strain-enabled stereoselective synthesis of skipped dienes.[3]



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3. Kadam, G. A.; Singha, T.; Rawat, S.; Hari, D.P. *ACS Catal.* **2024**, *14*, 12225-12233.

Bio-sketch

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Durga Prasad Hari received his MSc degree from IIT Madras in 2010. He then moved to the University of Regensburg, Germany, where he pursued his Ph.D. with Prof. Burkhard Koenig. In 2014, following his graduate education, he was a postdoctoral fellow in the laboratory of Prof. Jerome Waser at EPFL, Switzerland. In 2018, he joined the Aggarwal group at the University of Bristol as a Marie-Curie research fellow. Since March 2021, he has been holding an assistant professor position at the Indian Institute of Science, Bangalore. His research interests focus on discovering new reactivity in organic synthesis by harnessing the high reactivity of strain-embedded molecules and carbenes through photo- and electrochemical strategies.

Representative Publications:

1. Kadam, G. A.; Singha, T.; Rawat, S.; Hari, D.P. ACS Catal. **2024**, *14*, 12225-12233.
2. Das, K.; Pedada, A.; Singha, T.; Hari, D. P. *Chem. Sci.* **2024**, *15*, 3182-3191.
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4. Singha, T.; Kadam, G. A.; Hari, D.P. *Chem. Sci.* **2023**, *14*, 6930-6935.
5. Samim Mondal, A. R.; Ghorai, B.; Hari, D. P. *Org. Lett.* **2023**, *25*, 4974-4979.

N-Heterocyclic Carbene (NHC)-Catalyzed Synthesis of C-N, C-O and N-N Axially Chiral Molecules

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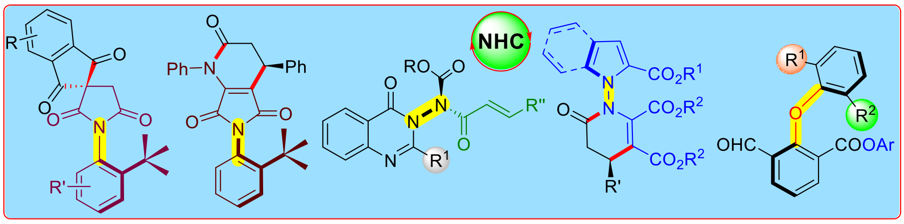
N-Heterocyclic carbene (NHC)-catalyzed umpolung of aldehydes is widely used for the unconventional access to target molecules.[1] Although the assembly of axially chiral C-C bonds leading to the atroposelective synthesis of biaryls and related compounds are well-known, the analogous synthesis of compounds bearing axially chiral C-heteroatom bonds are relatively rare using NHC catalysis. We have recently reported the NHC-catalyzed atroposelective synthesis of N-aryl succinimides having an axially chiral C-N bond via the desymmetrization of N-aryl maleimides.[2] Moreover, we have demonstrated the NHC-catalyzed kinetic resolution of N-aryl aminomaleimides and a facile synthesis of N-aryl phthalimides/maleimides bearing the C-N axis.[3,4] In addition, NHC-catalyzed selective amidation reaction leading to the atroposelective synthesis of N-N axially chiral 3-amino quinazolinones has been realized recently.[5] Further, we have uncovered the NHC-catalyzed synthesis of C-O axially chiral diaryl ethers via atroposelective esterification of dialdehyde-containing diaryl ethers via a desymmetrization strategy.[6] The details of these works will be presented.



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2. Barik, S.; Shee, S.; Das, S.; Gonnade, R. G.; Jindal, G.; Mukherjee, S.; Biju, A. T. *Angew. Chem. Int. Ed.* **2021**, *60*, 12264.
3. Barik, S.; Das, R. C.; Balanna, K.; Biju, A. T. *Org. Lett.* **2022**, *24*, 5456.
4. Barik, S.; Ranganathappa, S. S.; Biju. A. T. *Nat. Commun.* **2024**, *15*, 5755.
5. Balanna, K.; Barik, S.; Barik, S.; Shee, S.; Manoj, N.; Gonnade, R. G.; Biju, A. T. *ACS Catal.* **2023**, *13*, 8752.
6. Shee, S.; Ranganathappa, S. S.; Gadhave, M. S.; Gogoi, R.; Biju, A. T. *Angew. Chem. Int. Ed.* **2023**, *62*, e202311709.

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Subject Editor, *Current Science Journal*, Indian Academy of Sciences.

A. T. Biju received his M. Sc. from Sacred Heart College Thevara (affiliated to MG University, Kerala, India) and Ph.D. under the guidance of Dr. Vijay Nair at the CSIR-NIIST (Formerly RRL), Trivandrum, India. Subsequently, he has been a post-doctoral fellow with Prof. Tien-Yau Luh at the National Taiwan University, Taipei and an Alexander von Humboldt fellow with Prof. Frank Glorius at the Westfälische Wilhelms-Universität Münster, Germany. In June 2011, he began his independent research career at the CSIR-National Chemical Laboratory, Pune. In June 2017, he moved to the Department of Organic Chemistry, Indian Institute of Science, Bangalore, where he is a professor presently. His research focuses on the development of transition-metal-free carbon-carbon and carbon-heteroatom bond-forming reactions using strained molecules and N-heterocyclic carbene (NHC) organocatalysis, and their application in organic synthesis.

Dearomative Annulation: A Versatile Strategy to Spiro-/Fused Polycyclic Molecules

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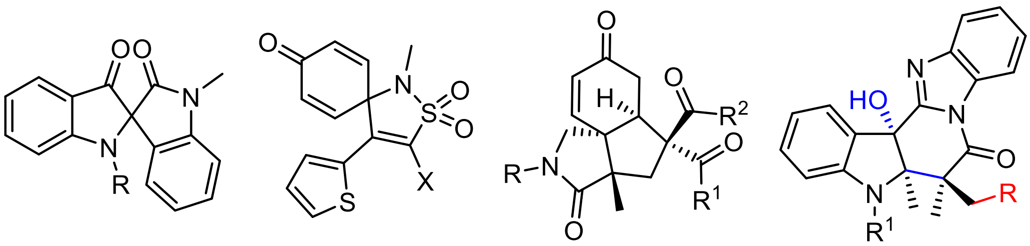
Abstract:

Aromatic compounds, as readily accessible and economical precursors, are ample in nature and are widely used in both industry and academia. As an essential chemical conversion of aromatic molecules, dearomatization is a significant process for the synthesis of various complex molecular entities including spirocyclic or fused polycyclic compounds. Over the past few decades, the development of handy synthetic strategies for the assembly of these *aza*-heterocycles with diverse functionalities has been the attention of research initiatives. In this direction, dearomatization is one of the important methods for the construction of complex molecular scaffolds including spirocyclic or fused polycyclic compounds. From the last two decades, synthesis of spiro-/fused polycylic molecules through alkyne/alkene-assisted dearomatization reactions have received substantial attention from synthetic organic chemists.[1] The present lecture will focus on the recent accomplishments on dearomative annulation reactions to access spiro-/fused polycylic compounds (Figure 1).[2-5]

Figure 1:



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2. Ch. Raji Reddy,* A. Theja, E. Srinivasu and M. Subbarao. *Org. Lett.* **2024**, *26*, 68-72
3. Ch. Raji Reddy,* Anjali Rathaur, B. Karuna Sagar A. Theja, Amol D. Patil and M. Subbarao; *Adv. Synth. Catal.*, **2024**, *in press.*
4. Ch. Raji Reddy,* Aratikumari S Prasad and U. Ajaykumar. *Org. Lett.* **2024**, *26*, 4904-4909.
5. Ch. Raji Reddy,* E. Srinivasu, A. Theja, E. Damodar and M. Subbarao, **2024** (under revision).

Bio-sketch

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Biosketch:

Dr. Raji Reddy has obtained M. Sc. from Osmania University in 1997. After completion of Ph. D. at CSIR-Indian Institute Chemical Technology in 2002, he moved as a post-doctoral fellow to University of South Florida, Tampa, USA (2002) and subsequently to University of Mississippi, USA (2002-2005). He returned India in 2005 and joined as a principal scientist in Sai Life Sciences, Hyderabad. After one year, he joined CSIR-IICT, Hyderabad as a scientist at the Department of Organic Synthesis & Process Chemistry and presently working as a Chief Scientist.

His research interests are both fundamental and applied research, include (i) the chemistry of propargylic alcohols and propiolamides; (jj) enyne-assisted annulation reactions, *ipso*-annulations and synthesis of bio-active natural products; (iii) Process development of APIs. Representative accomplishments are: processes for Favipiravir, Remdesivir, (*S*)-Pregabalin, key fragment of Eribulin mesylate and TLR 7/8 agonist molecule, used as an adjuvant in COVAXIN® (COVID-19 vaccine) have been developed and transferred to pharmaceutical organizations.

He is a recipient of CSIR-Technology Award-2021, NASI-Reliance Industries Platinum Jubilee Award-2020, CSIR-Technology Award-2020, CRSI Bronze Medal-2018, CDRI–Drug Research Excellence Award-2017, Dr. A K Singh Memorial-Young scientist award-2014, AVRA-Young scientist award-2011 and A P Akademi-Young scientist award-2007. He is also a Fellow of National Academy of Sciences (FNASc) and Telangana Academy of Sciences (FTAS).

He is an author of 175-publications, 12-patents, 3-review articles and 2-book chapters. Under his supervision 32-Students have been awarded Ph. D. degree. Presently, 12-research fellows are working for their Ph. D. He has also supervised 24-Master students for their dissertation

Representative Publications:

1. Ch. Raji Reddy,* A. Theja, E. Srinivasu and M. Subbarao. *Org. Lett.* **2024**, *26*, 68-72
2. Chada Raji Reddy,* Anootha N V, Uprety Ajaykumar, Nagender Punna, Luc Neuville and Geraldine Masson; *J. Org. Chem.* **2024**, *89, 7115-7124.*
3. Ch. Raji Reddy,* Aratikumari S Prasad and U. Ajaykumar. *Org. Lett.* **2024**, *26*, 4904-4909.
4. Chada Raji Reddy,* Karna Nair, Ejjirotu Srinivasu Muppidi Subbarao and René Grée, *J. Org. Chem.* **2024,** *89*, 2675-2682.
5. Chada Raji Reddy,* Veeramalla Ganesh, and Nagender Punna, *Chem.Commun* **2023,** *59*, 8600-8603.

Transforming Energetic Materials: Advancements in Tailored Green High-Energy Density Materials for Enhanced Performance

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Indian Institute of Technology, Kanpur, UP-208016
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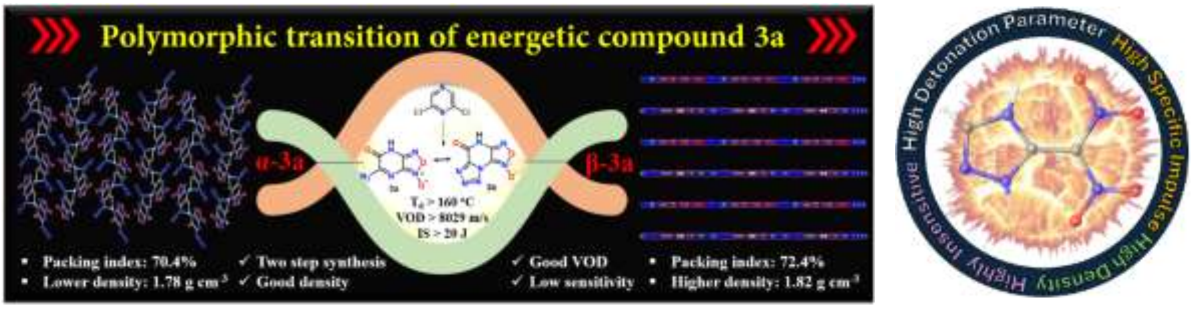
Abstract:
The evolution of energetic materials underscores the persistent challenge of synthesizing and developing green high-energy density materials and oxidizers. This presentation delves into the historical context of established explosives, including ammonium nitrate (AN), pentaerythritol tetranitrate (PETN), trinitrotoluene (TNT), and hexahydro-1,3,5-trinitro-1,3,5-triazine (RDX). It addresses their impact on the field and the safety and environmental sustainability challenges they present. Recent advancements in the synthesis of novel green high-energy density materials are introduced, highlighting compounds designed to overcome the limitations of traditional explosives. These innovative materials aim to offer enhanced performance while mitigating environmental impact. A comparative analysis of the energetic properties of these new compounds against established explosives such as TNT, RDX, HMX, FOX-7, and CL-20 will be presented. This overview provides insight into the current state and future directions of the field of energetic materials.

Figure:



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2. *Organic letters*, **2024**, *26*, 4788-4792
3. *Chemical Communications*, **2024**, *60*, 1646-1649
4. *ACS Applied Materials & Interfaces*, **2024**, *16*, 20670-20680
5. *Chemical communications*. **2023**, *59*, 4324-4327
6. *Journal of Materials Chemistry A*, **2022,** *10*, 22803-22811
7. *Journal of Materials Chemistry A*, **2022,** *10*, 12702-12712
8. *ACS Applied Materials & Interfaces*, **2022**, *14*, 49898-49908

Bio-Sketch of Speaker

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Experience:

1. Indian Institute of technology, Kanpur, India 2019-till
Assistant professor, Department of Chemistry

2. McMaster University, Hamilton, Canada
Postdoctoral fellow in the group of Prof. Jakob Magolan, **2017-2009**

3. University of Idaho, Moscow, USA-Department of Chemistry
Postdoctoral fellow in the group of Prof. J. M. Shreeve, **2015-2017**

4. University of Hyderabad, Hyderabad, India - School of Chemistry
Postdoctoral fellow in the group of Dr. K. Muralidharan, **2015**

Education:

1. **University of Hyderabad, Hyderabad, India - ACRHEM**
Ph.D. (Heterocyclic/Energetic Materials Chemistry), **August 2010–December 2014**, University of Hyderabad, Hyderabad, India. **"*Design and Synthesis of Nitrogen-rich Heterocyclic Compounds and Salts as Energetic Materials*"**

2. M.Sc. (Organic Chemistry), **2007-2009**, Osmania University, Hyderabad, India.

3. B.Sc. (Chemistry, Botany and Zoology), **2003-2006**, Osmania University, Hyderabad, India.

Modulating the key functional behaviour of flavin for bioimaging and biomedical applications

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Abstract: Multifunctional and multi-faceted naturally occurring biomolecular entity namely, flavin moiety, remains the most interesting chemical entity considering its involvement in numerous biological phenomena.[1] This, flavin entity as co-factor in numerous flavoenzymes has been found to be involvement in a diverse biochemical transformations and are very well studied and reported in literature. Expectedly, the fundamental understanding of the structure and activity associated with the flavoenzymes has paved the way for design and development of numerous synthetic catalytic designs for highly efficient and selective chemical transformation. While catalytic application around the flavin core have been thoroughly investigated, the inherent photophysical studies were largely limited to the understanding their behaviour in natural systems.[2] Synthetic modulations around flavin core to harness the photophysical properties as synthetic model for sensing and bioimaging is severely limited. Our group at IIT Hyderabad, is broadly interested in understanding and harnessing the inherent property of the flavin core for various activity. Here in this talk, I will be discussing about subtle chemical modification around the flavin core skeleton for a singular platform for bioimaging and biomedical applications.[3-4]

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1. A. Sancar, *Chem. Rev.*, **2003**, 103, 2203.
2. (a) A. Losi, K. H. Gardner and A. Möglich, *Chem. Rev*., **2018**, 118, 10659 (b) A. Kaur and E. J. New, *Acc. Chem. Res.*, **2019**, 52, 623 (c) S. Fukuzumi, K. Ohkubo, *Coord. Chem. Rev.* **2010**, *254*, 372-385
3. H. G. Agrawal, P. S. Giri, P. Meena, S. N. Rath, A. K. Mishra, *ACS Med. Chem. Lett.,* **2023***, 12, 14, 1857*
4. H. G. Agrawal, S. Khatun, A.K. Regnan, A. K. Mishra, Chem. Eur. J., **2024**, 30, e202401483
5. H. G. Agrawal, P. S. Giri, T. Sahoo, S. N. Rath, A. K. Mishra, *unpublished work*

Bio-sketch

Profile

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Institution IIT-Hyderabad

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Biosketch: Ashutosh Kumar Mishra obtained his master's degree in chemistry from DDU Gorakhpur university and doctoral degree from Indian institute of technology (IIT)-Kanpur working on metal-nucleobase interactions. Later he moved to Northwestern University (USA) as post- doctoral fellow to work on understanding the underlying mechanism and dynamic of charge transport phenomenon in synthetic model DNA systems. Moving back to India, he is currently serving as associate professor at Indian Institute of technology (IIT)-Hyderabad. His research group is interested in bioinspired model systems with subtle the flavin core chemical skeleton to fine tune the functional behavior for potential application in catalytic, bioimaging or order architecture.

Representative Publications:

1. H. G. Agrawal, S. Khatun, A.K. Regnan, A. K. Mishra, *Chem. Eur. J.*, **2024**, 30, e202401483
2. D. Mondal, I. Naskar, M. Deepa, A. K. Mishra, *Energy Adv.*, **2024**, 3, 1710
3. H. G. Agrawal, P. S. Giri, P. Meena, S. N. Rath, A. K. Mishra, *ACS Med. Chem. Lett.*, **2023**, *12*, *14*, *1857*
4. M.S.S.V. Mouli, A. K. Mishra, *Org. Biomol. Chem.*, **2023,** *21*, 5622
5. M.S.S.V. Mouli, D. Mondal, K. Kumari, S. K. Singh, A. K. Mishra, *Org. Biomol. Chem.***,** **2023**, *21*, 3311
6. M. S. S. V. Mouli, A. K. Mishra, *Inorganica Chem. Acta*, **2023**, 558, 121752
7. M.S.S.V. Mouli, S. Katyal A. K. Mishra, *Synlett*, **2023** *34*, 829-834
8. M. S. S. V. Mouli, A. K. Mishra, *Dyes Pigm.*, **2023**, 212, 111148
9. M. S. S. V. Mouli, A. K. Mishra, *CrystEngComm*, **2022**, 24, 2221-2225
10. M. S. S. V. Mouli, A. K. Mishra, *RSC Adv*, **2022**, 12, 3990

Biomimetic Studies on Metal Homeostasis and Detoxification

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Methylmercury (Me–Hg^{+}) is an extremely neurotoxic and ubiquitous environmental pollutant, which accumulates at high levels in food chains, mainly in fish and seafood, and therefore, consumption of contaminated foods poses a significant risk to human health. Exposure to ethylmercury (Et–Hg^{+}) is another serious concern in developing countries where Et–Hg^{+}-containing antimicrobial agent "*Thimerosal*" is commonly used as a preservative in multiuse vials of vaccines and other medicines. In nature, however, several microorganisms have been reported to detoxify organomercurials, including Me–$Hg^{+,}$ by converting them to less toxic biologically inert species. For instance, bacterial organomercurial lyase (MerB) catalyzes the protolytic cleavage of the otherwise inert Hg–C bond of Me–Hg^{+} and produces methane (CH_4) gas and less toxic Hg^{2+}, while a second enzyme mercuric ion reductase (MerA) subsequently reduces Hg^{2+} to volatile Hg^{0}.

Likewise, arsenic is another ubiquitous environmental toxin and human carcinogen that also poses a serious threat to human health.[3,4] However, in this case, methylation of inorganic arsenic (iAs) is recognized as an established detoxification process in organisms. S-adenosylmethionine (SAM) is a universal cofactor that methylates iAs(III) up to three times, with the help of As^{3+} S-adenosylmethionine methyltransferase, producing the less toxic methylated arsenic species, including dimethylarsenite ($DMAs^{3+}$).

On the other hand, copper ion is essential in our lives and used as a cofactor in several vital processes. However, high concentrations of copper can be deleterious as they promote Fenton-like reactions, thereby increasing the cellular ROS levels and leading to the oxidative damage of cellular constituents like proteins, lipids, and nucleic acids. Thus, it is essential to control copper concentration in the body strictly. This talk will focus on the homeostasis of copper and the detoxification pathways of mercury and arsenic-related compounds in the cellular system.

References & Notes:

1. Das, R.; Karri, R.; Chalana, A.; Roy, G* *Inorganic Chemistry*, **2024**, 63, 10455 (Highlighted on the *Front Cover Page* of the journal).
2. Rai, R. K.; Islam, A.; Pati, R, S.; Roy, G* *Chem. Eur. J.*, **2024**, xx, xxxx (just accepted).
3. Karri, R.; Das, R.; Rai, R. K.; Gopalakrishnan, A.; Roy, G* *Chem. Comm.* **2020**, 56, 9280.
4. Karri, R.; Chalana, A.; Binayak, Jayadev, S. K. M.; Roy, G* *Chem. Eur. J.*, **2019**, 25, 12810.
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6. Chalana, A.; Karri, R.; Das, R.; Kumar, B.; Rai, R, K.; Saxena, H.; Gupta, A.; Banerjee, M.; Jha, K. K.; Roy, G* *ACS Appl. Mater. Interfaces*, **2019**, *11*, 4766.
7. Banerjee, M.; Roy, G* *Inorganic Chemistry*, **2017**, *56*, 12739;
8. Banerjee, M.; Karri, R.; Chalana. A.; Das, R.; Rai, R. K.; Rawat, K. S.; Pathak, B.; Roy, G.* *Chem. Eur. J.*, **2017**, *23*, 5696 (Highlighted on the *Inside Cover Page* of the journal).
9. Banerjee, M.; Karri, R.; Rawat, K. S.; Muthuvel, K.; Pathak, B.; Roy, G.* *Angew. Chem. Int. Ed.*, **2015**, 54, 9323 (Highlighted on the *Inside Cover Page* of the journal).

Bio-Sketch of Speaker

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Education & Professional Experience

Jan2020-	Professor, Department of Chemistry, IIT Tirupati, Tirupati, A.P.
Jan2020–Dec 2023	Associate Professor, Dept. of Chemistry, IIT Tirupati, Tirupati, A.P.
July 2018–Jan 2020	Associate Professor, Dept. of Chemistry, Shiv Nadar University, U.P.
Nov2012 – June 2018	Assistant Professor, Dept. of Chemistry, Shiv Nadar University, UP.
Nov2011–Sept2012	Research Associate, The Scripps Research Institute, San Diego, USA.
Jan2008–Nov2011	Postdoctoral Fellow, Dept. of Physiology and Pharmacology, Oregon Health and Science University, Oregon, USA.
Aug2002–Oct2007	Ph.D, IPC, IISc, Bangalore, India.

Research

Research in our laboratory mainly focuses on two major areas, chemistry, and biology, at the interface of chemistry and biology. Our laboratory is involved in the chemical detoxification of various toxic heavy metals such as mercury, arsenic, and copper. Organomercurials are highly neurotoxic environmental pollutants that preferentially accumulate in the glia of the central nervous system (CNS). Thus, the detoxification of organomercurials is of critical importance. On the other hand, copper ion is essential in our lives and used as a cofactor in several vital processes. However, high concentrations of copper can be harmful as they promote Fenton-like reactions, thereby increasing the cellular ROS levels and leading to the oxidative damage of cellular constituents like proteins, lipids, and nucleic acids. Thus, it is essential to control copper concentration strictly in the body. We aim to understand how methylmercury, an extremely neurotoxic organomercurial, exerts its neurotoxicity and try to understand the detoxification pathways in the biological system. Our research group focuses on understanding the homeostasis of essential metals and the detoxification pathways of toxic heavy metals in the cellular system.

Awards & Recognitions

- "STARS-MoE Grant", 2023.
- *"Bronze Medal, 2020*", CRSI, 2020.
- "SERB CRG Grants", 2013, 2019, and 2023.
- "*Emerging Investigators 2019*", *Metallomics* journal, RSC.
- "Indo-French (IFCPAR/CEFIPRA)" Grant, 2016.
- "*Excellency Award*", 2014, Shiv Nadar University (SNU), Greater Noida, UP.
- "Prof. S Soundararajan Medal" *for Best Thesis, 2007, IPC, IISc, Bangalore*.
- "*Vasudevamurthy-Soundarajan Prize*" for "*Best Performance in the Course Work*", 2002, IPC, IISC, Bangalore.

Representative Publications:

Chem. Eur. J., **2024**, xx, xxxx; *Inorg. Chem.*, **2024**, 63, 10455; *J. Agric. Food Comm.* **2022**, 70, 9730; *Chem. Comm.* **2020**, 56, 9280; *Chem. Asian J.*, **2019**, 14, 4582; *Chem. Eur. J.*, **2019**, 25, 12810; *Inorg. Chem.*, **2019**, 58, 6628; *ACS Appl. Mater. Interfaces*, **2019**, *11*, 4766; *Metallomics*, **2019**, 11, 213; *Langmuir*, **2020**, 36, 328; *Org. Biomol. Chem.*, **2018**, *16*, 4243; *Inorg. Chem.*, **2017**, *56*, 12739; *Inorg. Chem.*, **2017**, *56*, 12102; *Chem. Eur. J.*, **2017**, *23*, 5696; *Proc. Natl. Acad. Sci., India, Sect. A Phys. Sci.*, **2016**, *86*, 611; *Angew. Chem. Int. Ed.*, **2015**, 54, 9323.

A Metalloenzyme-Based Engineered Biocatalytic Platform for Efficient Hydrocarbon Production

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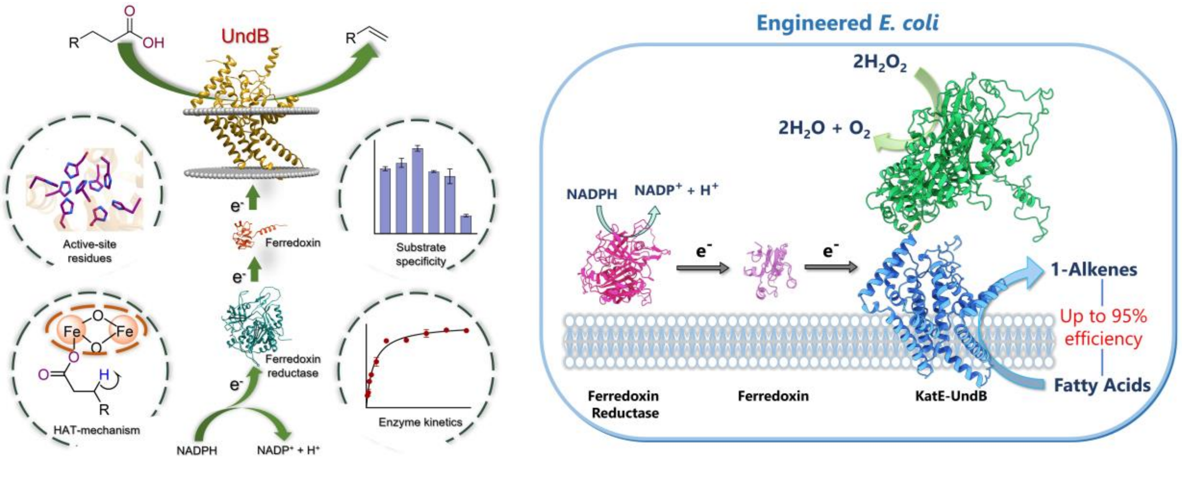
Abstract: Biosynthetically produced 1-alkenes hold immense value as sustainable alternatives to fossil fuels and find widespread applications in polymer, lubricant, and detergent industries. UndB is the only known membrane enzyme capable of converting naturally abundant fatty acids to 1-alkenes. However, despite diverse applications, UndB remains poorly understood since its discovery nearly a decade ago. Here, we present insights into the molecular basis of UndB catalysis and the mechanism of UndB reaction at the membrane interface. We unravel UndB as a diiron-enzyme that utilizes a conserved histidine cluster at the active site. We decipher the dependency of UndB activity on molecular oxygen and electrons and identify the most efficient redox partners of UndB. We elucidate the catalytic intricacies of UndB and establish it as the most efficient decarboxylase in producing industrially valuable medium-chain 1-alkenes. Further, we engineered UndB, tremendously improved the enzyme's activity, and developed a novel whole-cell biocatalyst utilizing the engineering UndB for highly efficient conversion (up to 95%) of naturally abundant free fatty acids to 1-alkenes (both aliphatic and aromatic). These findings hold promise for the sustainable high-titre production of 1-alkenes with a multitude of biotechnological applications such as biofuels and commodity chemicals.

Figure/Scheme:



References:

1. Iqbal, T., Murugan, S. **Das, D.*** ***Science Advances***, 2024, 10, eadl2492.
2. Murugan, S.; Iqbal, T. and **Das, D.*** ***Protein Science***, 2024, 33, e4893.
3. Iqbal, T.; Murugan, S.; Rajendran, K.; Sidhu, J. S. and **Das, D.*** ***ACS Catalysis***, 2023, 13, 23, 15516. [Front Cover]
4. Iqbal, T. and **Das, D.*** ***Biochemistry***, **2022**, 61, 10, 909–921 [Front Cover]
5. Iqbal, T.; Chakraborty, S.; Murugan S. and **Das, D.*** ***Chem. Asian J., 2022*** e202200105. [Front Cover]

Bio-sketch

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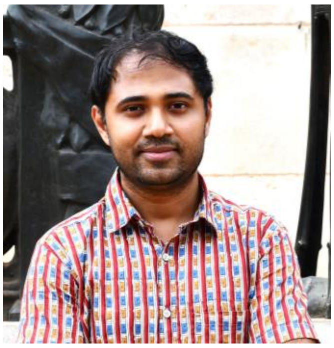

Debasis received his Ph.D. in Chemistry (Chemical Biology) from the University of Michigan, Ann Arbor, USA, in 2014. Followed by his postdoctoral work at MIT, USA, Debasis joined the Indian Institute of Science, Bangalore, as an assistant professor in 2019. His research area is interdisciplinary in nature, which has flavors of both Chemistry and Biology. His group focuses on the mechanistic understanding of various metalloenzymes and their applications. Employing various tools of chemistry, biochemistry, molecular biology, and microbiology, his group is exploring the function, kinetics, mechanism, and reaction intermediates of several poorly understood enzymes. The long-term goal of the work is to engineer and utilize these enzymes in green energy applications and therapeutics. He is an EMBO Global Investigator and recipient of the Excellence of Research Award 2013 given by University of Michigan, Excellence of Research Award 2024 and Excellence in Teaching Award 2024 given by IISc Bangalore.

Representative Publications:

1. Iqbal, T.; Murugan, S. and **Das, D.*** A Chimeric Membrane Enzyme and an Engineered Whole-cell Biocatalyst for Efficient 1-Alkene Production, ***Science Advances***, 2024, 10, eadl2492. [This article is featured by IISc Press The Times Of India, The Hindu, Deccan Herald, The New India Express, Energy World, LatestLY, BioEnergy Times, Neo Science Hub, Greenleaf, Udayavani), USA (EurekAlert!, Phys.org, MSN, Scienmag, Bioengineer.org), UK (AZoCleantech - The Online Clean Technology Community), Australia (Mirage), Germany (Germanic)].
2. Murugan, S.; Iqbal, T. and **Das, D.*** Functional Production and Biochemical Investigation of an Integral Membrane Enzyme for Olefin Biosynthesis. ***Protein Science***, 2024, 33, e4893
3. Iqbal, T.; Murugan, S.; Rajendran, K.; Sidhu, J. S. and **Das, D.*** Unraveling the Conversion of Fatty Acids into Terminal Alkenes by an Integral Membrane Enzyme, UndB. ***ACS Catalysis***, 2023, 13, 23, 15516. [This article is featured on the Front Cover of the journal, featured by IISc News, and the KERNEL magazine]
4. Sidhu, J. S.; Rajendran, K.; Mathew, A. B.; Iqbal, T. ; Saini, D. K. and **Das, D**.* Acetylcholine structure-based small activatable fluorogenic probe for specific detection of acetylcholinesterase, ***Analytical Chemistry, 2023, 95, 19, 7594–7602*** [This article is featured by IISc Press, PhysOrg, and several leading newspapers: Times of India, Hindustan Times, Deccan Herald, India Today, Today Headline, The Week Magazine, MedIndia, Mirage News, Latest LY, Alzforum etc.]
5. Iqbal, T. and **Das, D.*** Biochemical Investigation of Membrane-Bound Cytochrome b5 and Catalytic Domain of Cytochrome b5 Reductase from *Arabidopsis Thaliana*, ***Biochemistry, 2022, 61, 10, 909–921.*** [Featured as the **Front Cover** of the journal]

Understanding Mechanisms to Facilitate Rational Design of Short Cationic Antimicrobial Peptides

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Abstract:

Growing resistance in microbes against the known antimicrobials, coupled with the slowdown in the development of newer classes of antimicrobials both in academia and pharma industries, is a cause of eminent danger threatening the present-day human civilization. If not attended to, infections of resistant organisms might claim a great loss to human life by 2050 as predicted by WHO. Hence, there is a dire need for the development of alternate classes of compounds, effective against antimicrobial infections. Antimicrobial peptides (AMPs), a class of naturally occurring peptides with antimicrobial properties, and slow resistance development, holds immense promise in this regard. However, despite their potential, shortcomings like protease degradability, cytotoxicity, salt-sensitivity towards their activity have limited their commercial success. Researchers worldwide are working on improvement of the therapeutic potential of the AMPs. Though design through hit and trials, or from educated guesses from natural AMPs have led to some successes, rational design of efficient AMPs can be best optimized through understanding their underlying mechanisms of action. Our research focus is directed towards (1) development of robust, selective and potent AMPs, devoid of their present shortcomings from de novo/ template assisted design and (2) understanding their mechanism of action in molecular details using MD simulations. In addition to generating potent therapeutics, our studies establish basic understanding of the molecular mechanisms, which would enable rational design of other antimicrobial therapeutics in the future. Recently, we have also developed potent membrane active AMPs using the alchemical free energy simulations. Our long-term target is to be able to develop economically and commercially viable AMP therapeutics.

References and Notes:

1. Sarkar, T.; Ghosh, S.; Sundaravadivelu, P. K.; Pandit, G.; Debnath, S.; Thummer, R. P.; Satpati, P.; Chatterjee S. *ACS Infect. Dis.* 2024, 10, 562−581.
2. Pandit, G.; Chowdhury, N.; Mohid, Sk. A.; Bidkar, A. P.; Bhunia, A.; Chatterjee S. *ChemMedChem* **2021**, 16, 355-367.
3. Pandit, G.; Ilyas, H.; Ghosh, S.; Bidkar, A. P.; Mohid, Sk. A.; Bhunia, A.; Satpati, P.; Chatterjee. S. *J. Med. Chem.* **2018**, 61, 2614-2629.

Bio-sketch

Profile

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Biosketch: Sunanda completed her PhD from IISC Bangalore in 2009 under the mentorship of Prof. P. Balaram. Thereafter, she moved for her first postdoc (CNRS) with Prof. Marie Agnes Sari to University Paris Descartes, Paris, France in 2010 and for her second postdoc with Prof. Suparna Sanyal to Uppsala university, Sweden in 2012. Sunanda joined the Department of Chemistry, IITG in Dec 2013 as an Assistant Professor. She has been serving the department as an Associate Professor since 2021. Joined J. Med. Chemistry, ACS Publications, as an Associate Editor from Feb 2024.

Sunanda is a peptide chemist primarily interested in the development of peptide-based antimicrobial therapeutics. She is interested in the design, synthesis, structure, peptide-membrane interactions, biological activities of peptides and the mechanisms underlying their action.

Representative Publications:

1. Sarkar, T.; Ghosh, S.; Sundaravadivelu, P. K.; Pandit, G.; Debnath, S.; Thummer, R. P.; Satpati, P.; Chatterjee S. *ACS Infect. Dis.* **2024**, 10, 562−581.
2. S. Ghosh, S. Chatterjee, P.Satpati *J. Chem. Inf.Model*, **2023,** 63, 5823-5833.
3. S. Ghosh, S. Chatterjee, P.Satpati, J. Phys. Chem. B, 2022, 126, 5262-5273.
4. Ghosh, S.; Pandit, G.; Debnath, S.; Chatterjee, S.; Satpati, P. *RSC Adv*., **2021**, 11, 36836- 36849.
5. Pandit, G.; Chowdhury, N.; Mohid, Sk. A.; Bidkar, A. P.; Bhunia, A.; Chatterjee S. *ChemMedChem* **2021**, 16, 355-367.
6. Pandit, G.; Biswas, K.; Ghosh, S.; Debnath, S.; Bidkar, A. P.; Satpati, P.; Bhunia, A.; Chatterjee S. *BBA – Biomembranes* **2020**, 1862, 183177-183193.
7. Pandit, G.; Ilyas, H.; Ghosh, S.; Bidkar, A. P.; Mohid, Sk. A.; Bhunia, A.; Satpati, P.; Chatterjee. S. *J. Med. Chem*. **2018**, 61, 2614-2629.

Bio-inspired Designs for Dynamic and Complex Supramolecular Polymers

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Abstract:
The investigation of dynamic and adaptive supramolecular polymers, arising from monomer self-assembly, has entered a phase demanding greater structural and dynamic precision. Living supramolecular polymerization has emerged as a synthetic approach to craft assemblies with well-defined structures and dispersity. Concurrently, the pursuit of temporal control over dynamic materials is extending into the non-equilibrium realm. Despite the desirability of both controls, the strategies employed have largely been chemically distinct. Recognizing the importance of synergy between structural and temporal control, especially for the functional application of supramolecular polymers as adaptive materials, it is imperative to seek a common strategy. Drawing inspiration from the biological realm becomes crucial in navigating this conundrum.

Our laboratory is motivated by this philosophy and is actively engaged in comprehending both the thermodynamic and kinetic aspects of supramolecular polymerization. This presentation outlines our endeavors in understanding a pivotal concept in biological self-assembly: temporal control over aggregates through a chemical reaction. We believe this approach has the potential to address various challenges in supramolecular chemistry, including living supramolecular polymerization and dissipative assemblies. The talk will delve into our recent efforts to design reaction-coupled supramolecular polymers and explore bio-inspired design strategies aimed at expanding the structural diversity of supramolecular polymers.

Bio-sketch

Profile

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Biosketch:

Subi George is currently leading a supramolecular chemistry group at the New Chemistry Unit of JNCASR, Jawaharlal Nehru Centre for Advanced Scientific Research (JNCASR), Bangalore, India. Currently, He is also the Chair of New Chemistry Unit and also the Associate Editor of Chemical Science (RSC). His current research interests focus on Functional Supramolecular Polymers, Living and Non-equilibrium supramolecular polymerization, Supramolecular Chirality and Organic Phosphors.

He is the recipient of Shanti Swarup Bhatnagar (SSB) Prize for Science and Technology in Chemical Sciences Category for the year 2020. He is also the recipient of Swaranjayanti Fellowship from Department of Science and Technology of Government of India (2017), Asian Photochemistry Association (APA) Young Scientist award (2015), NASI-SCOPUS Young Scientist Award in Chemistry (2015), Chemical Research Society of India Bronze Medal (2015) and Materials Research Society of India Medal (2013). In 2019, he has been elected as the Fellow of Indian Academy of Sciences (FASc) and in 2023 he is elected as Fellow of Indian National Science Academy (FNASc). In 2021, he received CNR RAO National Prize for Chemical Research from CRSI. He is currently the member of Editorial Advisory Boards of JACS, Material Horizons, Organic Materials , ACS Materials-Au, PCCP and Chemistry Asian Journal.

Bio-sketch

Representative Publications:

1.

Abstract

Chemical Strategies to Address Protein Aggregation Diseases

Ishu Saraogi

Department of Chemistry
IISER Bhopal

Amyloidosis is a well-known, but poorly understood phenomenon caused by the aggregation of proteins, often leading to pathological conditions.[1] The aggregation of insulin, for example, poses significant challenges during the preparation of pharmaceutical insulin formulations commonly used to treat diabetic patients. Through screening of an in-house library, we have identified a small molecule, which causes a dose dependent reduction in insulin fibril formation. Biophysical analyses and docking results suggested that the inhibitor likely bound to partially unfolded insulin intermediates. Further, molecule-treated insulin had lower cytotoxicity, and remained functionally active in regulating cell proliferation in cultured *Drosophila* wing epithelium.[2]

Building up on this work, we have identified another molecule called PAD-S that completely inhibited insulin fibril formation.[3,4] The molecule acts as a chemical chaperone, by preventing the aggregation of insulin and preserving the native structure of the protein. Seeded aggregation kinetics with preformed insulin fibrils indicated that PAD-S likely inhibited primary nucleation and elongation events during the aggregation process. Structural-activity relationship analysis of the fragments of PAD-S for insulin aggregation inhibition underlines the importance of all the features of the molecule for optimal activity. PAD-S was also effective in disaggregating preformed insulin fibrils to non-toxic species. We found PAD-S to be highly effective against several commercial fast and slow acting insulin variants, e.g. Lispro and Glargine. The benign nature of PAD-S towards HEK293T cell lines and prevention of aggregation-induced toxicity by PAD-S treated insulin further highlights its potential use in commercial insulin formulations.

Publications:

- Das, A.; Shah, M.; Saraogi, I.*; "Molecular aspects of insulin aggregation and its inhibition using small molecules" *ACS Bio & Med Chem Au*, **2022,** *2*, 205
- Das, A.; Gangarde, Y.M.; Tomar, V.; Shinde, O.; Upadhyay, T.; Alam, S.; Ghosh, S.; Chaudhary, V.; Saraogi, I.*; "A small molecule inhibitor prevents insulin fibrillogenesis and preserves activity" *Mol. Pharm* **2020**, *17*, 1827
- Gangarde, Y.M.; Das, A.; Ajit, J.; Saraogi, I.* "Synthesis and evaluation of arylamides with hydrophobic side chains for insulin aggregation inhibition" *ChemPlusChem* **2021**, *86*, 750
- Das, A.; Gangarde, Y.M.; Pariary, R.; Bhunia, A.; **Saraogi, I.***; "An amphiphilic small molecule drives insulin aggregation inhibition and amyloid disintegration" *Int. J. Biol. Macromol.* **2022,** *218*, 981

Bio-sketch

Profile

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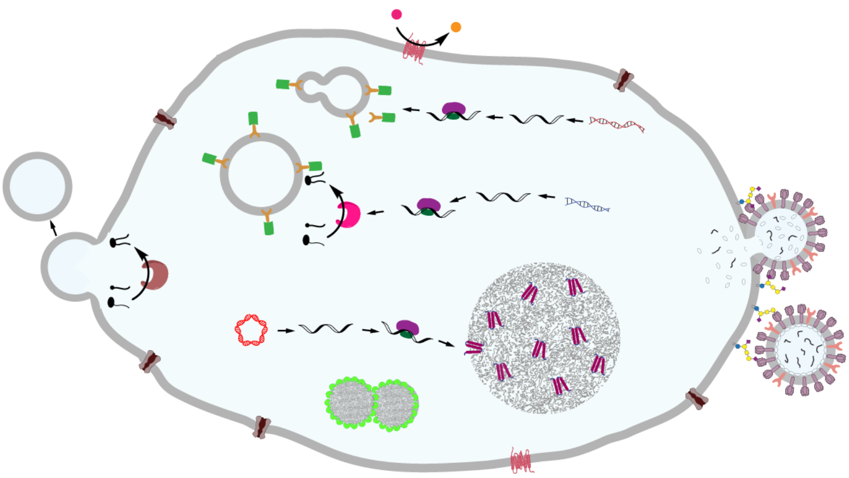
Ishu Saraogi received her BSc in Chemistry from University of Calcutta, and a MS in Chemistry from Indian Institute of Science, Bangalore working with Prof. T. N. Guru Row. In 2003, she joined Yale University to pursue a PhD under the supervision of Prof. Andrew Hamilton followed by a postdoctoral stint at Caltech with Prof. Shu-ou Shan. In 2013, Dr. Saraogi joined Indian Institute of Science Education and Research Bhopal, where she works on developing chemical tools to modulate biomolecular interactions. Their research group focuses on the development of novel antibacterial and anti-amyloidogenic agents, as well as on chemical manipulation of nucleic acids for interesting biological applications. She is a recipient of the Ramanujan and POWER fellowships from the Science and Engineering Research Board (SERB), India. Their work was recently featured in the ChemBioTalents collection by the journal ChemBioChem (Wiley). She serves on the editorial advisory boards of ChemBioChem (early career) and ACS Chemical Health & Safety. She was recently awarded the Prof. Dhananjay Nasipuri Memorial Lecture Award by the Indian Chemical Society, and was one of the Thieme Journal Awardees for 2024.

Title: Origins of Life to Viruses: A Chemical Synthetic Biology Approach

Name: Ahanjit Bhattacharya*
Indian Institute of Science Education and Research Bhopal
(Email: ahanjit@iiserb.ac.in)

Abstract: Compartmentalization is a defining feature of all forms of life.[1] Here we describe a chemical synthetic biology approach to understand the importance of compartmentalization in the context of origins of life and also in biological organisms. Various lipid architectures were used to build functional artificial cells and organelles. We utilized giant vesicles to recapitulate the basic membrane-bound structure of cells.[2] To model membrane-rich organelles such as the endoplasmic reticulum, we described a novel bicontinuous lipid sponge phase lipid droplet system.[3] With their nanoporous structure consisting of an interconnected network of bilayers, lipid sponge droplets can sequester hydrophobic and hydrophilic molecules in a programmable manner at concentrations comparable to that in cells. The droplets can further sequester and release proteins rapidly and reversibly to control enzymatic reactions in response to external stimuli. Next, to understand the origins of cellular compartmentalization, we explored various minimal chemoenzymatic pathways for *de novo* generation of lipid membranes.[4–6] We demonstrated a few primitive modes of growth and division of such membrane compartments to provide a hint at how earliest cells may have proliferated. Given their central role in cellular physiology, lipid membranes are also key to understanding the fundamentals of many infectious diseases. For example, pathogens like viruses hijack the dynamical processes of the cellular membrane systems to gain entry. We describe the application of surface-immobilized lipid vesicles mimicking endosomes to model the events concerning cellular attachment, endosomal membrane fusion, and genome transfer of enveloped viruses such as influenza.[7]

Figure/Scheme (if any):



References and Notes:

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3. A. Bhattacharya, H. Niederholtmeyer, K. A. Podolsky, R. Bhattacharya, J.-J. Song, R. J. Brea, C.-H. Tsai, S. K. Sinha and N. K. Devaraj, *Proc. Natl. Acad. Sci.*, 2020, 202004408.
4. A. Bhattacharya, H. Brea, Roberto J, Niederholtmeyer and N. K. Devaraj, *Nat. Commun.*, 2019, **10**, 300.
5. A. Bhattacharya, C. J. Cho, R. J. Brea and N. K. Devaraj, *J. Am. Chem. Soc.*, 2021, **143**, 11235-11242.
6. A. Bhattacharya, L. Tanwar, A. Fracassi, R. J. Brea, M. Salvador-Castell, S. Khanal, S. K. Sinha and N. K. Devaraj, *J. Am. Chem. Soc.*, 2023, **145**, 27149-27159.
7. A. Bhattacharya, N. Bagheri and S. G. Boxer, *Anal. Chem.*, 2024, **96**, 13033-13046.

Bio-sketch

Profile

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Biosketch: Ahanjit Bhattacharya is an Assistant Professor of Chemistry at the Indian Institute of Science Education and Research, Bhopal. He is the Principal Investigator of the Chemical Synthetic Biology Laboratory. His core philosophy of research is "learning about biology through building". Ahanjit graduated in Chemistry with minor in Biotechnology from IIT Kharagpur as the Prime Minister of India Gold Medalist (2014), Ahanjit carried out his doctoral research at the University of California San Diego under the guidance of Neal Devaraj. Here, he worked on designing artificial cellular systems from fundamental chemical and biochemical building blocks. Ahanjit's major accomplishments are the development of programmable lipid compartments as artificial cells and organelles and designing minimal biochemical strategies for synthesis of membrane-forming lipids. His experience with lipids and soft matter physics inspired him to gain expertise around membrane biophysics during postdoctoral tenure in the lab of Steven Boxer. At Stanford, Ahanjit has worked on biophysical mechanisms of fusion of enveloped viruses like influenza. He has also studied structure-function relationships in archaeal bipolar lipids to shed light on cellular physiology of extremophilic archaea. His association with the Stanford Center for Innovation in Global Health as a postdoctoral affiliate inspired him to develop low-cost solutions to human health problems in the developing world. Ahanjit's research work led to several awards including his recognition as one of the CAS Future Leaders Top 100 (2024), and Reaxys PhD Prize Finalists (2020). Ahanjit enjoys teaching and received the Postdoc Teaching Certificate from Stanford in recognition of his comprehensive teaching training and practice. Ahanjit is passionate about communicating science and making it a transformational force for betterment of society and humanity.

Representative Publications:

1. **A. Bhattacharya**, N. Bagheri, S. G. Boxer. A fluorogenic pseudo-infection assay to probe transfer and distribution of influenza viral contents to target vesicles. *Anal. Chem.* **2024**, 96, 13033-13041.

2**. A. Bhattacharya**, I. D. Falk, F. R. Moss III, K. N. Tran, N. Z. Burns, S. G. Boxer. Structure-Function Relationships in Pure Archaeal Bipolar Tetraether Lipids. *Chem. Sci.* **2024**, 15, 14273-14286.

3. **A. Bhattacharya**, C. J. Cho, R. J. Brea, N. K. Devaraj. Expression of Fatty Acyl-CoA Ligase Drives One-Pot De Novo Synthesis of Membrane-Bound Vesicles in a Cell-Free Transcription-Translation System. *J. Am. Chem. Soc.* **2021**, 143, 11235-11242.

4. **A. Bhattacharya**, H. Niederholtmeyer, K. A. Podolsky, R. Bhattacharya, J. Song, R. J. Brea, C. H. Tsai, S. K. Sinha, N. K. Devaraj. Lipid Sponge Droplets as Programmable Synthetic Organelles. *Proc. Natl. Acad. Sci. USA* **2020**, 117, 18206-18215.

5. **A. Bhattacharya**, R. J. Brea, H. Niederholtmeyer, N. K. Devaraj. A Minimal Biochemical Route towards *de novo* Formation of Synthetic Phospholipid Membranes. *Nat. Commun.* **2019**, 10, 300.

Title: Bioinspired Materials using Oxime Chemistry and Non-Natural Amino Acids

Name: Alexander Baker, Ph.D.
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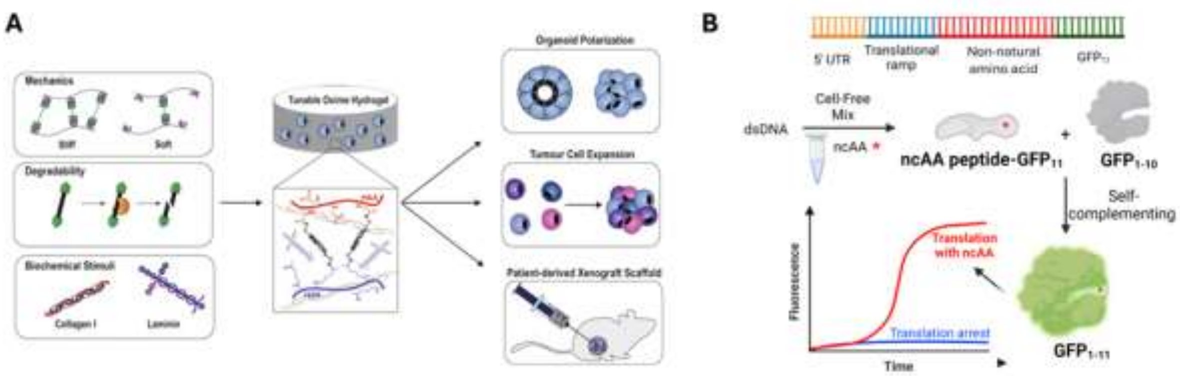
Abstract:

Bioinspired materials continue to offer promising solutions to a variety of medical, agricultural, and industrial problems. This research talk Dynamic covalent chemistry offers a new class of stress relaxing biomaterials to mimic soft tissues for complex 3D in vitro cancer models. To capture the physicochemical attributes of cancer tissue and achieve the desired cellular phenotype we synthesized a biomimetic oxime crosslinked hydrogel composed of hyaluronan and matrix metalloproteinase-cleavable peptide. Tumour organoids were prepared from patient cells isolated from tumour biopsies grown in the oxime hydrogel. We observed a differential response to drugs when patient organoids were cultured in our hydrogel vs laminin-rich mouse sarcoma protein extract Matrigel®. The hyaluronan-based hydrogel showed superior reproducibility in establishing patient-derived xenografts (PDX) tumour growth compared to Matrigel®. In the case of PDX grown in Matrigel® the tumours showed skewed macrophage polarization based on the proportion of alternatively activated resident murine macrophage cells. A second story focused on a bio-inspired protein-based material synthesized using cell-free protein expression focuses on identification of non-canonical amino acids which expand the genetic code for protein engineering applications.

Figure/Scheme:



Scheme**:** Application of oxime chemistry and non-canonical amino acids. **A)** Oxime chemistry hydrogels as a responsive material to support 3D cell growth in vitro and in vivo **B)** Determination of novel non-canonical amino acid incorporation using split-fluorescent protein assays.

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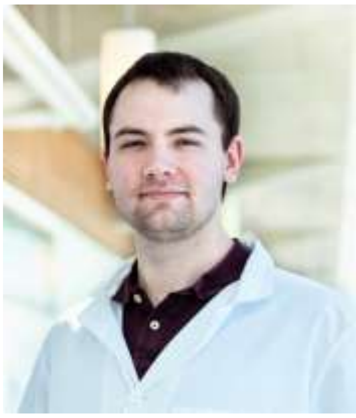
1. **Baker, A.E.G.**; Bahlmann, L.C.; Xue, C.; Lu, Y.H.; Cruickshank, J.; Cescon, D.W.; Shoichet, M.S. (2022) Materials Today. 56, 96-113.
2. **Baker, A.E.G.**; Cui, H.; Ballios, B.G.; Ing, S.; Yan, P.; Wolfer, J.; Wright, T.; Dang, M.; Gan, N.Y.; Cooke, M.J.; Ortín-Martínez, A.; Wallace, V.A.; van der Kooy, D.; Devenyi, R.; Shoichet, M.S. (2021) Biomaterials. 271 120750.

Bio-sketch

Profile



Alexander E.G. Baker
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Biosketch: Dr. Alexander Baker is an Assistant Professor in the Department of Chemistry at Dalhousie University (July 2023). He pursued undergraduate studies (B.Sc.) as a combined Honors in Chemistry, Biochemistry at Dalhousie University, before proceeding to a PhD in Chemical Engineering and Collaborative Specialization in Biomedical Engineering. The focus of his research involved click chemistry hydrogels and 3D in vitro drug screening models for cancer with Dr. Molly Shoichet at the University of Toronto. As a postdoctoral fellow Dr. Baker concentrated on the design of an intraocular hydrogel to treat retinal detachment in Dr. Shoichet's lab. He later joined Dr. Keith Pardee's synthetic biology research group (University of Toronto) as a postdoctoral fellow. Here research focus included developing a multiplexed diagnostic against Lyme disease caused by caused by borrelia bacteria and expansion of the genetic code with non-canonical amino acids for therapeutic applications. The Baker research group specializes in cell-free incorporation of non-natural amino acids in adhesive biomaterials and conductive hydrogels for regenerative medicine applications.

Representative Publications:

1. https://onlinelibrary.wiley.com/doi/abs/10.1002/adma.201901166
2. https://linkinghub.elsevier.com/retrieve/pii/S014296122100106X
3. https://www.sciencedirect.com/science/article/abs/pii/S1369702122000232

Copper(I)-Catalyzed Proto/Carboboration of 1,3-Diynes: An Easy and Sustainable Access to Borylated Enynes and Dienes

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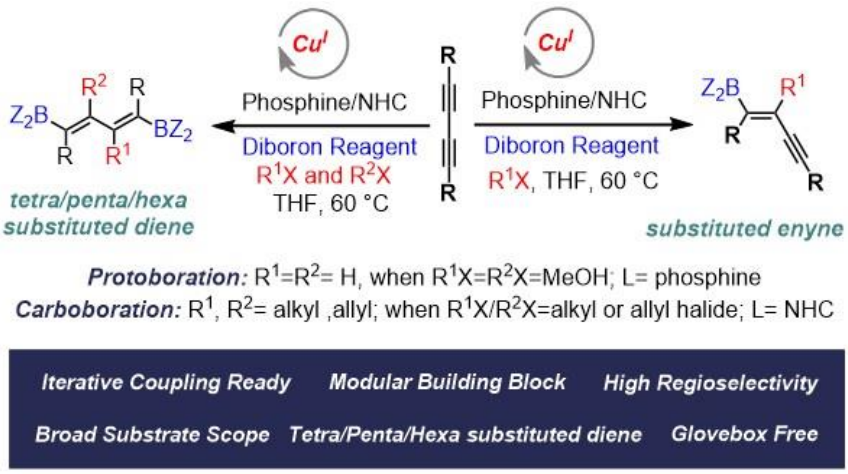
Abstract:

Targets with high structural complexity can be easily assembled using small, modular building blocks similar to a 'Lego' construction using Iterative chemistry.[1-3] Organoboron compounds have been in the spotlight as versatile building blocks in natural product synthesis. Here, we present a sustainable, glovebox-free regioselective protoboration of 1,3-diynes using a stable diboron source and Cu^{I}/phosphine as a catalyst to access stable enynyl and dienyl boronate esters in a single operation. Then, we developed the first copper-catalyzed carboboration of 1,3-diynes, in which a simultaneous C−B and C−C bond formation was achieved in a single operation using a Cu^{I}/NHC catalyst. The methodology provides easy access to highly sterically encumbered penta- and hexa-substituted dienes. A wide range of electrophiles have been successfully employed. DFT studies supported the regioselective incorporation of electrophiles. The products were employed in iterative coupling to obtain densely functionalized 1,3-dienes and polyenes.[4,5]



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5. Ghosh, S.; Kumar, S.; Chakrabortty, R.; Ganesh, V. *Org. Lett.* **2024**, *26*, 6574.

Bio-sketch

Profile

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Venkataraman Ganesh received his early education from Bishop Heber College Tiruchirappalli (2001-2004) and joined the Integrated Ph.D. program (Chemical Sciences) at Indian Institute of Science (IISc) Bangalore (2004). Ganesh obtained his Ph.D. in 2013, working with Prof. S. Chandrasekaran as a CSIR-Shyama Prasad Mukherjee (CSIR-SPM) fellow. He had postdoctoral stints as a JSPS fellow (2013–15) with Prof. M. Shibasaki at BIKAKEN, Japan, and as a Newton International Fellow (2016–18) with Prof. V. K. Aggarwal at the Univ. of Bristol, UK. He started his independent research career in 2018 at the Dept. of Chemistry, Indian Institute of Technology Kharagpur, India, and held the Ramanujan fellowship till 2023 (SERB, India). His research interests include exploiting transition-metal catalysts and boron chemistry to develop new synthetic methodologies and mechanistic studies.

Representative Publications:

1. Ghosh, S.; Kumar, S.; Chakrabortty, R.; Ganesh, V.* *Org. Lett.* **2024**,26, 6574.
2. Biswas, K.; Malik, S.; Ganesh, V.* *J. Org. Chem.* **2024**, *89*, 11014.
3. Mondal, S.; Biswas, K.; Ganesh, V.* *Adv. Synth. Catal.* **2024**, *366*, 3277.
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7. Mondal, S.† Ballav, T.† Tofayel, S. M.; Ganesh, V.* *Org. Lett.* **2023**, *25*, 3941.
8. Biswas, K.; Khamrai. A; Malik, S.; Ganesh, V.* *Org. Lett.* **2023**, *25*, 1805.
9. Ghosh, S.; Chakrabortty, R.; Kumar, S.; Das, A.; Ganesh, V.* *ACS Catal.* **2022**, 12, 11660.

Chemistry of Imidates: Application in Glycochemistry

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Abstract:

Functionalized organic molecules are an important class of compounds that are ubiquitously present as a key structural motif in natural products, and biologically active compounds. The introduction of the required functional motif into the desired system while satisfying the parameters of sustainable chemistry such as cost and atom economy is high in demand. Therefore, the direct functionalization of robust and unreactive C-H (sp^2/sp^3) bonds provides an alternate, effective, and desirable tool for organic chemists to convert them into valuable chemical commodities.[1] Imidates are versatile chemical compounds that have garnered significant interest in organic synthesis due to their ability to serve as valuable intermediates for various functionalization reactions. The unique chemistry of imidates offers synthetic chemists a plethora of opportunities for diversifying molecular structures and accessing complex organic molecules efficiently.

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

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3. Kumar, Y**.,** Jaiswal, Y., Kumar, A., *Org.Lett*. **2019**. 21, 3108.
4. Kumar, Y**.,** Shaw, M., Thakur, R., Kumar A., *Org. Letter,* **2020**, 22, 5, 1908.

Bio-Sketch of Speaker

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Career profile:

- Associate Professor, IIT Patna **5th Dec. 2019**
- Assistant Professor, IIT Patna: **2014-2019**
- Research Investigator-Biocon-Bristol Myers Research Center, Bangalore: **2012- 2013**
- Postdoctoral Fellow-University of Konstanz, Germany: **2010-2012**
- Postdoctoral Fellow -City University of New York, USA: **2008-2009**
- Ph. D. IIT Kanpur, India: **2008**
- M. Sc. Delhi University: **2002**

Honours and awards:

- Editorial Board Member: **Journal of Carbohydrate Chemistry from 2024**
- CRSI-Bronze medal award **2023**
- Council Member, CRSI-**2023-2026**
- Executive Member ACIT **2023-2026**
- Life-member- CRSI, India
- Life-member-ISCB, India
- Life-member, ACIIT, India

AK research group is primarily involved in the design and development of cost and atom-economical strategies for the syntheses of important functional organic molecules utilizing the chemistry of primary amides and imidates. The chemistry of ubiquitous amides and imidates functional groups has been well explored for the distal functionalization of robust C-H bonds of electronically complex molecules such as carbohydrates and aliphatic compounds. Indeed, our group is also involved in the glycodiversification aspects of carbohydrate chemistry.

Representative Publications:

1. *Chem.Commun.* **2022**, *58,11304*
2. *J. Org. Chem.* **2021**, *86, 9744*
3. *Org. Letter*, **2020**, *22, 5, 1908*
4. *Org. Letter*, **2020**, *22,4,1605*
5. *J. Org. Chem.* **2019**, *84, 589*
6. *Org.Lett.* **2018**, *20, 4964*
7. *Org.Lett.* **2018**,*20,4964*
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10. *J. Org. Chem.* **2016**, *81, 6617*

Diverse Boronic Esters: Sustainable Methodologies for Synthesis through Fe and Co catalysis and applications

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Organoborane compounds are of interest to chemical, medicinal, and materials scientists because of their stability and ability to undergo selective transformations into diverse functional groups through various established protocols.[1] The predominant methods for synthesizing organoboron compounds typically employ either hydroboration or borylation protocols, utilizing metal catalysis.[2] Although organoborane compounds are versatile, their traditional synthesis relies on organometallic reagents and precious-metal catalyst systems. Notably, catalysts like Pd, Pt, Rh, Re, Ru, and particularly Ir have been developed over the past decades for this purpose.[3] This highlights the importance of discovering new catalysts with earth-abundant 3d transition metals like manganese, iron, and cobalt instead of relying on rare and precious metals. In our lab we strive to develop milder and effective methodologies to obtain valuable boronic esters, containing varied features. We used inexpensive and challenging substrates, available in feed stock in nature, like aryl[4] and alkyl halides,[5a,b] substituted alkenes,[6] aldehydes,[7] N-heterocycles,[8a] and alkynes.[8b] These transformations shows the potential of the carefully designed Cobalt and Iron complexes. We have also discovered the first 1,2-metallate rearrangement reaction involving the selenium nucleophile, utilising the diborylated product of carbonyl functionalities,[9] thus adding one more example to the plethora of value to boronic ester moieties. Key results and mechanistic findings will be discussed.

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(2) (a) Burgess, K.; Ohlmeyer, M. J. *Chem. Rev.* **1991**, *91*, 1179– 1191. (b) Marder, T.B.; Norman, N.C. *Topics in Catalysis.* **1998**, *5*, 63–73. (c) Neeve, E. C.; Geier, S. J.; Mkhalid, I. A. I.; Westcott, S. A.; Marder, T. B. *Chem. Rev.* **2016**, *116*, 9091– 9161.

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(4) Verma, P. K.; Mandal, S.; Geetharani, K. *ACS Catal.* **2018**, *8*, 4049-4054.

(5) (a) Verma, P. K.; Sujit Prasad, K.; Varghese, D.; Geetharani, K. *Org. Lett.* **2020**, *22*, 1431-1436. (b) Siddiqui, S.; Bhawar, R.; and Geetharani, K. *J. Org. Chem*. **2021**, *86*, 1948-1954.

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Bio-sketch

Profile

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Biosketch:

Geetharani was born and raised in Madurai, Tamilnadu, India. She began her independent research career as an Assistant Professor at department of inorganic and physical chemistry, Indian Institute of Science Bangalore, India in 2016. She was promoted to an Associate professor in 2022. She is a recipient of DST-Inspire Faculty Award. She has been elected as Young Scientist/Affiliate by all three Science Academies in India. She received the SERB-Women Excellence Award from the President of India. She is also an Editorial member of Chemistry – An Asian Journal and a member of the Early Career Advisory Board of the European Journal of Inorganic Chemistry. Her research interests are in the areas of catalysis, main group and organometallic chemistry.

Representative Publications:

1. Keerthika, K.; Bazil Muhammed, S.;Geetharani, K.* Synthesis of Trifluoromethylated Ketones from ,-Unsaturated Ketones via Catecholboron Enolates, **J. Org. Chem., 2024**.
2. Meher, N.; Suryavansi, M.; Geetharani, K.* Regioselective Hydroboration of Unsymmetrical Internal Alkynes Catalyzed by Cobalt Pincer-NHC Complex, **Org. Lett., 2024**, *26*, 5862-5867.
3. Keerthika, K.; Bazil Muhammed, S.;Geetharani, K.* A Metal-free and Operationally Simple Radical Trifluoromethylative Borylation of Unactivated Alkenes, **Chem. Eur.J., 2023, e202303468.**
4. Paul, S.; Verma, P. K.; Kashyap, A.; Mondal, R.; Geetharani, K.* Approach to the Synthesis of gem-Thiolated Alkylboronates via Cobalt-Catalyzed Diboration of Aldehydes, **Org. Lett., 2023**, 25, 2901-2906.
5. Meher, N. K.; Verma, P. K.; Geetharani, K.* Cobalt-Catalyzed Regioselective 1,2-Hydroboration of N-Heteroarenes, **Org. Lett., 2023, 25, 87-92**
6. Verma, P. K.; Meher, N. K.; Geetharani, K.* Homolytic Cleavage of Diboron(4) Compounds by Diazabutadienes. *Chem Commun.* **2021**, *57*, 7886 – 7889. Highlighted on the Cover Page of the Article.
7. Verma, P. K.; Souvik, M.; Geetharani, K.,* Efficient Synthesis of Aryl Boronates via Cobalt-Catalyzed Boryla-tion of Aryl Chlorides and Bromides. *ACS Catal.* **2018**, *8*, 4049-4054. Highlighted in Synfacts 2018, 14(07), 0746.

Transition Metal Catalysis towards C–H and C–C Bond Activation: From Biaryl Frameworks to Natural Product Scaffolds

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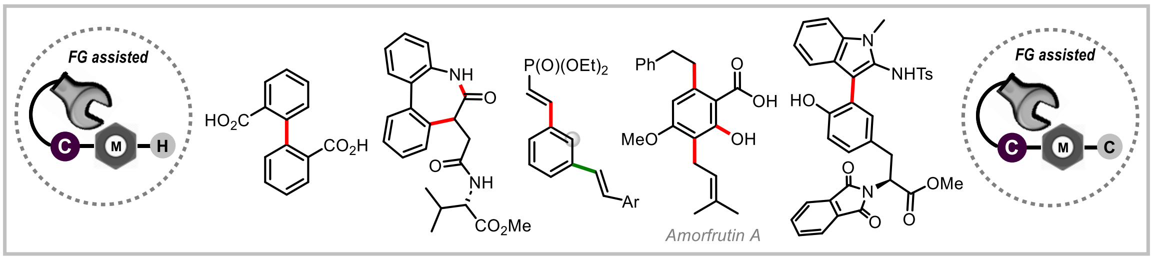
Abstract:

Sustainable synthetic strategies to embrace molecular complexity from simple precursors are fundamental in contemporary organic chemistry. In this context, transition metal-catalyzed regio- and stereoselective functionalization of otherwise inert C–H and C–C bonds is particularly promising.[1] We have explored the use of carboxylic acids, amides, free amines, and alcohols as versatile directing groups for a range of position-selective reactions, including olefination, annulation, and dimerization, employing versatile ruthenium and cobalt catalysts.[2] Additionally, we have developed methods for C–H ruthenation-enabled decarboxylative hydroarylation of alkenes, leading to *meta*- and *para*-functionalization, as well as one-pot deformylative arene functionalization with carbenes, producing unsymmetrical biaryldiols and heterobiaryl amino alcohols.[2b,d] Recently, we have also advanced a Wacker-type reaction using a nucleopalladation strategy, which promotes diverse functionalization of unactivated olefins.[2a] These strategies have applications in synthesizing and the late-stage functionalization of bioactive molecules.[2] This presentation will overview recent advancements from our laboratory in transition-metal-catalyzed C–H and C–C bond activation of arenes and olefins.



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2. Selected papers: (a) N. Ballav, S. N. Saha, S. Yadav, and M. Baidya, *Chem. Sci.* **2024**, *15*, 4890. (b) C. K. Giri, T. Singh, S. Mondal, S. Ghosh, and M. Baidya, *ACS Catal.* **2024**, *14*, 11286 (c) Chowdhury, D.; Ghosh, S.; Reddy, K. S. S. V.; Yamijala, S. S. R. K. C.; Baidya, M. *ACS Catal.* **2023**, *13*, 12543. (d) A. Mandal, H. Sahoo, S. Dana, and M. Baidya, *Org. Lett.*, **2017**, *19*, 4138. (e) Dana, S.; Chowdhury, D.; Mandal, A.; Chipem, F. A. S.; Baidya, M. *ACS Catal.* **2018**, *8*, 10173. (f) A. Mandal, J. Selvakumar, S. Dana, U. Mukherjee, and M. Baidya, *Chem. Eur. J.* **2018**, *24*, 3448.

Bio-sketch

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Biosketch:
Mahiuddin Baidya studied chemistry at the Indian Institute of Technology Kanpur (IITK), India. He obtained his PhD in 2009 from Ludwig-Maximilians-Universität München (LMU), Germany under the supervision of Prof. Herbert Mayr. After postdoctoral studies with Prof. Hisashi Yamamoto at The Universality of Chicago, USA and Molecular Catalyst Research Center in Japan with JSPS fellowship, he joined at the Department of Chemistry, Indian Institute of Technology Madras, as an Assistant Professor in 2014, and was promoted to Professor in 2022. His research interest includes the development of novel concepts on transition-metal catalysis, organocatalysis, and visible-light photocatalysis for organic synthesis, and the synthesis of bioactive natural products and drug candidates. As an independent researcher at IIT Madras, he has more than seventy research publications in peer-reviewed journals of international repute.
He is a recipient of the INSA-Young Scientist Medal (2017), NASI-Young Scientist Platinum Jubilee Award (2017), Institute Research & Development Award (IRDA IIT M, 2018), AVRA Young Scientist (2021), Merck Young Scientist Awards (2021), CRS Bronze Medal (2023), and CRSI Bronze Medal (2025) and also became an Associate of the Indian Academy of Sciences (IAS) in 2017. Recently, he also received the *Best Teacher Award (Chemistry)* from IIT Madras. He served as an Early Career Advisory Board (ECAB) member of *ACS Catalysis* and also is an International Advisory Board Member of *Chemistry - An Asian Journal*.

Representative Publications:

1. Three-component dicarbofunctionalization of allylamines *via* nucleopalladation pathway: unlocking *vicinal* and *geminal* selectivity; N. Ballav, S. N. Saha, S. Yadav, and M. Baidya, *Chem. Sci.* **2024**, *15*, 4890.
2. Ruthenium-catalyzed deformylative C–C activation and carbene insertion towards diversity-oriented synthesis of unsymmetrical biaryldiols and heterobiaryl amino alcohols; C. K. Giri, T. Singh, S. Mondal, S. Ghosh, and M. Baidya, *ACS Catal.* **2024**, *14*, 11286.
3. Metal-free site-selective functionalization with cyclic diaryl λ^3-chloranes: suppression of benzyne formation for ligand-coupling reactions; K. Patra, M. P. Dey, and M. Baidya, *Chem. Sci.* **2024**, *DOI: 10.1039/D4SC04108A.*
4. Cobalt(III)-catalyzed free amine directed site-selective allylation in 2-aminobiaryls with vinyl cyclopropanes; D. Chowdhury, S. Ghosh, K.S.S.V. P. Reddy, S. S.R.K.C. Yamijala, and M. Baidya, *ACS Catal*. **2023**, 13, 12543.

Iodine(III) Catalyzed Stereoselective Functionalization and Rearrangement of Olefins for Organic Synthesis

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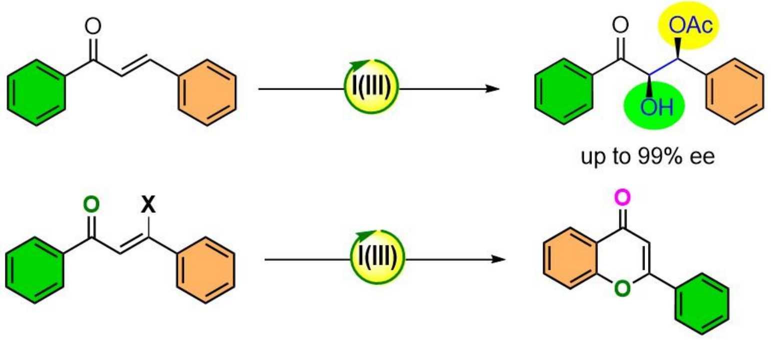
Abstract:

Hypervalent iodine reagents have recently garnered increasing attention for the oxidative functionalization of π-bonds, enabling access to complex molecular scaffolds from simple and widely available substrates. Pyrazolines, pyrazoles and isoxazoles are the privileged motifs found in numerous marketed drugs and natural products possessing vital properties like antidepressant, anti-inflammatory, antiviral, antibacterial, etc. Editing them with a heteroatom(s) often improves/expands the clinical efficacy of the parent molecules and opens new domains for applications through easy manipulations of these functionalities. We have recently developed highly efficient iodine(III) catalyzed methods for the preparation of heterofunctionalized pyrazolines and pyrazoles/isoxazoles. Unprecedented enantioselective methods for the *syn*-hydroxy-oxyacylation of enones and rearrangement of chalcones have also been reported.



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3. Singh, V.; Kumar, D.; Mishra, B. K.; Tiwari, B. *Org. Lett.* **2023**, *25*, 7089.
4. Pandey, C. B.; Singh, V.; Tiwari, B. *ChemRxiv* DOI: 10.26434/chemrxiv.14345981.v2.

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Dr. Bhoopendra Tiwari received his B.Sc. (Chem. Hons) and M.Sc. (Organic Chemistry major) from Tripura University. He obtained his Ph.D. from CSIR-Indian Institute of Chemical Technology, Hyderabad under the guidance of Dr. S. Chandrasekhar in 2010. Subsequently, he joined the lab of Prof. Robin Y. Chi as a Research Associate at Nanyang Technological University, Singapore.

Dr. Tiwari joined MACS-Agharkar Research Institute, Pune, an autonomous research institute of Department of Science and Technology (DST), Govt. of India, as a Scientist-D in 2013. Subsequently, he moved to Centre of Biomedical Research, Lucknow as an Assistant Professor in the Department of Biological and Synthetic Chemistry in 2014. Currently, he serving as an Associate Professor. His research group is actively engaged in the development of novel asymmetric synthetic methods and organic synthesis using organocatalysis (NHC and Hypervalent Iodine catalysis). He has received CBMR Research Excellence Award 2022. He has published around 50 research articles and several patents.

Representative Publications:

1. Singh, V.; Mishra, B. K.; Kumar, D.; Tiwari, B. *Org. Lett.* **2024**, *26*, 385.
2. Verma, R. S.; Khatana, A. K.; Verma, D.; Tiwari, B. *Chem. Commun.* **2024**, *60*, 5306.
3. Singh, V.; Kumar, D.; Mishra, B. K.; Tiwari, B. *Org. Lett.* **2023**, *25*, 7089.
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8. Verma, R. S.; Khatana, A. K.; Kumar, S.; Tiwari, B. *Chem. Commun.* **2020**, *56*, 7155

Photocatalytic Systems for Energy and Environmental Applications

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Abstract: Energy and environment are the major problems across the world. Water pollution is an emerging problem due to rapid population growth and modern industrialization. Wastewater contains organic (such as phenolic derivatives, polycyclic aromatic hydrocarbons etc.) and inorganic compounds (e.g. heavy metals) which can cause serious disorder. Apart from these pollutants, there is also a category of emerging contaminants e.g. pharmaceuticals, pesticides, personal care products, etc. Conventional wastewater treatment plants (WWTPs) are not capable of removing such pollutants. Photocatalysis is an advanced oxidation process, considered an effective technique for treating wastewater laden with organic contaminants. In this talk, I will present our group's recent work about visible light activated nanostructured photocatalysts for wastewater remediation applications. Developed materials are reusable, and their nanostructures do not change after repetitive usage. Development of inexpensive prototype photochemical reactor will also be discussed towards continuous flow operation. Finally, I will talk about our recent efforts to develop photocatalysts for CO_2 to fuel conversion applications.

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Bio-sketch

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Biosketch: Dr. Raju Kumar Gupta is currently a Professor at the Department of Chemical Engineering, Indian Institute of Technology Kanpur, India and is associated with Department of Sustainable Energy Engineering and Kotak School of Sustainability, IIT Kanpur since their inception. Prof. Gupta received Ph.D. degree in Chemical and Biomolecular Engineering from National University of Singapore, Singapore in 2010. He joined as an Assistant Professor at the Department of Chemical Engineering, Indian Institute of Technology Kanpur, India in 2012. Prof. Gupta's research group has made important contributions to the area of sustainable materials, green synthesis, nanostructured materials for wastewater treatment and energy storage applications. His current research interests are photocatalysis for water remediation and CO_2 capture & conversion to fuels, water generation *via* desalination, perovskite solar cells and energy storage devices based on batteries. Prof. Gupta has been recipient of several fellowships and awards for his outstanding career in academic and research fields. Some of the fellowships and awards include DST Inspire Faculty Award 2013, IEI Young Engineer Award (2014-15), Young Scientist Award (2014-15), P. K. Kelkar Young Faculty Research Fellowship 2018, Distinguished Young Alumnus Awards 2021, PK Kelkar Young Faculty Fellowship 2022 and Fellowship of the Royal Society of Chemistry (FRSC) 2022. He has authored more than 135 research articles in international journals, 7 patents, 3 edited books, 18 book chapters, guest edited special issues for several international journals, and his work has been cited more than 10000 times. Prof. Gupta is an editorial board member of several international journals, as well as a member of scientific bodies. Some of his significant appointments include Founding Editor for Elsevier journal *'Sustainable Chemistry One World'*; Associate Editor for Elsevier journal *'Solar Energy'*; Editorial Board member for Nature Research journal *'Scientific Reports'*, Wiley journals *'IET Nanodielectrics'* & *'Journal of Polymer Science'*, Elsevier journals *'Current Opinion in Green and Sustainable Chemistry'* & *'Materials Today Sustainability'*; Editorial Advisory Board member for ACS journal *'Environmental Science & Technology Water'*, Royal Society of Chemistry journals *'Nanoscale Horizons'*, *'Reaction Chemistry & Engineering'* and *'Molecular Systems Design & Engineering'*.

Stimuli assisted energy storage: Going towards super-batteries

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Abstract:
Energy storage plays a critical role in meeting future energy demands. Particular sector of interest in the current scenario is improving urban transport which causes much distress to the environment through pollution. Electric vehicles with conventional lithium ion batteries are alternatives, but establishing the infrastructure and slow charging times coupled with limitations of charging cycles, forcing researchers to look for alternative technologies. Supercapacitors are one such alternative to try for. Supercapacitors have huge power density with practically unlimited cyclic stability, but lacks specific energy density. Researchers are designing systems to bring a reasonable balance between power density and energy density, namely super-batteries. Higher energy density in supercapacitors can be achieved by precisely designing systems by controlling Faradaic and non-Faradaic processes at the electrode/electrolyte interface. Our research approach has been dedicated in enhancing the specific capacitance under external stimuli through improvements in charge transfers and mass transport governed mainly by diffusion processes in the supercapacitor devices. We present here some of our preliminary results on the influence of external stimuli in designing super-batteries.

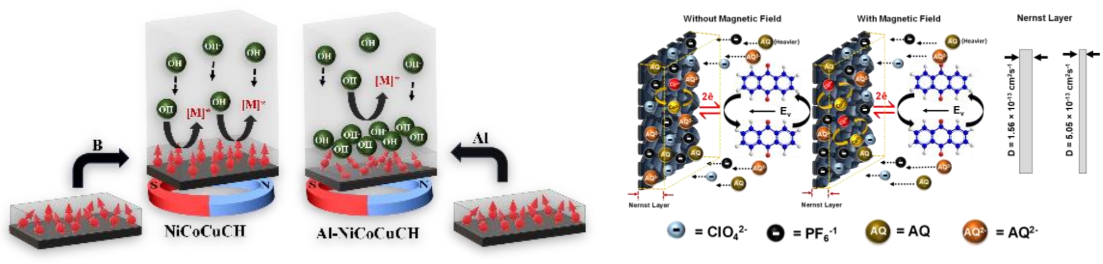

Figure 1: (Left) Mechanistic understanding of external magnetic field assisted supercapacitor; (Right) Flexible electrode under the influence of external magnetic field

References: (1) Peeyush Pandey, Mohammad Qureshi; ACS Appl. Mater. Interfaces; 15, 39435, 2023; (2) Peeyush Pandey, Mohammad Qureshi; ACS Appl. Mater. Interfaces; ACS Appl. Mater. Interfaces, 16, 44665, 2024

Bio-sketch

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Biosketch:

Mohammad Qureshi received his Ph.D. in 2005 from IIT Kanpur on "Design and development of white light emitting organic light emitting diodes,". After a postdoc position at Forshungzentrum, Juelich, Germany, he returned in 2008 to IIT Guwahati as an assistant professor. He is currently working as a Professor at the department of chemistry, IIT Guwahati. He is focused on a fundamental understanding of interfacial energy transfers to design efficient energy storage and generation systems. His recent interests are on developing supercapacitors by controlling diffusion and capacitive contributions through external stimuli such as magnetic field and light.

Representative Publications:

1. Peeyush Pandey, Anjana Singha, Sourav Bhowmick, Mohammad Qureshi *, **ACS Appl. Mater. Interfaces**, 16, 44665, 2024.
2. Anjana Sigha, Peeyush Pandey, Alpana Sahu, Mohammad Qureshi*, **J. Phys. Chem. Lett.** 15, 2123, 2024.
3. Peeyush Pandey, Sourav Bhowmick, Mohammad Qureshi*, **ACS Appl. Mater. Interfaces**, 15, 39435, 2023.
4. Sourav Bhowmick, Mohammad Qureshi*, **ACS Appl. Mater. Interfaces**, 15, 5466, 2023.
5. Ching Thian Moi, Alpana Sahu, Mohammad Qureshi* **ACS Appl. Mater. Interfaces**, 15, 5336, 2023.
6. Pronoy Dutta, Sujit Kumar Deb, Amalika Patra, Abhisek Majumdar, Golam Masud Karim, Chintak Kamalesh Parashar, Manoj Kumar Mohanta, Mohammad Qureshi, Uday Narayan Maiti, **Adv. Func. Mater**. 32 2204622 2022
7. Sourav Bhowmick, Arijeet Sarangi, Ching Thian Moi, Sudip Chakraborty and Mohammad Qureshi*, **ACS. Appl. Mater. Interfaces**, 14, 52204, 2022

Thin Films of Molecular Functional Materials: Possible Materials for Future Electronics

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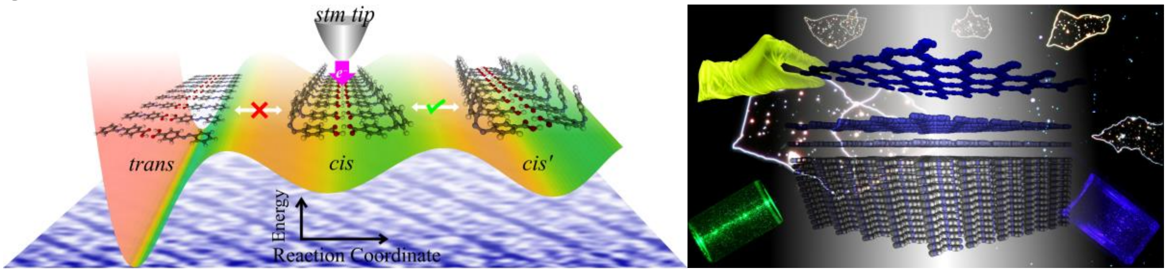
Abstract: Thin films of semiconducting molecules have increased a lot of attention in modern electronic devices. The library of molecules offers different electronic functionalities like switches, diodes, memories, wires etc. The unique self-assembling property of molecules is an added advantage in fabricating devices using well-ordered array of these electronic functionalities. In this talk I will discuss two major aspects of molecular materials on surfaces. a) The assembly and switching of different azobenzene (AB) derivatives on graphite surface. Using external triggers (photons and electrons), we demonstrate that the AB derivatives can be switched between two states namely trans and cis on surface. The switching efficiency can be controlled by various external factors. b) Two dimensional (2D) molecular materials with tuneable electronic properties. We use a combination of atomic force microscopy (AFM), scanning tunnelling microscopy (STM), tunnelling spectroscopy and density functional calculations to address the above examples.

Figure/Scheme:



References and Notes:

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2. Hariom Birla et al., *J. Phys. Chem. C* 2023, 127, 17039.
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4. Himani Malik et al., *J. Phys. Chem. Lett.* 2021, 12, 5463
5. Vipin Mishra et al., *ACS Appl. Mater. Interfaces*, 2020, 12, 51122.

Bio-sketch

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Biosketch:

Thiruvancheril G. Gopakumar completed his BSc (Chemistry) and MSc (Physical Chemistry) from Mahatma Gandhi University, Kerala in 1998 and 2001, respectively. After spending a year at National Chemical Laboratory, Pune, India, he moved to Germany for PhD. He completed his PhD in 2006 at Chemnitz University of Technology, Germany in experimental condensed matter physics and continued there as a post-doctoral fellow till 2008. Then he moved to Christian-Albrechts-University, Kiel, Germany and worked as research associate till 2013. In 2013 he joined Indian Institute of Technology, Kanpur, India as an Assistant Professor. Till 2023 he is Professor at Indian Institute of Technology, Kanpur, India.

His major research areas are molecular thin films, 2D molecular materials for electronic applications, electronic structure of molecular materials, condensed matter, surface science, scanning tunnelling microscopy and atomic force microscopy. So far, he has supervised six PhDs and mentored around 16 Master theses. He has around 55 research articles and two book chapter contributions. He was awarded the Young Research Fellowship of Ministry of Electronics and Information Technology and the excellence in teaching award by IIT Kanpur.

Representative Publications:

1. Diksha Srivastava et al., ACS Appl. Mater. Interfaces 2024, 16, 30485.
2. Hariom Birla et al., J. Phys. Chem. C 2023, 127, 17039.
3. Richa Arjariya et al., Nanoscale, 2023,15, 13393.
4. Khushboo Yadav et al., Appl. Surf. Sci., 2022, 612, 155747
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Low-dimensional Halide Perovskites for High-performance Photodetection

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$ Equal contribution

Abstract:

In the field of optoelectronics, halide perovskite semiconductors are driving significant advancements that could reshape next-generation technologies. Metal-halide perovskites, particularly when produced with minimal structural disorder, enhanced thermal resistance, and photostability, stand out as a disruptive material class. Among them, 2D perovskites with Ruddlesden-Popper (RP) and Dion-Jacobson (DJ) phases offer superior moisture and heat stability due to the hydrophobic alkyl ammonium spacers, which act as barriers between inorganic octahedral layers, forming quantum well-like structures. This poster will focus on our strategies for designing 2D and 0D halide perovskites and their application in visible light photodetection, demonstrating how electronic properties can be modulated based on the perovskite composition.[1,2]

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Professional Career	2006~2008	Postdoc, Bar-Ilan University, Israel
	2008~2010	Postdoc, Drexel Nanotechnology Institute, USA
	2010~2015	Assistant Professor, IISER Kolkata
	2015~2019	Associate Professor, IISER Kolkata
	2016~2020	Founder Chair, Centre for Adv. Funct. Mater., IISER Kolkata
	2019~present	Professor, IISER Kolkata
Research Interests	1. Photovoltaics and optoelectronics with hybrid perovskite; 2. Electrocatalysis; 3. Metal-air & photorechargeable batteries	
Awards & Recognitions *(last 5 years)*	Life Fellow, Indian Chemical Society Editorial Advisory Board Member, ACS Applied Energy Materials Editor, Indian Journal of Chemistry SERB-STAR Award CRSI Bronze Medal Editorial Advisory Board Member, Journal of Materials Chemistry A	

Abstracts & Bio-Sketches – Posters

FORCE-IICS 2024 Conference
October 3 – 6, 2024

@Uday Samudra Backwater Resort,
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Modulating Biocatalysis to Promote Antioxidant Response

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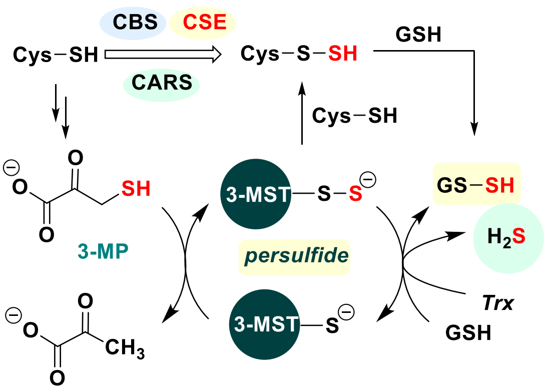
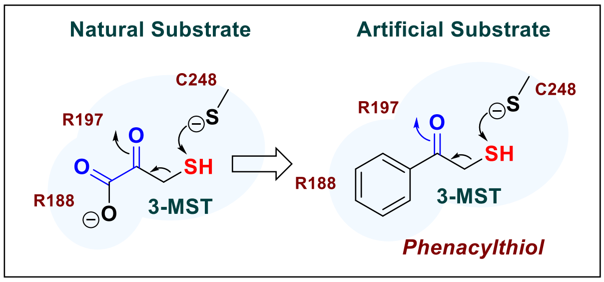
Abstract: Hydrogen sulfide (H_2S), persulfides (RS-SH), and related sulfur species are produced in nearly all cells and have diverse roles including as antioxidants.[1] Cysteine is the primary source of such sulfur species in cells, and enzymes that generate H_2S include cystathionine β-synthase (CBS), cystathionine γ-lyase (CSE), cysteinyl-tRNA synthetase (CARS) as well as 3-mercaptopyruvate sulfurtransferase (3-MST).[2] In an attempt to promote endogenous antioxidant response, our lab designed and developed artificial substrates for 3-MST, an enzyme whose natural substrate is 3-mercaptopyruvate (3-MP), and produces a persulfide, which is cleaved by thioredoxin (Trx) to generate H_2S. The first generation of artificial substrates showed excellent antioxidant and anti-inflammatory properties in both cellular and animal models.[3] Using a computational structure-guided approach, we designed and developed a new series of artificial substrates for 3-MST. These compounds were found to enhance endogenous persulfides, and protect cells from oxidative stress-induced cell death. Together, we provide evidence that underscores a new therapeutic paradigm of using small molecules to promote cells' own antioxidant response.





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2. Pedre, B.; Talwar, D.; Barayeu, U.; Schilling, D.; Luzarowski, M.; Sokolowski, M.; Glatt, S.; Dick, T. P. *Nat. Chem. Biol.* **2023**, *19* (4), 507–517.
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Bio-sketch

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Harinath Chakrapani completed his undergraduate and post-graduate studies in Chemistry from Loyola College (1994-97) and Indian Institute of Technology Madras (1997-99), respectively. In the fall of 1999, he moved to Duke University, USA to pursue his doctoral studies, which he completed in Dec. 2005. After a brief stint as a postdoctoral research associate at Wake Forest University, USA, he moved to the Center for Cancer Research, National Cancer Institute USA as a Visiting Fellow in Aug 2006. He joined Indian Institute of Science Education and Research Pune in July 2009 and is currently Professor. His primary research interests are in the area of physical and mechanistic organic chemistry, with applications in understanding biological responses to stress, circumventing mechanisms of antimicrobial resistance, and prodrug design and delivery.

Recent Publications

1. Manna, S.; Agrawal, R.; Yadav, T. Anand Kumar, T.; Kumari, P. Dalai, A.; Kanade, S. Balasubramanian, N. Singh, A.; **Chakrapani, H.** "Orthogonal Persulfide Generation through Precision Tools Provides Insights into Mitochondrial Sulfane Sulfur" *Angewandte Chemie International Edition* **2024**, in press https://doi.org/10.1002/anie.202411133
2. Chaudhary, B.S.; Anand Kumar, T.; Vashishta, A.; Tejasri, S.; Kumar, A. S.; Agarwal, R.; **Chakrapani, H.** "An Esterase-Cleavable Persulfide Donor with No Electrophilic Byproducts and a Fluorescence Reporter" *Chemical Communications*, **2024**, 60, 1727-1730.
3. Sawase, L.; Anand Kumar, T.; Mathew, A. B.; Khodade, V. S.; Toscano, J. P.; Saini, D. K.; **Chakrapani, H "**β-Galactosidase-activated nitroxyl (HNO) donors provide insights into redox cross-talk in senescent cells" *Chemical Communications*, **2023**, *59*, 12751-12754.
4. Sawase, L.; Jishnu, C.V.; Manna, S..; **Chakrapani, H.** "A modular scaffold for triggerable and tunable nitroxyl (HNO) generation with a fluorescence reporter" *Chemical Communications*, **2023**, *59*, 3415-3418.
5. Bora, P.; Sathian, M.B.; **Chakrapani, H.** "Enhancing Cellular Sulfane Sulfur Through β-glycosidase-Activated Persulfide Donors: Mechanistic Insights and Oxidative Stress Mitigation" *Chemical Communications*, **2022**, *58*, 2987–2990.
6. Bora, P.; Manna, S.; Nair, M.; Sathe, R.M.S.; Singh, S.; Adury, V.S.S.; Gupta, K.; Mukherjee, A.; Saini, D. K.; Kamat, S.S.; Hazra, A. B.; **Chakrapani, H.** "Leveraging an Enzyme/ Artificial Substrate System to Enhance Cellular Persulfides and Mitigate Neuroinflammation" *Chemical Science*, **2021**, *12*, 12939-12949.

Integrated omics approaches for the identification of short polypeptides in plants: A case study

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Microproteins with molecular weight less than 10 kDa have been gaining attention over the past few years as important regulatory molecules in all three domains of life, namely, microbes, plants and animals. Low molecular weight polypeptides are involved in the regulation of diverse physiological, morphological, and defense-related processes in plants.[1] Due to their transient existence, intermediate size, and polar nature, they are not often identified in a typical phytochemical analysis. At the transcript level, they are encoded by short open reading frames (sORF) and are usually excluded in conventional transcriptome analysis, for the fear of leading to false-positives. Recently, considerable advance has been made in the identification sORF from RNA-seq data, and many sORF that could translate to microproteins are being predicted. Ribosome profiling offers more accurate prediction of sORF that have protein coding potential.[2] Proteo-genomics that includes a combination of proteomics, transcriptomics, and ribosome profiling techniques, are the currently followed procedures for the identification and characterization of microproteins in genomes. [3, 4]

In plants, sORF-encoded microproteins have been identified both at transcriptome level and proteome level only for a few model plants such as *A. thaliana*, *Maize* etc. [4,5] In CSIR-CIMAP, we are exploring short polypeptides from Medicinal and Aromatic Plants (MAPs) by combining information derived from transcriptomic and proteomics studies on semi-purified plant extracts. The poster will focus on the medicinal plant, *Rauvolfia serpentina*.

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3. Wu, H., Song, G., Walley, J., and Hsu, P. The Tomato Translational Landscape Revealed by Transcriptome Assembly and Ribosome Profiling. *Plant Phys.* 2019, 181(1), 367–380.

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5. Wang, P., Yao, S., Kosami, K., Guo, T., Li, J., Zhang, Y., Fukao, Y., Kaneko-Kawano, T., Zhang, H., She, Y., Wang, P., Xing, W., Hanada, K., Liu, R., and Kawano, Y. Identification of endogenous small peptides involved in rice immunity through transcriptomics- and proteomics-based screening. *Plant Biotech. J.* 2020, 18(2), 415–428.

Bio-sketch

Profile

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Employment and Education

- **Employment** 2023 – till now: Senior Principal Scientist, CSIR-CIMAP, Lucknow
  2018– 2023: Principal Scientist, CSIR-CIMAP, Lucknow
  2013 – 2018: Senior Scientist, CSIR-CIMAP, Lucknow
  2011 – 2013: Scientist Fellow, CSIR-CIMAP, Lucknow
  2010 - 2011 Research Associate, Molecular Biophysics Unit, Indian Institute of Science, Bangalore. (Mentor: Prof. P. Balaram)
  2009: Guest Researcher, Department of Biochemistry and Organic Chemistry, Uppsala University, Sweden. (Mentor: Prof Lars Baltzer)

- **Ph. D.** 2009; Department of Physics, Indian Institute of Science, Bangalore.
  Topic: X-Ray Crystallographic Studies of Designed Peptides.
  (Research Supervisor: Prof. N. Shamala)
- **M. Sc.** 2001; School of Chemical Sciences, Mahatma Gandhi University. (Organic Chemistry)
- **B. Sc.** 1998; University of Kerala. (Chemistry)

- **Current Research Interests:**
  - Polypeptides from medicinal plants
  - Structural Biology of plant proteins
  - Crystallographic studies of peptides containing modified non-natural amino acids

Bio-sketch

- Number of publications: 49 (https://scholar.google.com/citations?hl=en&user=JM1bQ94AAAAJ)

Representative Publications:

1. Thakur, S., Vasudev, P.G. In silico characterization of a MYB TF (WsMYB46) from the medicinal plant *Withania somnifera* L. predicting its probable role in secondary cell wall biosynthesis. *Genet Resour Crop Evol* (2024). DOI: 10.1007/s10722-024-01951-2
2. Verma, M., Sarfraz, A., Hasan, I., Vasudev, P. G., Khan, F. Structure-Activity Relationship studies on VEGFR2 tyrosine kinase inhibitors for identification of potential natural anticancer compounds. *Medicinal Chemistry* (2024), DOI: 10.2174/0115734064247526231129080415
3. Verma, M., Trivedi, L., Vasudev, P. G. Interaction Patterns of Pyrazolopyrimidines with receptor proteins. *J. Chem. Ed. Model.* (2023) 63 (8), 2331-2344. DOI: 10.1021/acs.jcim.2c01315.
4. Debnath, S., Kumar, D., Vasudev, P. G., Chatterjee, S. Helices in Peptides Containing Differentially Geminally Di-substituted γ Amino Acid Residues. *ChemistrySelect* (2022) 8:25, e202301352. DOI: 10.1002/slct.202301352.
5. Yadav, S.K., Archana, Singh, R. Insecticidal fern protein Tma12 is possibly a lytic polysaccharide monooxygenase. *Planta* (2019) 249, 1987–1996.

A helium nanodroplet spectrometer to study molecular aggregation at ultracold temperatures

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Abstract: Helium droplets are clusters of helium atoms formed by the supersonic expansion of precooled helium gas (at temperatures of 4–25 K and backing pressures of 10–80 bar) through a 5-micron diameter nozzle.[1-2] These droplets achieve an equilibrium temperature of approximately 0.4 K and exist in a superfluid state. Molecules of interest can be easily embedded within the droplets, allowing the study of molecular aggregation using mass spectrometry and infrared spectroscopy.[1-4] Due to the weak interaction between the doped molecules and the helium droplets, the resulting infrared spectra closely resemble gas-phase spectra, providing valuable insights into isolated molecular behaviour.

We have recently constructed a helium nanodroplet spectrometer in our laboratory at IIT Kanpur. In this presentation, I will demonstrate the performance of the spectrometer by showcasing our results from the mass-spectrometric analysis of acetonitrile clusters. Additionally, I will discuss our plans to integrate the spectrometer with a high-resolution infrared laser, which will enable us to perform mass-selective infrared spectroscopy of molecular processes relevant to fundamental and interstellar chemistry.

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2. Yang, S.; Ellis, A. M. *Helium Droplets: A Chemistry Perspective.* Chem. Soc. Rev. 2013, 42 (2), 472–484.
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4. Mani, D.; De Tudela, R. P.; Schwan, R.; Pal, N.; Körning, S.; Forbert, H.; Redlich, B.; Van Der Meer, A. F. G.; Schwaab, G.; Marx, D.; Havenith, M. *Acid Solvation versus Dissociation at "Stardust Conditions": Reaction Sequence Matters.* Sci. Adv. 2019, 5 (6).

Bio-sketch

Profile

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Institution: Department of Chemistry, IIT Kanpur.

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Biosketch: Devendra Mani earned his Ph.D. in 2014 from the Indian Institute of Science (IISc) Bangalore, specializing in microwave spectroscopy of weakly bound molecular clusters. He then pursued postdoctoral research at Ruhr University Bochum, Germany, where he focused on infrared spectroscopy in helium nanodroplets. In 2020, he joined the Department of Chemistry at IIT Kanpur as an assistant professor, where he is currently working. His research group has built the first helium nanodroplets spectrometer in India. His research interests span high-resolution gas-phase spectroscopy, particularly emphasizing the use of helium nanodroplets to investigate molecular aggregation and chemical reactions at ultracold temperatures.

Representative Publications:

1. R. Gupta, S. Singha and D. Mani, Cooperativity between Intermolecular Hydrogen and Carbon Bonds in ZY···CH_3CN/CH_3NC···HX Trimers (ZY = H_2O, H_2S, HF, HCl, HBr, NH_3, and H_2CO; HX = HF, HCl, and HBr), J. Phys. Chem. A, 128, 4605-4622 (2024).

2. D. Mani, T. K. Roy, J. Khatri, G. Schwaab, S. Blach, C. Hölzl, H. Forbert, D. Marx, M. Havenith, Internal Electric Field-Induced Formation of Exotic Linear-Acetonitrile Chains, J. Phys. Chem. Lett. 13 (29), 6852–6858 (2022).

3. G. Schwaab, R.P. de Tudela, D. Mani, N. Pal, T. K. Roy, F. Gabas, R. Conte, L. D. Caballero, M. Ceotto, D. Marx, M. Havenith, Zwitter Ionization of Glycine at Outer Space Conditions due to Microhydration by Six Water Molecules, Phys. Rev. Lett. 128, 033001 (2022).

4. D. Mani, R.P. de Tudela, R. Schwan, N. Pal, S. Körning, H. Forbert, B. Redlich, A. F. G. van der Meer, G. Schwaab, D. Marx, M. Havenith, Acid solvation versus dissociation at "stardust conditions": Reaction sequence matters!, Science Advances, 5 (6): eaav8179 (2019).

Transforming Energetic Materials: Advancements in Tailored Green High-Energy Density Materials for Enhanced Performance

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Indian Institute of Technology, Kanpur, UP-208016
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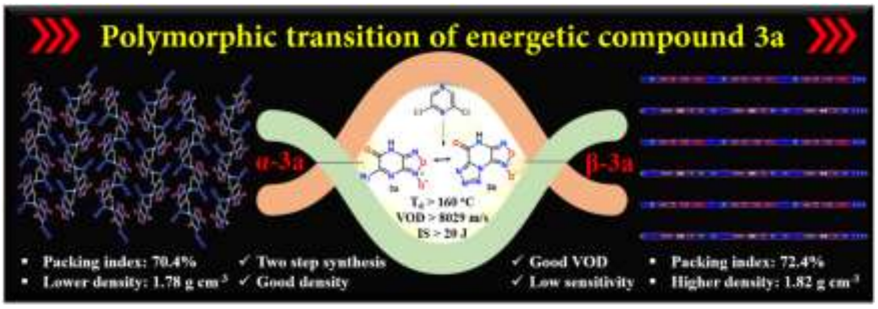
Abstract:
The evolution of energetic materials underscores the persistent challenge of synthesizing and developing green high-energy density materials and oxidizers. This presentation delves into the historical context of established explosives, including ammonium nitrate (AN), pentaerythritol tetranitrate (PETN), trinitrotoluene (TNT), and hexahydro-1,3,5-trinitro-1,3,5-triazine (RDX). It addresses their impact on the field and the safety and environmental sustainability challenges they present. Recent advancements in the synthesis of novel green high-energy density materials are introduced, highlighting compounds designed to overcome the limitations of traditional explosives. These innovative materials aim to offer enhanced performance while mitigating environmental impact. A comparative analysis of the energetic properties of these new compounds against established explosives such as TNT, RDX, HMX, FOX-7, and CL-20 will be presented. This overview provides insight into the current state and future directions of the field of energetic materials.

Figure:



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1. *Organic letters*, **2024**, *28*, 6006-6011
2. *Organic letters*, **2024**, *26*, 4788-4792
3. *Chemical Communications*, **2024**, *60*, 1646-1649
4. *ACS Applied Materials & Interfaces*, **2024**, *16*, 20670-20680
5. *Chemical communications*. **2023**, *59*, 4324-4327
6. *Journal of Materials Chemistry A*, **2022,** *10*, 22803-22811
7. *Journal of Materials Chemistry A*, **2022,** *10*, 12702-12712
8. *ACS Applied Materials & Interfaces*, **2022**, *14*, 49898-49908

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Experience:

1. Indian Institute of technology, Kanpur, India 2019-till
Assistant professor, Department of Chemistry

2. McMaster University, Hamilton, Canada
Postdoctoral fellow in the group of Prof. Jakob Magolan, **2017-2009**

3. University of Idaho, Moscow, USA-Department of Chemistry
Postdoctoral fellow in the group of Prof. J. M. Shreeve, **2015-2017**

4. University of Hyderabad, Hyderabad, India - School of Chemistry
Postdoctoral fellow in the group of Dr. K. Muralidharan, **2015**

Education:

1. **University of Hyderabad, Hyderabad, India - ACRHEM**
Ph.D. (Heterocyclic/Energetic Materials Chemistry), **August 2010–December 2014**, University of Hyderabad, Hyderabad, India. **"*Design and Synthesis of Nitrogen-rich Heterocyclic Compounds and Salts as Energetic Materials*"**

2. M.Sc. (Organic Chemistry), **2007-2009**, Osmania University, Hyderabad, India.

3. B.Sc. (Chemistry, Botany and Zoology), **2003-2006**, Osmania University, Hyderabad, India.

Construction of Five-membered Heterocycles through Electrosynthesis

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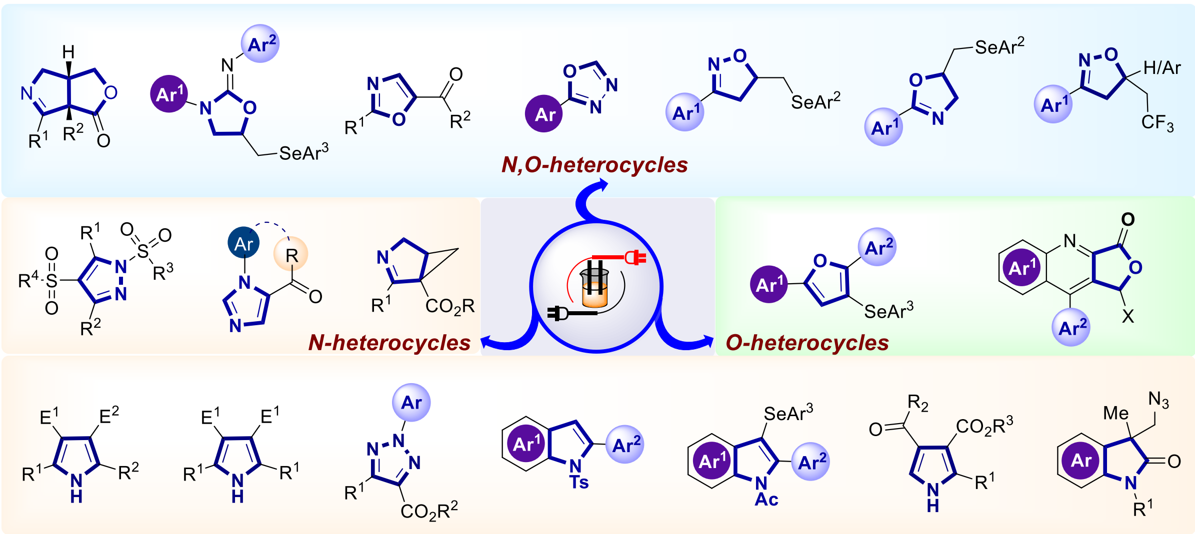
Abstract: Five-membered heterocycles have been recognized as one of the prime candidates for pharmaceutical industries due to their omnipresence in numerous biologically relevant natural products and drug molecules.[1] Among the FDA-approved medications, 39% of the pharmacological compounds are nitrogen-containing five-membered heterocycles in which 62% of molecules are aromatic and the remaining 38% are non-aromatic ring systems.[2] In this premise, electro-organic synthesis has emerged as a cutting-edge alternative to fabricate complex molecular architectures by constructing a diverse array of C–C and C–het bonds by employing electrons as redox elements.[3] During the last five years, our group has contributed significantly in the field of organic electrosynthesis by developing unique synthetic routes to obtain different aromatic and alicyclic heterocyclic frameworks.[4] Depending upon the heteroatom present in the core ring structure, the synthesized manifolds are categorized into three sections: a) *N*-heterocycles, b) *O*-heterocycles and c) *N*,*O*-heterocycles. Implementation of these electrosynthetic protocols offered additional benefits in terms of chemo- and regioselectivity, cost-effectivity and reduced waste generation compared to the established traditional reagent-based methodologies.



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2. Vitaku, E.; Smith, D. T.; Njardars, J. T. *J. Med. Chem.* **2014**, *57*, 10257−10274.
3. Yan, M.; Kawamata, Y.; Baran, P. S. *Chem. Rev.* **2017**, *117*, 13230−13319.
4. De Sarkar *et al.* https://www.redoxlab.in

Bio-sketch

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Suman De Sarkar received B.Sc. (2005) and M.Sc. (2007) degrees in Chemistry from University of Calcutta and IIT Kanpur, respectively. He obtained his Ph.D. in November 2010 from University of Muenster under the supervision of Prof. Armido Studer. Afterward, he worked as a postdoctoral researcher in the research group of Prof. Karl Gademann at the University of Basel (2011-2013) and with Prof. Lutz Ackermann as an Alexander von Humboldt Postdoctoral Fellow at the University of Goettingen (2013-2015). In October 2015 he joined IISER Kolkata, as an Assistant Professor and in September 2019 was promoted to the post of Associate Professor. His research interests are the application of redox-mediated transformations in organic synthesis with a special focus on electrochemistry and photocatalysis.

Selected Publications:

1. T. Mandal, S. Mallick, M. Islam, **S. De Sarkar***, *ACS Catal.* **2024**, *14*, 13451.
2. S. K. Saha, S. Mallick, A. Nath, **S. De Sarkar***, *Org. Lett.* **2024**, *26*, 7330.
3. M. Baidya, D. Maiti, L. Roy*, **S. De Sarkar***, *Angew. Chem., Int. Ed.* **2022**, *61*, e202111679.
4. D. Maiti, K. Mahanty, **S. De Sarkar***, *Org. Lett.* **2021**, *23*, 1742.
5. **S. De Sarkar***, *Angew. Chem., Int. Ed.* **2016**, *55*, 10558.

Awards/Achievements:

- CRSI Bronze Medal **2025** (Announced)
- Editorial Board member of Tetrahedron & Tetrahedron Letters **2024**
- Member of the Early Career Advisory Board of Asian Journal of Organic Chemistry
- Thieme Chemistry Journals Award 2023
- Fellow of the Indian Chemical Society
- DSM Science & Technology Award, Netherlands (**2011**)
- D. C. Mukherjee Gold Medal award (**2005**)

Guide RNA engineering of CRISPR-Cas9 for improved gene editing

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Abstract:

CRISPR/Cas9 is a binary system that has an effector Cas9 nuclease and a single guide RNA (sgRNA) that together forms a ribonucleoprotein complex and carry out double strand cleavage of its DNA target. Though the system is very precise and easy to manipulate, it has its own challenges such as sgRNA stability, less access to certain region of chromosomes, off-targeting effects and delivery. All of these mentioned challenges reduces the efficiency and limits its use. To overcome these challenges, modifications are focused on either Cas9 protein or sgRNA or both. Herein, we showed that the incorporation of an RNA secondary structural element, a three way junction (3WJ), at different positions of sgRNA increased the cleavage efficiency of CRISPR-Cas9 system with better cellular stability. The RNA 3WJ motif utilized was a part of packaging RNA of Phi29 bacteriophage DNA packaging motor, and has been used as a basic structural motif in RNA nanotechnology for constructions of various 2D and 3D RNA nanostructures for their use in therapy. The RNA 3WJ motif also shows exceptional thermal stability and chemical stability in serum. We showed here that by introducing 3WJ core sequence at different sgRNA loops will significantly improve sgRNA stability, and thus enhances cleavage efficiency in addition to the cellular stability of CRISPR-Cas9 system.

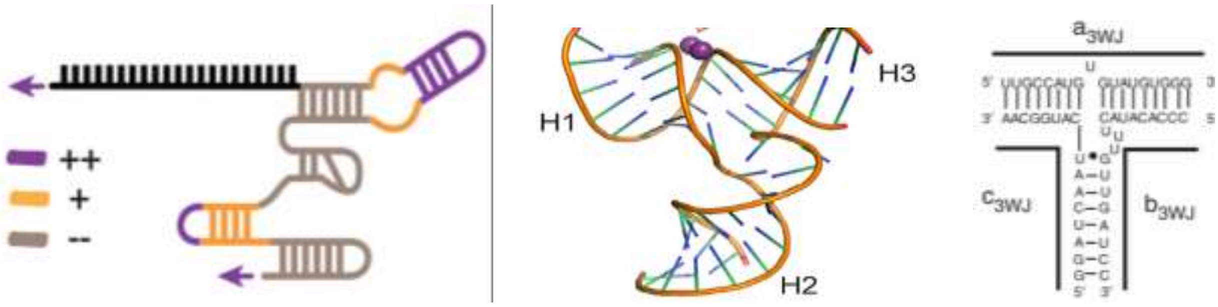

Figure: Schematic showing sgRNA regions where modifications can be tolerated, and crystal structure and secondary structure of phi29 3WJ.

Reference:

1. Allen D, Rosenberg M and Hendel A (2021) Using Synthetically Engineered Guide RNAs to Enhance CRISPR Genome Editing Systems in Mammalian Cells. *Front. Genome Ed.* 2:617910.

Bio-sketch

Profile

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Dr. Ashwani Sharma completed his PhD in 2011 from National Chemical Laboratory (NCL), Pune. He did his post-doctoral studies from University of Utah and Markey Cancer Centre, University of Kentucky, USA from 2011–2015. After coming back to India, he joined as DST young scientist in Indian Institute of Chemical Technology (IICT), Hyderabad for a short span of one year. He joined IISER Tirupati as an Assistant Professor in 2017 and promoted to Associate Professor in 2023. His area of interest is RNA biology. His lab work on RNA nanotechnology for targeted drug delivery, developing RNA aptamers, ribozymes and utilizing them in the detection of small molecules as well as macromolecules, RNA engineering for efficient gene editing, and to understand the role of various non-coding RNAs in the cell.

Representative Publications:

1. Soni, R.; Krishna, A. M.; More, S. H.; Sharma, A. Reversible modulation of aptamer-ligand binding in RNA light-up aptamers containing G-quadruplex using chemical stimuli. *Chembiochem* **2023**, *24*, e202200574

2. Soni, R.; Sharma, D.; Krishna, A. M.; Sathiri, J.; Sharma, A. Highly efficient Baby Spinach-based minimal modified sensor (BSMS) for nucleic acid analysis. *Org. Biomol. Chem.* **2019**, *17*, 7222

Enantioselective Cu(BINAP)-Catalyzed Hydrocupration

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Abstract: Enantiomerically enriched complex alcohols are presented in wide range of small molecule therapeutics and biologically active natural polyketides. Therefore, exploring the general methods for the enantioselective synthesis of substituted alcohols is an attractive target in organic synthesis. Here, we have developed the Cu(I)-catalyzed enantioselective hydrocupration[1-2] for the synthesis of complex 1,2-*syn-sec,tert*-diols, α-hydroxy allyl ketones and propargyl alcohols using reductive coupling of carbon-carbon π-bonds with carbonyl compounds

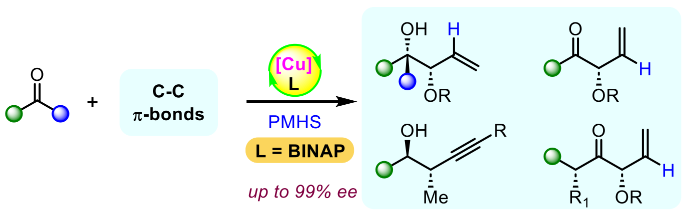

Figure 1. Enantioselective hydrocupration to access chiral alcohols

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Bio-sketch

Profile

Dr. Rambabu Chegondi

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Rambabu Chegondi received his M.Sc. (2003) degree from University of Hyderabad and completed Ph.D. (2009) in Organic Synthesis from Indian Institute of Chemical Technology (CSIR-IICT), Hyderabad under the supervision of Dr. S. Chandrasekhar. In 2009, he moved to The University of Kansas, USA to work with Prof. Paul R. Hanson as a postdoctoral researcher. He joined CSIR-IICT, Hyderabad as CSIR-Pool-Scientist (SRA) in 2014 as an independent researcher. He is currently a Principal Scientist at the OS&PC department, CSIR-IICT, focusing on the development of new enantioselective desymmetrization methodologies and new process development of key APIs. He has received the Eli Lilly Asia Best Thesis Award 2009, AVRA-Young Scientist Award-2019, Thieme Chemistry Journals Award, and SERB-STAR Award. He is an FRSC and currently an Editorial Advisory Board Member of Organic Letters.

Representative Publications:

1. 1. Jadhav, S. B.; Dash, S. R.; Maurya, S.; Nanubolu, J. B.; Vanka, K.; Chegondi, R. *Nat. Commun.* **2022**, *13*, 854.
2. 2. Gollapelli, K. K.; Patil, V. B.; Vinaykumar, A.; Chegondi, R. *Chem. Sci.* **2021**, *12*, 1544.
3. 3. Thopate, S.B.; Jadhav, S.B.; Nanubolu, J. B.; Chegondi, R. *ACS Catal.* **2019**, *9*, 10012.
4. 4. Gollapelli, K. K.; Donikela, S.; Manjula, N.; Chegondi, R. *ACS Catal.* **2018**, *8*, 1440.
5. 5. Gollapelli, K. K.; Kallepu, S.; Govindappa, N.; Nanubolu, J. B.; Chegondi, R. *Chem. Sci.* **2016**, *7*, 4748.

Title: A Versatile Step-Growth Polymerization Route to Enzymatically Degradable Functional Polyesters and Their Biomedical Implications

Name: Dr. Anindita Das
Institution: Indian Association for the Cultivation of Science (IACS), Kolkata, India
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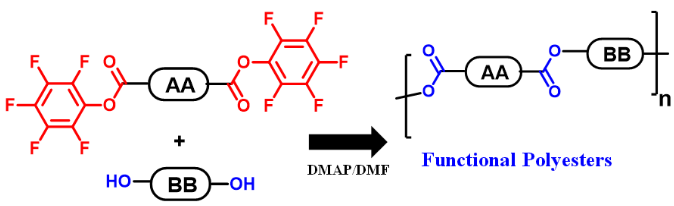
Abstract: Our work describes a versatile and efficient step-growth polymerization route to functional aliphatic polyesters through an organo-catalyzed transesterification reaction between an activated pentafluorophenyl-diester of adipic acid (AA) and various structurally different diols (BB) (Scheme 1).[1] The use of an activated diester enables us to obtain a near quantitative reaction under mild conditions with no requirement of by-product (pentafluorophenol) removal, which remains a major drawback in the conventional polyester synthesis with non-activated diesters. Enzymatic degradation of the resultant polyesters has been demonstrated, which can be tuned by playing with the hydrophobicity of the polyester backbone. Following the same synthetic strategy, water dispersible amphiphilic, cationic polyesters with pendant naphthalene monoimide (NMI) derivatives were prepared by pre-quaternization of the fluorescent monomers with different alkyl chain ends in order to design polyesters with positively charged hydrophobic pendant moieties. These amphiphilic polyesters produced fluorescent nanoparticles in water, which exhibit broad-spectrum antibiotic properties against both gram-positive and gram-negative bacteria depending upon the nature of the cationic side chains.[2] The intrinsic fluorescent nature of the nanoparticles enabled us to study their interactions with bacterial cells by fluorescence live-dead assay, which provided us insights of bacterial disruption by membrane perturbation similar to the mechanism followed by host defense peptides. The facile synthetic methodology enables us to investigate systematic structure-activity relationships in such rarely reported dye-conjugated polyester backbones, which suggests the dual role of the aliphatic chain and the aromatic dyes in conferring biocidal activity, selectively against the bacterial cells. Some of these cationic polyesters exhibit remarkably high cellular uptake by the endocytic pathway and mitochondrial targeting ability following lysosomal escape.[3] Further, this methodology enables us to design and prepare biotin-functionalized polyesters that exhibit selective uptake in cancer cells, thus showing their potential for targeted drug delivery applications. This presentation will showcase multiple aspects of our newly established synthetic methodology for functional polyesters and their biomedical implications.



Scheme 1. Synthetic scheme for functional polyesters from activated pentafluorophenyl ester of adipic acid and structurally different diols.

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1. S. Biswas, A. Das, *Chem. Eur. J.* **2023**, 29, e202203849
2. S. Biswas, R. Barman, M. Biswas, A. Banerjee, A. Das, *Polym. Chem.* **2024**, 15, 2753
3. S. Biswas, P. Rajdev, A. Banerjee, A. Das (manuscript under preparation)

Bio-sketch

Profile

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Biosketch: 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, The Netherlands (2016–2017). She started her independent research career at the IACS in 2017. Her research interests include supramolecular polymerization of functional π-systems and macromolecules by directional non-covalent interactions, crystallization-driven macromolecular assemblies, and functional degradable polymers.

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).

Representative Publications:

1) Chakraborty, C.; Rajak, A.; Das, A. *Nanoscale* **2024**, *16*, 13019-13028
2) Biswas, S.;ǂ Barman, R.;ǂ Biswas, M.; Banerjee, A.; Das, A. *Polym. Chem.* **2024,** *15*, 2753-2762 (ǂ equal contribution)
3) Khanra, P.; Rajdev, P.; Das, A. *Angew. Chem. Int. Ed.* **2024**, *63*, *e20240048* (VIP)
4) Rajak, A.; Das, A. *Angew. Chem. Int. Ed.* **2023**, *62*, e202314290
5) Khanra, P.; Singh, A. K.; Roy, L; Das, A. *J. Am. Chem. Soc.* **2023**, *145*, 5270

6) Biswas, S.; Das, A. *Chem. Eur. J*. **2023**. *29*, e202203849
7) Rajak, A.; Das, A. *Angew. Chem. Int. Ed.* **2022**, *61*, e202116572 (Hot Paper)
8) Jamadar, A; Singh, A. K.; Roy, L*; Das, A. *J. Mater. Chem. C* **2021**, *9*, 11893

7-Azaspiro [3, 5]-nonane Substituted Aurones: Selective towards Gram-negative Bacteria

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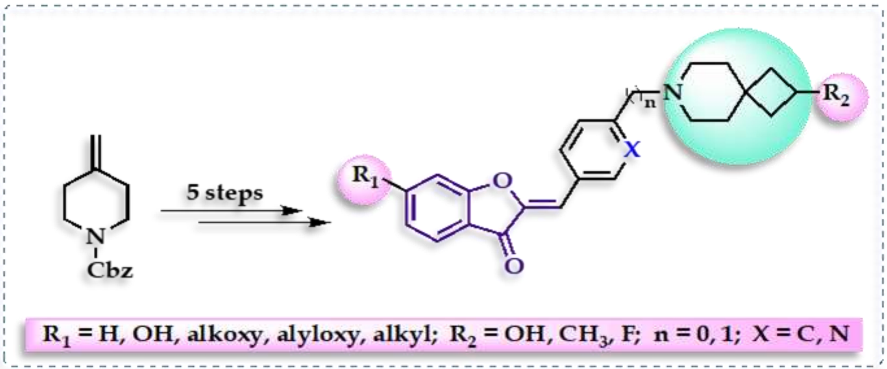
Abstract: Aurones are naturally occurring structural isomers of flavones that have diverse bioactivities including antimicrobial, anti-inflammatory, antitumor, antimalarial, antioxidant and neuropharmacological activities. Herein we report the design, synthesis and evaluation of novel 7-azaspiro [3, 5]-nonane substituted aurones for antibacterial activity against Gram-positive and Gram-negative bacteria. Preliminary antibacterial susceptible testing results indicate that these novel aurones demonstrate promising selectivity towards Gram-negative *vs* Gram-positive bacteria and have a potential to be optimized further for potent Gram-negative activity.



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4. Hasanpour, A.H *et al. Antimicrob. Resist. Infect. Control*. **2023**, 12. DOI: 10.1186/s13756-023-01210-6
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6. Zheng, Y. *et al.*, *Bioorg. Med. Chem. Lett*. 2014, 24: 3673-82. DOI: 10.1016/j.bmcl.2014.06.081

Bio-sketch

Profile

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Biosketch: Prof. Summon Koul completed her Masters degree in Organic Chemistry (1998) from University of Kashmir and PhD from University of Jammu (2003). During her PhD, she worked extensively on the "Isolation, Characterization and semisynthetic conversions of biologically active Natural Products". She worked as Research Associate in Indian Institute of Science, Bengaluru followed by Post-Doctoral Fellow in Simon Fraser University, British Columbia, Canada where she worked on total synthesis of Triquinacenes. She worked in Advinus Therapeutics – A TATA Enterprise as a drug discovery Scientist and leader for more than 13 years. She worked as a program leader on in-house and collaborative drug discovery research projects with reputed multinational pharma companies like Merck, USA; Johnson and Johnson, USA and Takeda, Japan. In the role of program leader, she has handled multi-crore projects and has been recognized twice for Best Scientist Awards in the Company for achieving milestones before stipulated timelines. She has worked in the fields of Cardiovascular Diseases, Metabolic disorders and Inflammation. During this span, she has also led CRO discovery projects in Eurofins Advinus (Advinus Therapeutics was acquired by Eurofins Ltd. in 2017) in collaboration with companies like Medicines for Malaria Venture (MMV), Switzerland; Astellas Pharma, Japan; Nostrum Biodiscovery, Barcelona, Spain; and Foundation of Neglected Disease Research (FNDR), Bengaluru, India. Summon has about 20 publications in international journals of repute, 1 book chapter, 7 US and 1 Indian patents to her credit. She has guided several summer trainee students in the company for their MS dissertations and advised employees working for the external PhD programs. She is currently guiding 4 PhD students in the new academic role in the University and has recently received SERB-SURE Grant as a Principal Investigator.

Representative Publications:

1. Summon Koul* *et al*. Design and synthesis of novel, potent and selective hypoxanthine analogs as adenosine A_1 receptor antagonists and their biological evaluation. *Bioorg. Med. Chem*. **2017**, *25*, 1963
2. Summon Koul* *et al*. Stereo-controlled total syntheses of ieodomycins A and B using D-glucose based chiral pool approach. *Tetrahedron Lett*. **2013**, *54*, 2489.
3. Summon Koul* *et al*. Design and synthesis of novel spirocyclic carboxylic acids as potent and orally bioavailable DGAT1 inhibitors and their biological evaluation. *Bioorg. Med. Chem. Lett*., **2022**, *62*, 128632.
4. Ashish Patil and Summon Koul* Role of Biosynthesis and Catabolism of Neurotransmitters in Drug Discovery for Anxiety and Depression. *Curr. Pharm. Des*. **2024**. DOI: 10.2174/011381612830991324070409533

Naphthalene-Derived Hyperbranched Polymeric Aggregates for Monitoring Azoreductage Activity Under Hypoxic Conditions

Narayan Das and Raja Shunmugam*
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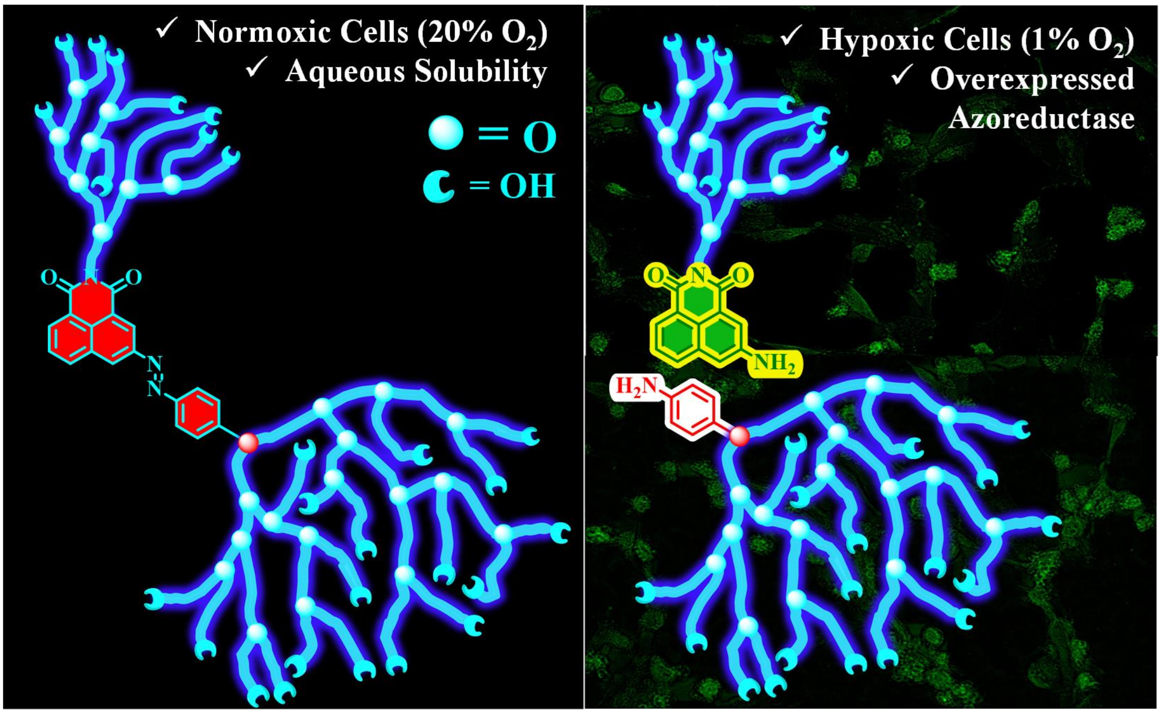
Abstract: The design and synthesis of macromolecules by introducing controlled branching via hyperbranch polymerization gained recent attention from the scientific community due to its diverse application in the biomedical field, from diagnosis to drug delivery.[1] This article emphasizes the development of a naphthalene-derived, self-assemble hyperbranch polymer (**PNapAzo**) in an aqueous medium where the azo bond works as a stimuli-responsive function in the presence of an overexpressed enzyme in hypoxic microenvironment. Here, the monomer is completely water-insoluble. On the other hand, our polymer is completely soluble in an aqueous medium due to rich hydrophobicity on both sides of the monomer. Due to the compound's amphiphilic nature and extensive hydrogen bonding, it shows excellent twisted-rod-like morphological architecture, increasing the concentration of the polymer from below CAC to above CAC. It is well documented that the azo bond reduced very easily in the presence of azoreductase enzyme, which is beautifully explained by our polymer.[2] Initially, our polymer remains nonfluorescent in the absence of azoreductage. On the other hand, in the presence of azoreductage extracted from E. coli bacterial cells, our polymer shows intense green fluorescence at 550 nm in a hypoxic microenvironment. The same phenomenon was also proved by sodium dithionite (mimic of azoreductase) for both monomer and polymer with the help of mass spectrometry and gel permeable chromatography. It is also established that our polymer can monitor the level of azoreductage selectively in hypoxic cell lines over normoxic cell lines.



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2. Zhu C.; Zou Z.; Huang C.; Zeng J.; Liu N.; Li J.; Yang R.; Chem. Commun., **2019**, 55, 3235-3238.

Raja Shunmugam

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Raja Shunmugam *received his bachelor's degree in 1994, and a master's degree in 1996 from V. O. C. College, Manonmaniam Sundaranar University, Tamil Nadu. He received his Ph. D. from the Indian Institute of Technology Madras under Professor R. Dhamodharan. He then joined Professor Gregory N Tew's laboratory in the Polymer Science and Engineering Department at the University of Massachusetts, Amherst as a postdoctoral research associate from 2003 to August 2008. From September 2008 to 2013, he was an Assistant Professor in the Department of Chemical Sciences at the IISER-Kolkata. From January 2014 to September 2018, he was an Associate Professor in the Department of Chemical Sciences at the IISER-Kolkata. He was the Head of the Department from February 2014 to March 2016. From October 2018 onwards, he has been a full Professor in the Department of Chemical Sciences. He was a recipient of the prestigious Ramanujan Fellowship from the Department of Science and Technology, Government of India. He received the Joint Runner-Up award in the 6th NATIONAL AWARD FOR TECHNOLOGY INNOVATION under the Polymeric Materials category, on 20 January 2016, for Arsenic sensing work. He also received the Joint Winner Award in the 7th NATIONAL AWARD FOR TECHNOLOGY INNOVATION under the Polymeric Materials category, on 01 March 2017, for developing a sensor for nerve agents. In 2018, his group received the Joint Runner-Up award in the National Award for Technology Innovation under the polymeric Materials category for developing a New Polymer for Drug Delivery application. Raja is the recipient of the coveted NASI-Reliance Industries Platinum Jubilee Award for the year 2019. Under his guidance, 15 Ph.D. students already graduated, and currently, seven students are undergoing their Ph.D. degrees. Raja has published 122 International peer-reviewed publications, six Book Chapters, and one book. He also owns five patents to his credit.*

Low-dimensional Halide Perovskites for High-performance Photodetection

Anamika Mondal,[$] Arnab Mandal,[$] Shresth Gupta, and Sayan Bhattacharyya*
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$ Equal contribution

Abstract:

In the field of optoelectronics, halide perovskite semiconductors are driving significant advancements that could reshape next-generation technologies. Metal-halide perovskites, particularly when produced with minimal structural disorder, enhanced thermal resistance, and photostability, stand out as a disruptive material class. Among them, 2D perovskites with Ruddlesden-Popper (RP) and Dion-Jacobson (DJ) phases offer superior moisture and heat stability due to the hydrophobic alkyl ammonium spacers, which act as barriers between inorganic octahedral layers, forming quantum well-like structures. This poster will focus on our strategies for designing 2D and 0D halide perovskites and their application in visible light photodetection, demonstrating how electronic properties can be modulated based on the perovskite composition.[1,2]

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Bio-Sketch of Speaker

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IISER Kolkata

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Academic Records	1996; University of Calcutta (B.S.) 1998; University of Kalyani (M.S.) 2006; Indian Institute of Technology (IIT) Kanpur (Ph.D)
Professional Career	2006~2008 Postdoc, Bar-Ilan University, Israel 2008~2010 Postdoc, Drexel Nanotechnology Institute, USA 2010~2015 Assistant Professor, IISER Kolkata 2015~2019 Associate Professor, IISER Kolkata 2016~2020 Founder Chair, Centre for Adv. Funct. Mater., IISER Kolkata 2019~present Professor, IISER Kolkata
Research Interests	1. Photovoltaics and optoelectronics with hybrid perovskite; 2. Electrocatalysis; 3. Metal-air & photorechargeable batteries
Awards & Recognitions *(last 5 years)*	Life Fellow, Indian Chemical Society Editorial Advisory Board Member, ACS Applied Energy Materials Editor, Indian Journal of Chemistry SERB-STAR Award CRSI Bronze Medal Editorial Advisory Board Member, Journal of Materials Chemistry A

Utilising simple building blocks for complex catalytic functions

Dibyendu Das

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IISER Kolkata, India

Abstract:

Significant gaps remain in our understanding of how functional biopolymers and the complex reaction networks underlying metabolic activities emerged during the origins of Earth's biosphere. In this context, extant proteins, evolved over millions of years, carry out an impressive array of responsibilities, from catalysis and molecular recognition to the out-of-equilibrium work such as motility and load bearing. One of the goals of our lab is to investigate the possible origins of such advanced enzymatic functions from simple building blocks and short peptides.[1-3] Via my poster, I will show our attempts to develop simple chemical-based systems that can demonstrate advance enzyme like traits. Further, I will show how simple chemicals can be driven to access higher energy self-assembled states, just as seen in natural microtubules.[4-5]

References and Notes:

1. Singh, A.; Parvin, P.; Saha, B.; Das, D.* Nat. Rev. Chem. (Accepted)
2. Soumili Roy, Janmejay Laha, Antara Reja and Dibyendu Das* J. Am. Chem. Soc. 2024, 146, 32, 22522-22529.
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4. Sarkhel, B.; Chatterjee, A.; Das, D.* J. Am. Chem. Soc. 2020, 142, 4098-4103.
5. Goswami, S.; Reja, A.; Pal, S.; Singh, A.; Das, D.* J. Am. Chem. Soc. 2022, 144, 19248-19252.

Bio-sketch

Profile

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Dibyendu Das is an Associate Professor at the Department of Chemical Sciences of IISER Kolkata, West Bengal, India. He obtained his PhD at Indian Association for the Cultivation of Science (IACS), India and postdoctoral training from Emory University, USA. His research group is interested in emerging field of systems chemistry, chemical evolution and peptide nanotechnology.

Awards and Distinctions

1. Featured in "75 under 50 scientists shaping today's India" compendium. On National Science Day, Honorable Minister of State for the Ministry of Science &Technology, Dr. Jitendra Singh released this coffee table book published by Vigyan Prasar. The book mentions the profiles of 75 scientists under the age of 50 shaping today's India.
2. Awarded Swarnajayanti Fellowship in Chemical Science 2020, DST, Govt of India. (https://dst.gov.in/swarna-jayanti-fellow-develop-intelligent-materials-taking-inspiration-living-matter).
3. Awarded CRSI Bronze Medal for the year 2023.
4. Article featured in the virtual issue of the JACS Early Career Investigators as an outstanding work published in 2020.
5. Awarded Indian Peptide Society-Young Scientist Award (IPS-YSA) for excellence in Peptide Research for the year 2021.
6. Early Career Advisory Board of ACS Chemical Reviews 2020-2021.
7. Selected as an Associate of the Indian Academy of Sciences (IASc) 2019.
8. Advisory Board of Materials Horizons, 2021.
9. International Advisory Board (IAB) of AsianJOC, 2021 onwards.

Representative Publications:

1. Allosteric dipeptide assemblies - JACS, 2024
2. Short peptide amidase - Proc. Natl. Acad. Sci. U.S.A 2024
3. Non-equilibrium self-assembly - Nat. Rev. Chem. 2024
4. Short Peptide Based Reductase - Nat. Commun. 2024
5. Chemotactic Amylobots - Nat. Commun. 2023
6. Photomodulated Protometabolism by Short Peptide - JACS, 2023
7. COF-Peptide Biomimetic Catalysts - JACS, 2023
8. Charge-Selective Catalysis - JACS, 2022

Photoredox/Nickel Dual Catalysis for C(sp2)-C(sp3) Cross Electrophile Coupling Reaction Using Mesylate of phenols and Primary Alcohols as the Latent Electrophile Sources

Sayan K. Jana, Rayan Bhattacharya‡, Purusattam Dey‡, Sunit Chakraborty, and Biplab Maji *

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Abstract:

Forming the C–C bond is one of the central goals in synthetic organic chemistry. The drawbacks of the traditional cross-coupling reaction between an electrophile with an organometallic nucleophile demanded an alternative synthetic protocol. In the last decade, visible light photoredox catalysis has emerged as a powerful arsenal in organic synthesis.[1] Cross-electrophile coupling has rapidly become essential to synthesizing C(*sp2*)-C(*sp3*) bonds, ubiquitous in various natural products and drug molecules.[2] Primarily, aryl halides with a different alkyl radical precursor make the C(*sp2*)-C(*sp3*) bond. Alcohol is a 'native' functional group, and the utilization of alcohol as an alkyl coupling partner is advantageous in terms of its commercial availability and inert reactivity.[3,4] Herein, we describe a photoredox/nickel dual catalytic strategy for alkyl-aryl cross-electrophile coupling.[5] Two alcohol coupling partners were taken, activated by mesylation, and utilized in a cross-coupling reaction. Besides several challenges to activating similar coupling partners with equal reactivity, we are pleased to have archived our cross-coupled product with an excellent yield. A dual ligand with a suitable nickel catalyst and an appropriate photocatalyst combination furnishes fruitful results. Several phenol and alkanol derivatives give the desired product a good to excellent yield, irrespective of their steric and electronic nature. A detailed mechanistic study has been performed, and it concludes that the role of the photoredox cycle and a metallaredox cycle operating at a specific rate is necessary. It reveals the photocatalytic SET event and formation of alkyl radicals in our reaction.

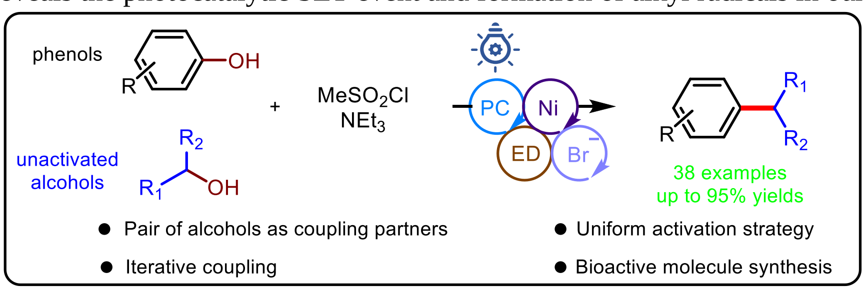

Figure. C(sp2)-C(sp3) Cross Electrophile Coupling[5]

For the synthetic utility of the reaction, we have employed this strategy in various drug fragment syntheses, iterative cross-coupling starting from alcohol. Also, scale-up and one-pot reaction has been performed to show synthetic applicability. In summary, we have successfully executed cross-electrophile coupling using abundant feedstock phenols and unactivated primary alcohols as carbon sources. Our innovation involved activating both coupling partners using the same activator and designing a photoredox/nickel dual catalysis system that enabled cross-selective coupling of similarly reactive sulfonate esters of the aryl and alkyl electrophiles.

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4. S. K. Jana, M. Maiti, P. Dey, B. Maji, *Org. Lett.* **2022**, *24*, 1298. 5.
5. S. K. Jana, R. Bhattacharya, P. Dey, S. Chakraborty, B. Maji, *ACS Catal.* **2024**, 14172.

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2013-2015: Postdoc: Chubu University, Mentor: Prof. Hisashi Yamamoto
2016: Alexander von Humboldt fellow: Westfälische Wilhelms-Universität Münster, Mentor: Prof. Frank Glorius
2016-2021: Assistant Professor, Indian Institute of Science Education and Research Kolkata
2021-: Associate Professor, Indian Institute of Science Education and Research Kolkata

Research focus: Organic synthesis, catalysis, and mechanistic studies.

Awards:
2024: Chirantan Rasayan Sanstha® (CRS) Bronze Medal (2024)
2024: Associate of the West Bengal Academy of Science & Technology (WAST)
2021: "2021 Young Investigator Award ", Sponsored by Molecules
2021: Merck Young Scientist Award (runner-up) in Chemical Science
2021: INSA Medal for Young Scientists
2021: Associate of the Indian Academy of Sciences (IASc)
2020: NASI-Young Scientist Platinum Jubilee Award (2020) in Chemical Sciences
2019: Thieme Journal Award

Selected publication:

- S. K. Jana, R. Bhattacharya, P. Dey, S. Chakraborty, B. Maji, *ACS Catal.* **2024**, *44*, 14172.
- A. Jati, A. K. Mahato, D. Chanda, P. Kumar, R. Banerjee, B. Maji, J. *Am. Chem. Soc.* **2024**, *146*, 23923.
- A. Jati, S. Dam, S. Kumar, K. Kumar, **B. Maji**, *Chem. Sci.* **2023**, *14*, 8624-8634.
- S. Waiba, K. Maji, M. Maiti, B. Maji, *Angew. Chem. Int. Ed.* **2023**, *Angew. Chem. Int. Ed.* **2023**, *62*, e202218329.
- P. Rai, K. Maji, S. K. Jana, B. Maji, *Chem. Sci.* **2022**, *13*, 12503-12510.
- A. Jati, K. Dey, M. Nurhuda, M. A. Addicoat, R. Banerjee, B. Maji, J. *Am. Chem. Soc.* **2022**, *144*, 7822-7833.
- S. Waiba, M. Maiti, B. Maji, *ACS Catalysis* **2022**, *12*, 3995-4001.
- S. K. Jana, M. Maiti, P. Dey, B. Maji, *Org. Lett.* **2022**, *24*, 1298-1302.

Challenging antimicrobial resistance (AMR) with cationic chlorpromazine-peptide conjugates as potent antibacterial agents

Presenter(s) name: Meenu Kumari*
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Indian Institute of Technology Kanpur, UP, 208016, India
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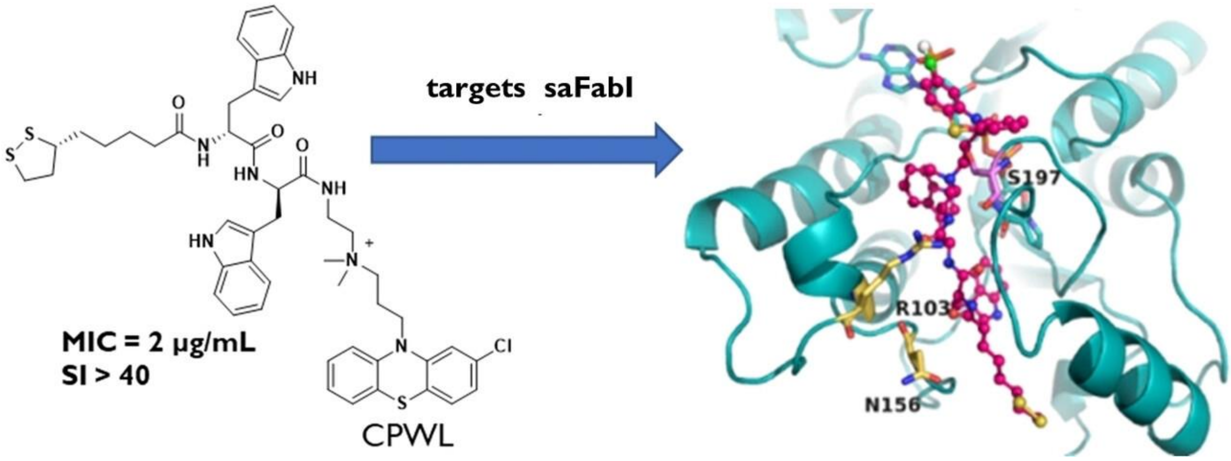
Abstract:

Antimicrobial resistance (AMR) has been noted by WHO as a particular important issue harming human health and productivity globally. The severity of the issue is unprecedented, prompting the development of innovative antimicrobial scaffolds aimed at new bacterial targets. Here, we rationally designed and synthesized three derivatives of cationic chlorpromazine peptide conjugates CPWPA, CPWLA and CPWL intended to target multidrug-resistant (MDR) bacteria. The most potent compound, CPWL, of all the conjugates evaluated, showed promising antibacterial activity against clinical, MDR *S. aureus*, with no cytotoxicity. The molecular docking experiment confirmed that CPWL possessed a very high affinity for *S. aureus* enoyl reductase (saFabI). Furthermore, CPWL anti-bacterial action against saFabI was corroborated by MD simulation studies. Thus, our findings highlight cationic chlorpromazine-peptide conjugates as promising scaffolds for the development of saFabI inhibitors to target severe staphylococcal infections.



References and Notes:

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Bio-sketch

Profile

Name: Meenu Kumari
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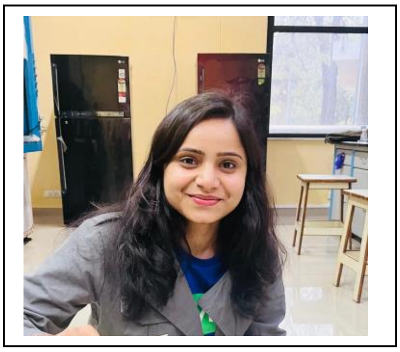

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Crafting and Characterization of Custom Surfaces Using Self-Assemblies of Tri-Carboxylic Acid Derivatives

Arunima Das, Richa Arjariya, Thiruvancheril G. Gopakumar, Sandeep Verma
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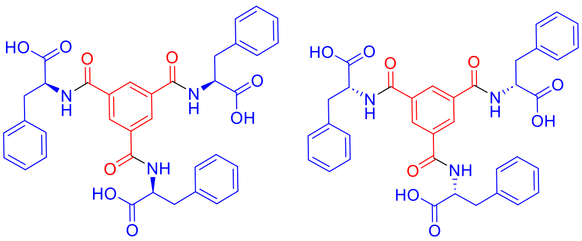
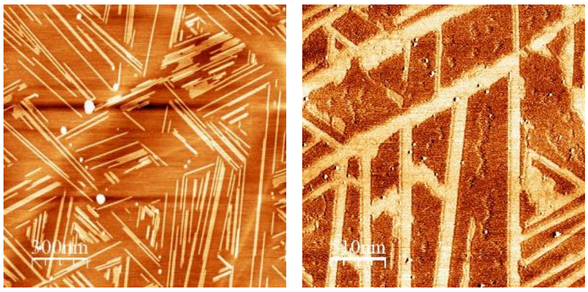
Abstract: Molecules with carboxylic acid moieties exhibit vast structural diversity in surface-supported self-assembly due to their tendency to form H-bonds. Carboxylic acid groups attached to planar, aromatic moieties give rise to extensive self-assembled frameworks owing to their π-π stacking interactions. Earlier studies have reported the 1D fibres and nanotube formation by the self-assemblies of benzene-1,3,5 tricarboxamides (BTAs).[1] Motivated by the ability of amino acids to form extensive hydrogen bonds, our group has fabricated Phenylalanine functionalized BTA molecules which revealed interesting polymorph structures under STM.[2] AFM analysis of these molecules on graphite surface has shown two types of self-assemblies: 1D islands and 1D chain. This observation is supported by data collected from FE-SEM experiments and other techniques. This property of phenylalanine functionalized BTA molecules can be explored for the design and fabrication of custom surfaces for various applications.

Figure:



Phe-functionalized BTA molecules



AFM images on graphite surface

Notes: STM – Scanning Tunnelling Microscopy, AFM – Atomic Force Microscopy, FE-SEM – Field Emission Scanning Electron Microscopy

References:

1. Matsumoto, N. M.; Lafleur, R. P. M.; Lou, X.; Shih, K. C.; Wijnands, S. P. W.; Guibert, C.; Rosendaal, J. W. A. M. V.; Voets, I. K.; Palmans, A. R. A.; Lin, Y.; Meijer, E. W. *J. Am. Chem. Soc.* **2018**, *140*, 13308-13316.
2. Arjariya, R.; Kaur, G.; Sen, S.; Verma, S.; Lackinger, M.; Gopakumar, T. G. *Nanoscale* **2023**, *15*, 13393.

Bio-sketch

FORCE-IICS 2024

Profile

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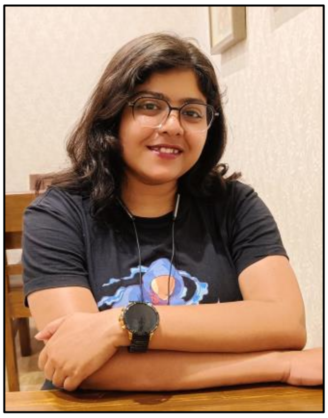

I have completed BSc. in Chemistry from Lady Brabourne College, University of Calcutta in 2019, and MSc. from National Institute of Technology (NIT), Jamshedpur in 2021. I was awarded silver medal for the first position in the Department of Chemistry, NIT Jamshedpur. I joined for PhD in Department of Chemistry, IIT Kanpur under the supervision of Prof. Sandeep Verma in January 2023 and received Prime Minister Research Fellowship (PMRF) in August 2023. I am conducting my research on fabrication of custom surfaces using self-assemblies of amino acid and nucleobase derived molecular frameworks. I have been selected for joint PhD program in IIT Kanpur and La Trobe University, Melbourne, Australia.

Multi-equilibria system for precise carboxylic acid engineering in proteins

Dwaipayan Biswas,[a‡] Rajib Molla,[a‡] Rohith Singudas,[a‡] Lucky Ojha,[a] Divya Bindra,[b] Saurabh Rai,[a] Ragendu V.,[a] Saptarshi Mukherjee,[a] Ram Kumar Mishra,[b] Vishal Rai[a]

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Abstract:

Complexity to simplicity: The platforms for engineering chemical bonds fuel the chemical industry. Historically, its focus on small molecules created a bias for the shortest pathways and irreversible transformations. While it served well, the rapid biopharma growth in recent years requires new principles for selective bond formation with biomolecules, such as proteins. This paper demonstrates that a complex multi-equilibria system[1] can create an opportunity for multiple reaction pathways[2]. Against conventional wisdom, it can render highly selective outcomes when applied to a complex substrate, such as protein, offering exclusive control over a specific pathway[3]. For example, a four-Component Reaction can render a four-Component Product (4CR-4CP). Besides, the pathway can be switched entirely (e.g., 4CR-4CP to 4CR-2CP or 3CR-2CP). The pathway-selectivity remains unaltered even at >90% bioconjugation. The exclusive control over chemoselectivity, site-selectivity, and modularity accompanies the pathway-selectivity (>36 examples). It redefines the pre-established principles and presents three methods for single-site carboxylate modification[4], a highly challenging protein targetome. It offers dual-probe engineering of diverse tags, including FRET pairs. It labels carboxylate in insulin without affecting its receptor binding and downstream signaling. The method renders homogeneous antibody-fluorophore and drug conjugates (AFC and ADC), enabling antigen-specific cellular labeling and antiproliferative activity. This work establishes the capability of multi-equilibria systems to convert complexity to simplicity and opens the gateway for a discovery space.

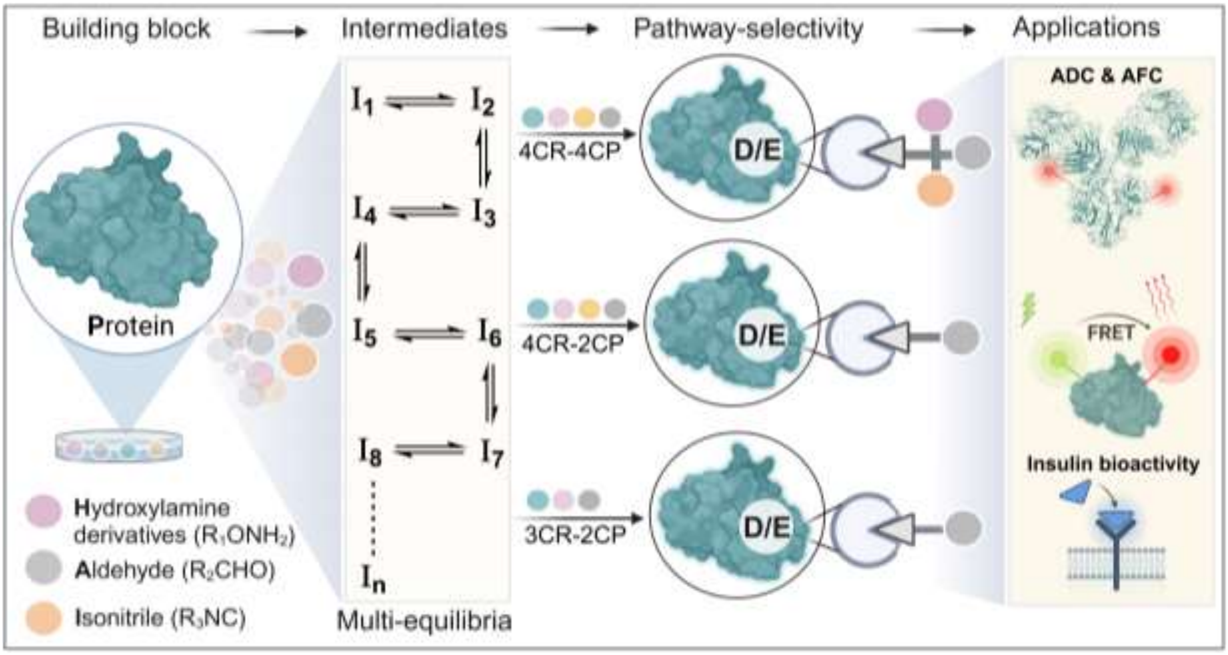

Figure: Multi-equilibria system for precise engineering in proteins and antibody.

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(1) Disintegrate (DIN) Theory Enabling Precision Engineering of Proteins. Chauhan, P.; V., R.; Kumar, M.; Molla, R.; V. B., U.; Rai, V. *ACS Cent. Sci.* **2023**, *9* (2), 137–150.

(2) Chemical Technology Principles for Selective Bioconjugation of Proteins and Antibodies. Chauhan, P.; V, R.; Kumar, M.; Molla, R.; Mishra, S. D.; Basa, S.; Rai, V. *Chem. Soc. Rev.* **2024**, *53* (1), 380–449.

(3) Protein–Protein Interaction in Multicomponent Reaction Enables Chemoselective, Site-Selective, and Modular Labeling of Native Proteins. Molla, R.; Joshi, P. N.; Reddy, N. C.; Biswas, D.; Rai, V. *Org. Lett.* **2023**, *25* (34), 6385–6390.

(4) Modular Diazo Compound for the Bioreversible Late-Stage Modification of Proteins. Jun, J. V.; Petri, Y. D.; Erickson, L. W.; Raines, R. T. *J. Am. Chem. Soc.* **2023**, *145* (12), 6615–6621.

Bio-sketch

Profile

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Dwaipayan obtained his Bachelor of Science (B.Sc.) in Chemistry from Ramakrishna Mission Vivekananda Centenary College, Rahara, West Bengal, in 2020, followed by a Master of Science (M.Sc.) in Chemistry from the Indian Institute of Technology (IIT) Hyderabad in 2022. Currently, he is pursuing his Doctor of Philosophy (PhD) in Chemistry at the Indian Institute of Science Education and Research (IISER) Bhopal under the supervision of Prof. Vishal Rai. He was awarded the prestigious Prime Minister's Research Fellowship (PMRF) in 2023. His research focuses on developing a chemical toolbox for the precision engineering of proteins and antibodies at IISER Bhopal.

Representative Publications:

1. Protein-protein interaction in multicomponent reaction enables chemoselective, site-selective, and modular labeling of native proteins. Molla, R.; Joshi, P. N.; Reddy, N. C.; **Biswas, D.**; Rai, V. *Org. Lett.* **2023**, *25*, 6385-6390.

Nickel-Photoredox Dual Catalysis Mediated Carbamoylation of Benzoyl Chlorides.

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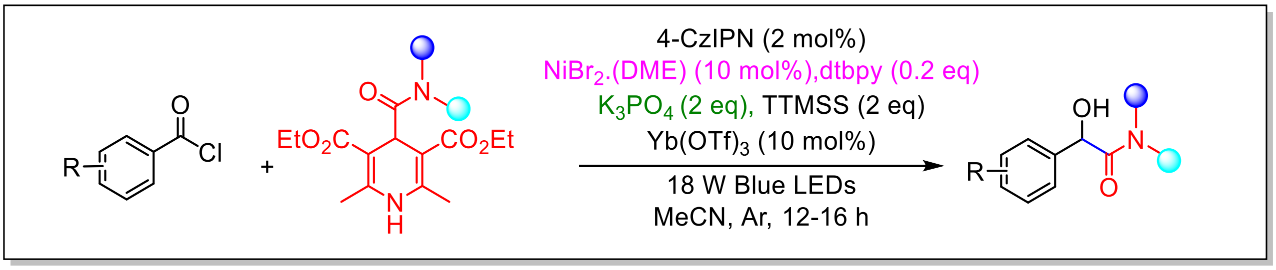
Abstract:

The field of dual photocatalysis has recently experienced rapid growth, emerging as a highly effective method for functionalizing organic molecules under mild conditions.[1-4] Herein, we have exploited the concept of cross-electrophile coupling by combining photoredox and nickel catalysis to synthesize α-hydroxy amides from commercially accessible benzoyl chloride and readily available dihydropyridines, which serve as precursors for carbamoyl radicals. The mild reaction conditions of the method make it compatible with substrates containing sensitive functional groups, enabling the incorporation of an amide scaffold into biologically important heterocycles.

Scheme:



References and Notes:

1. Melchiorre *et al*., Angew. Chem. Int. Ed. **2020**, *59*, 5248 – 5253
2. MacMillan *et al.*, *Chem. Rev*. **2022**, 122, 2, 1485–1542.
3. Doyle *et al.*, J. Am. Chem. Soc. **2024**, 146, *22*, 15331–15344
4. Paixão *et al*., *Adv. Synth. Catal*. **2020**, *362*, 2367-2374.

Bio-sketch

Profile

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Biosketch:

I grew up in Jaipur, Rajasthan, where I completed my schooling at Kendriya Vidyalaya. I then pursued a Bachelor of Science degree from the University of Rajasthan in 2017, followed by a Master's in Chemistry from Dr. B R Ambedkar National Institute of Technology, Jalandhar in 2020. During my M.Sc., I conducted a one-year project focused on synthesizing Nano-catalysts and optimizing their use in preparing biologically active compounds.

After completing my post-graduation, I worked as a Project Assistant at the Centre for Nano and Soft Matter Sciences, Bangalore, for six months, where I focused on the organic synthesis of liquid crystals. I later joined CSIR-CDRI in 2022 as a Project Associate -1, working on the project (HCP0041) "Antiviral Mission CSIR: Discovery & Preclinical Development of Antivirals for COVID-19 & Other Diseases." In 2023, I began my Ph.D. at IIT Kanpur under the supervision of Prof. Anand Singh, currently working on dual Nickel-Photoredox catalysis.

Representative Publications:

1. K. S. Krishnamurthy, D. S. Shankar Rao, S. Sharma, and C. V. Yelamaggad, *Structure, stability, and electro-optic features of nematic drops in 1'', 7''-bis (4-cyanobiphenyl-4'-yl) heptane–surfactant binary systems*, Phys. Rev. E **105**, 024709 (2022).

Electrifying Indolizines for Selective C-H Bond Functionalization

Satpal Singh Badsara*
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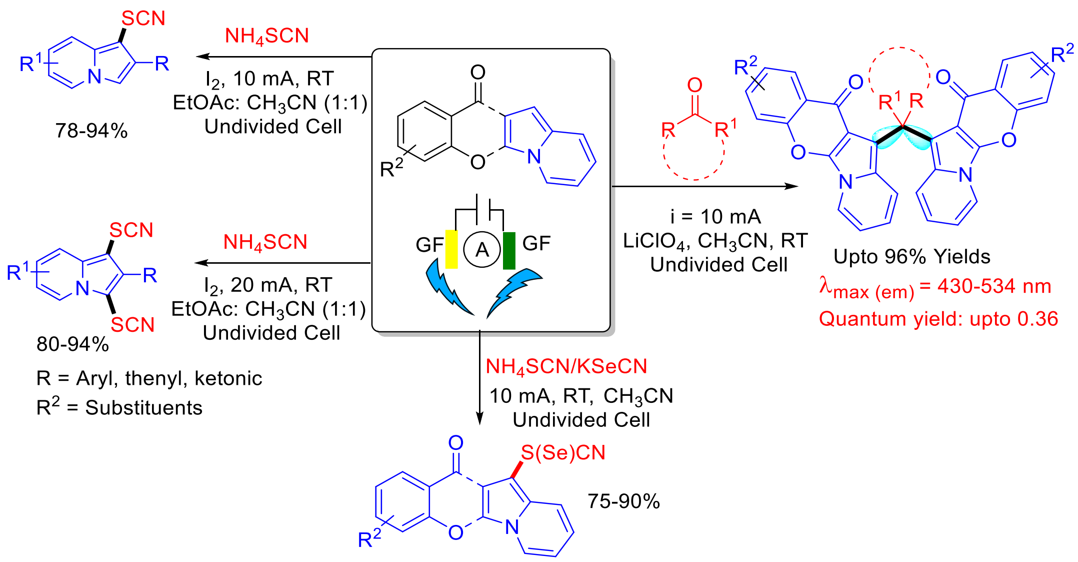
Abstract: Electro-catalysis has emerged as a green and sustainable alternative for the construction of carbon-carbon and carbon-heteroatom bonds over traditional methods.[1] We have recently developed a fast, scalable, transition metal-free, electrochemical sp2 geminal functionalization of carbonyls enabled by anodic oxidation of non-pre-functionalized chromone-fused indolizines (CFIs) to access the triarylmethanes (TRAMs) for the first time.[2] Also, an electrochemical, selective and divergent C-H chalcogenocyanation of indolizine frameworks was also developed by our group.[3] In my presentation, details about these results will be provided.



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2. Jat, P.; Badsara*, S.S. *J. Org. Chem.* **2024**, *89*, 12263-12276.
3. Ucheniya, K.; Jat, P.; Chouhan, A.; Yadav, L.; Badsara*, S. S. *Org. Biomol. Chem.*, **2024**, *22*, 3220-3224.

Bio-sketch

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Biosketch: Dr. Badsara obtained M.Sc. degree from Banaras Hindu University in 2006 and Ph.D. degree from the University of Hyderabad, India in 2013 (with Professor Deevi Basavaiah). During 2013-14, he was a postdoctoral fellow with Prof. Chin-Fa Lee at National Chung Hsing University, Taiwan. Since 2014, he is working as Assistant Professor at the University of Rajasthan, Jaipur India. His research interest mainly includes Electro-organic synthesis, transition metal-free approaches for organic synthesis and Baylis-Hillman chemistry.

Awards and Achievements

- Selected for the Chemical Research Society of India (CRSI) Bronze Medal -2025.
- ISCB Young Scientist Award-2019 in Chemical Sciences by Indian Society of Chemists and Biologists, India.
- DST INSPIRE Faculty Award-2015

Representative Recent Publications:

1. P. Jat, S. S. Badsara*, *J. Org. Chem.* **2024**, *89*, 12263-12276.
2. K. Ucheniya, P. Jat, A. Chouhan, L. Yadav, S. S. Badsara*, *Org. Biomol. Chem.*, **2024**, *22*, 3220-3224.
3. P. K. Jat, L. Yadav, A. Chouhan, K. Ucheniya, S. S. Badsara*, *Chem. Commun.*, **2023**, 59, 5415-5418.
4. K. Ucheniya, A. Chouhan, L. Yadav, P. K. Jat, S. S. Badsara*, *J. Org. Chem.*, **2023**, *88*, 6096.
5. A. Chouhan, K. Ucheniya, L. Yadav, P. Jat, A. Gurjar, S. S. Badsara*, *Org. Biomol. Chem.*, **2023**, *21*, 7643-7653.
6. P. K. Jat, K. K. Dabaria, R. Bai, L. Yadav, S. S. Badsara*, *J. Org. Chem.*, **2022**, *87*, 12975-12985.
7. Z-W. Chen, R. Bai, P. Annamalai, S. S. Badsara*, C-F. Lee*, *Chem. Asian J.* **2024**, Accepted article, doi.org/10.1002/asia.202400780

Title: Streamlined Synthesis of Eudesmane Sesquiterpenoids through Site-switchable Olefin Functionalization Strategy

Name: Kiran Kumar Pulukuri*
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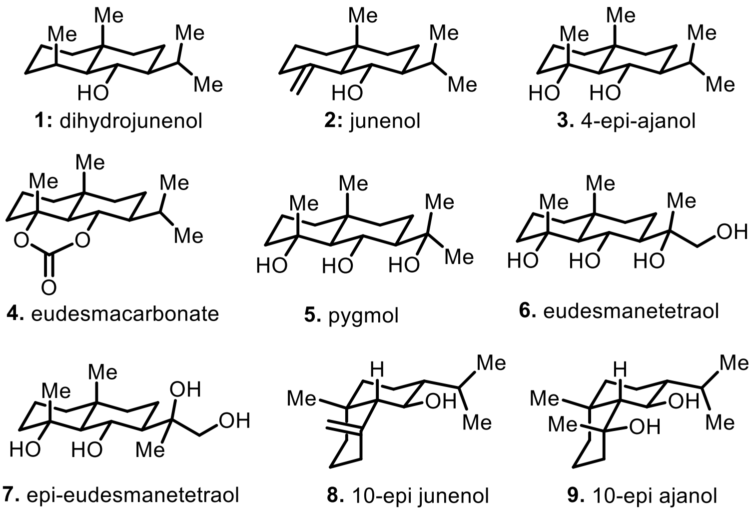
Abstract: Site-selective functionalization in the synthesis of natural products holds profound significance in organic synthesis and drug discovery. Nature intricately crafts the complex structures of natural products through selective functionalization of C-H bonds, olefins, and other functional groups. Over the past decade, site-selective oxidation of C-H bonds and alcohol groups have been extensively explored, leading to elegant syntheses of various natural products. However, selective functionalization of olefins has received comparatively less attention despite their potential for diverse derivatization. Our research group is actively engaged in the total synthesis of bioactive natural products by employing selective olefine functionalization strategies. In this poster, we will highlight the synthesis of eudesmane terpenes to showcase the effectiveness of selective olefin functionalization in the synthesis of complex terpenes (Figure).[1]

Figure/Scheme (if any):



Chemical Structures of Selected Eudesmane sesquiterpenes 1-9.

References and Notes:

1. Asuthosh Panigrahy and Kiran Kumar Pulukuri*, *ChemRXIV*. **2023**, DOI: 10.26434/chemrxiv-2023-3fldg-v2.

Bio-sketch

Profile

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Biosketch: Dr. Kiran earned his B.Sc in 2005 and M.Sc (Chemical Sciences) in 2007 from Pondicherry University. He subsequently joined the CSIR-IICT for his Ph.D. program, focusing on synthesis of complex natural products and glycopeptides under the guidance of Dr. T. K. Chakraborty. In 2013, he completed and submitted his thesis at CDRI-Lucknow, before proceeding to the Rice University for post-doctoral studies. There, he spent six years in the lab of Prof. K. C. Nicolaou as postdoctoral fellow and research scientist.

In 2019, Dr. Kiran started his independent career as an assistant professor in the Department of Chemistry at IISER-Tirupati. His research interests encompass a diverse range of topics, including Total Synthesis of Natural Products, Synthetic Methodology, Asymmetric Catalysis, Electro Organic Synthesis, and Natural Product-based Drug Discovery.

Representative Publications:

1. Asuthosh Panigrahy and Kiran Kumar Pulukuri*, *ChemRXIV*. **2023**, DOI: 10.26434/chemrxiv-2023-3fldg-v2.

Ligand Modification for the Preparation of Difluoroboron Complexes and Their Cations

Darakashan Parveen, Rahul Kumar Yadav, Dipak Kumar Roy*
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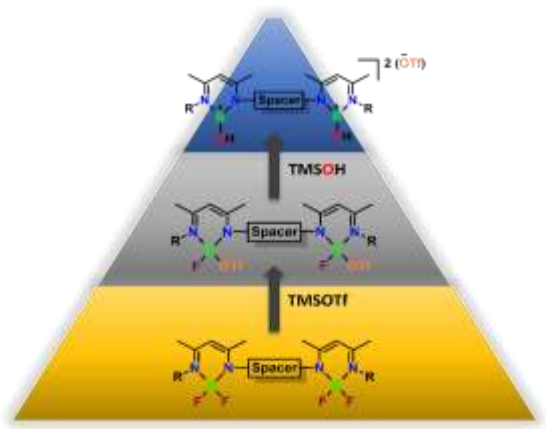
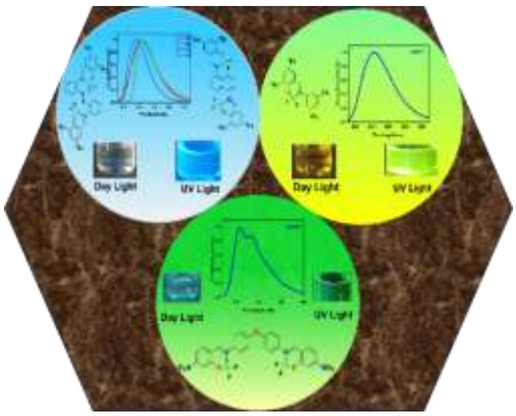
Abstract: Ligand design involves the strategic creation and modification of molecules that can able to produce a molecule with certain features. By fine tuning electronic and steric factors via change in substitution pattern of the ß-diiminate moiety gives an opportunity to showcase the different properties in difluoroborane compounds. A series of N, O and N, N donor-based mono- and binuclear four-coordinated difluoro boron complexes were synthesized. Depending on the substitution and spacer, these N, O donor complexes exhibit intense blue, green and yellow emission in solution states, whereas the N, N donor complexes were very weak in fluorescence intensity. With an aim to produce cationic boron species fluoride abstraction reaction was carried out. Although we were successful in preparing the cationic boron species with the N, N substituted boron complexes, the N, O donor BDI ligands were not helpful in making the boron cations. The details of the boron cations and the photophysical study of these boron complexes are going to be discussed in this presentation.





References and Notes:

1. X. Tan and H. Wang, *Chem. Soc. Rev.*, **2022**, *51*, 2583-2600.
2. W. E. Piers, S. C Bourke and K. D. Conroy, *Angew. Chem. Int. Ed.*, **2005**, *44*, 5016-5036.
3. D. Parveen, R. K. Yadav, B. Mondal, M. Dallon, Y. Sarazin, D. K. Roy, *Dalton Trans.*, **2024**, *53*, 14139-14143.

Bio-sketch

Profile

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Education Details

- Ph.D. (Organometallic Chemistry): Indian Institute of Technology Madras, India, 2015
- M.Sc. (Chemistry): Ramakrishna Mission Residential College, Narendrapur (University of Calcutta), India, 2010
- B.Sc. (Chemistry as major): Ananda Mohan College (University of Calcutta), India, 2008

Professional Appointments

- Feb. 2019 – till date: Assistant Professor, Department of Chemistry, Indian Institute of Technology Indore, India
- Jan. 2018 – Jan. 2019: SERB Overseas Postdoctoral fellow at University of Würzburg, Germany with Prof. H. Braunschweig
- Feb. 2016 – Dec. 2017: Postdoctoral fellow at University of Würzburg, Germany with Prof. H. Braunschweig
- June 2015 – Dec. 2016: Research Associate at Indian Institute of Technology Madras with Prof. Sundargopal Ghosh

Awards and Honours

- Overseas Post-Doctoral Fellowship, SERB, Dept. of Science and Technology, Govt. of India, 2016-17
- "Werner prize”- Best Ph.D. thesis in Inorganic and Analytical Chemistry, Indian Institute of Technology Madras, India, 2016

Representative Publications:

1. Saha, K., Roy, D. K., Dewhurst, R. D., Ghosh, S., Braunschweig, H., *Acc. Chem. Res.*, **2021**, *54*, 1260.
2. Roy, D. K., Troester, T, Fantuzzi, F., Dewhurst, R. D., Lenczyk, C., Radacki, K., Pranckevicius, C., Engels, B., Braunschweig, H., *Angew. Chem. Int. Ed.*, **2021**, *60*, 3812.
3. Parveen, D., Yadav, R. K., Roy, D. K., *Chem. Commun.*, **2024**, *60*, 1663.
4. Parveen, D., Yadav, R. K., Mondal, B., Cordier, M., Sarazin, Y., Roy, D. K., *Dalton Trans.*, **2024**, *53*, 14139.

Copper(I)-Catalyzed Proto/Carboboration of 1,3-Diynes: An Easy and Sustainable Access to Borylated Enynes and Dienes

Venkataraman Ganesh*
Department of Chemistry, Indian Institute of Technology Kharagpur, Kharagpur, West Bengal -721302, India.
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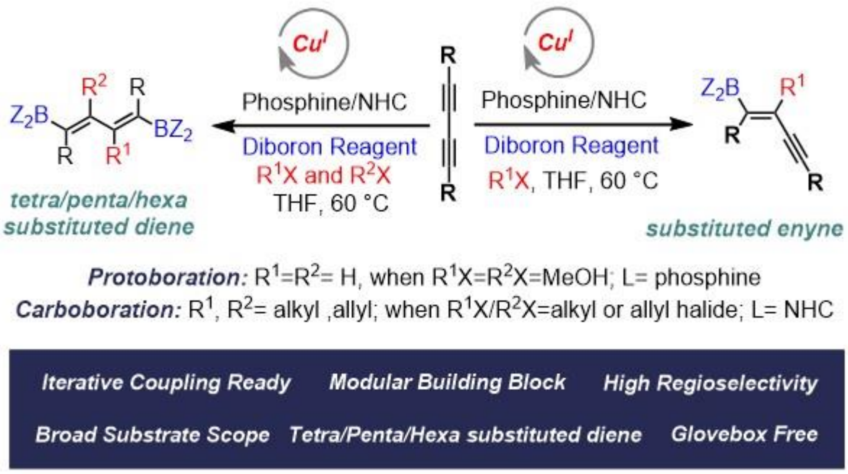
Abstract:
Targets with high structural complexity can be easily assembled using small, modular building blocks similar to a 'Lego' construction using Iterative chemistry.[1-3] Organoboron compounds have been in the spotlight as versatile building blocks in natural product synthesis. Here, we present a sustainable, glovebox-free regioselective protoboration of 1,3-diynes using a stable diboron source and Cu^{I}/phosphine as a catalyst to access stable enynyl and dienyl boronate esters in a single operation. Then, we developed the first copper-catalyzed carboboration of 1,3-diynes, in which a simultaneous C−B and C−C bond formation was achieved in a single operation using a Cu^{I}/NHC catalyst. The methodology provides easy access to highly sterically encumbered penta- and hexa-substituted dienes. A wide range of electrophiles have been successfully employed. DFT studies supported the regioselective incorporation of electrophiles. The products were employed in iterative coupling to obtain densely functionalized 1,3-dienes and polyenes.[4,5]



References and Notes:

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4. Ghosh, S.; Chakrabortty, R.; Kumar, S.; Das, A.; Ganesh, V. *ACS Catal.* **2022**, *12*, 11660.
5. Ghosh, S.; Kumar, S.; Chakrabortty, R.; Ganesh, V. *Org. Lett.* **2024**, *26*, 6574.

Bio-sketch

Profile

Ganesh Venkataraman

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Venkataraman Ganesh received his early education from Bishop Heber College Tiruchirappalli (2001-2004) and joined the Integrated Ph.D. program (Chemical Sciences) at Indian Institute of Science (IISc) Bangalore (2004). Ganesh obtained his Ph.D. in 2013, working with Prof. S. Chandrasekaran as a CSIR-Shyama Prasad Mukherjee (CSIR-SPM) fellow. He had postdoctoral stints as a JSPS fellow (2013–15) with Prof. M. Shibasaki at BIKAKEN, Japan, and as a Newton International Fellow (2016–18) with Prof. V. K. Aggarwal at the Univ. of Bristol, UK. He started his independent research career in 2018 at the Dept. of Chemistry, Indian Institute of Technology Kharagpur, India, and held the Ramanujan fellowship till 2023 (SERB, India). His research interests include exploiting transition-metal catalysts and boron chemistry to develop new synthetic methodologies and mechanistic studies.

Representative Publications:

1. Ghosh, S.; Kumar, S.; Chakrabortty, R.; Ganesh, V.* *Org. Lett.* **2024**,26, 6574.
2. Biswas, K.; Malik, S.; Ganesh, V.* *J. Org. Chem.* **2024**, *89*, 11014.
3. Mondal, S.; Biswas, K.; Ganesh, V.* *Adv. Synth. Catal.* **2024**, *366*, 3277.
4. Ghosh, S.; Rooj, A.; Chakrabortty, R.; Ganesh, V.* *Org. Lett.* **2024**, *26*, 4024.
5. Chakrabortty, R.; Ghosh, S.; Ganesh, V.* *Org. Lett.* **2024**, *26*, 792.
6. Khamrai, A.; Ganesh, V.* *Chem. Commun.* **2023**, *59*, 11141.
7. Mondal, S.† Ballav, T.† Tofayel, S. M.; Ganesh, V.* *Org. Lett.* **2023**, *25*, 3941.
8. Biswas, K.; Khamrai. A; Malik, S.; Ganesh, V.* *Org. Lett.* **2023**, *25*, 1805.
9. Ghosh, S.; Chakrabortty, R.; Kumar, S.; Das, A.; Ganesh, V.* *ACS Catal.* **2022**, 12, 11660.

Title: Design and synthesis of novel chiral phase transfer catalysts and their applications in asymmetric synthesis

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Abstract:

A phase-transfer catalyst (PTC) helps in shifting a reactant from one phase to another phase, where the reaction takes place[1]. PTC has made significant advances in catalysis and is identified as a versatile methodology in academia and industry, bestowed to the use of environment-friendly reagents and water as a solvent, ease of handling the catalysts, mild reaction conditions, and applicability in large-scale processes. The scope of chiral PTC is wide and large including asymmetric alkylation, alkynylation, aromatic nucleophilic substitution, hydroxylation, Mannich-type reaction, Michael addition, spirocyclization, desymmetrization, epoxidation, and kinetic resolution. It also has extensive applications in sulfenylation, asymmetric biomimetic transamination, and base-free asymmetric conjugate addition[2,3,4]. However, only a few effective chiral PTC catalysts have been reported and used in practical asymmetric transformations. It is found that two quaternary nitrogen centers are more effective in binding with anionic intermediates than a single quaternary nitrogen center to provide enantioenriched product. This poster illustrates our ongoing research efforts in the area of phase transfer catalysis related to the development of novel doubly quaternized binaphthyl-based chiral phase transfer catalysts (PTC).

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2. Hashimoto, T. and Maruoka, K. Recent Development and Application of Chiral Phase-Transfer Catalysts. *Chem. Rev.* **2007**, *107*, 5656−5682.
3. Maruoka, K.; Lee, H.J. Recent Asymmetric Phase-Transfer Catalysis with Chiral Binaphthyl-Modified and Related Phase-Transfer Catalysts over the Last 10 Years. *The chemical record* **2023**, e202200286.
4. Penso, M., Albanase, D. New Trends in Asymmetric Phase Transfer Catalysis. *Eur. J. Org. Chem.* **2023**, *26*, e202300224.

Bio-sketch

Profile

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Career Profile:

- ✓ Ph.D. candidate, Department of Chemistry, IIT Madras, India.
- ✓ M.Sc., Department of Chemistry, Modern College of ASC, Pune 2020,
- ✓ B.Sc., Department of Chemistry, Nutan Maratha College, Jalgaon. India.

Awards

- ✓ Prime Minister Research Fellowship (PMRF) July-2023
- ✓ Junior Research fellowship (JRF) Chemical Science, Feb-2022
- ✓ Maharashtra State Eligibility Test (MH-SET) Chemistry, Dec-2020, Eligibility Test for Assistant Professor.
- ✓ Graduate Aptitude Test in Engineering (GATE) Feb-2020.

Bio-sketch

Photocatalyst Free Visible-Light-Induced Fluoroalkylative Oximation of Aryl Olefins

Nisha Rawat, Tavinder Singh and Anand Singh*

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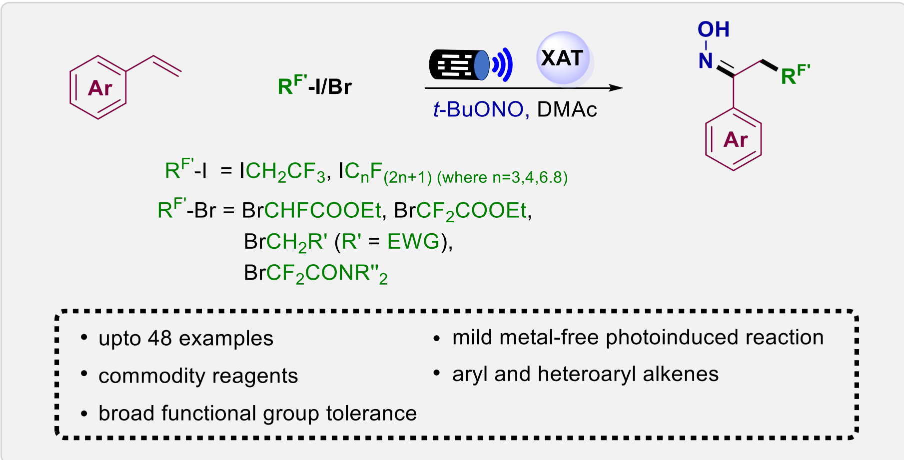
Abstract:

1,2-Difunctionalization of alkenes has emerged as a powerful tool for achieving novel and challenging organic transformations.[1] We have developed a catalyst-free photochemical protocol for the fluoroalkylation-oximation of styrenyl olefins using halogen atom transfer (XAT)[2] strategy. Given the importance of fluorinated organic molecules in the domains of pharmaceuticals and agrochemcials, the direct incorporation of nitrogen and fluoroalkyl moieties provides access to novel scaffolds with brevity.[3,4]

Figure:



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2. Juliá, F.; Timothée, C.; Leonori, D. *Chem. Rev.* **2022**, *122*, 2.
3. Inoue, M.; Sumii Y.; Shibata, N. *ACS Omega*. **2020**, *5*, 10633.
4. Chandra, G.; Singh-V, D.; Mahato-K, Gopal.; Patel, S. *Chem. pap.* **2023**, *77*, 4085.

Bio-sketch

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Postdoctoral Fellow (Postdoc): Indian Institute of Technology Kanpur, India (April, 2023-present); Supervisor: Prof. Anand Singh

Institute Postdoctoral Fellow: Indian Institute of Technology Bombay, India (August,2022-April, 2023); Supervisor: Prof. M. Ravikanth

Ph.D.: Indian Institute of Technology Bombay, India (July,2017- August, 2022); Supervisor: Prof. M. Ravikanth

M.Sc.: D.S.B. Campus, Nainital, Kumaun University, Uttarakhand, India (2015)

B.Sc.: Sri Venkteswara College, University of Delhi, India (2013)

Achievements and Awards

- 2016-Qualified CSIR-UGC-NET-JRF-June 2016 (All India rank- 46).
- Qualified Graduate Aptitude Test in Engineering in 2016.
- 2017- Awarded UGC-Junior Research Fellowship.
- 2019- Awarded UGC-Senior Research Fellowship.

Bio-sketch

Representative Publications

1. **Rawat, N.**; Thorat, K. G.; Kumar, S.; Ravikanth, M*. Synthesis of Expanded Hetero 2,6-Pyrihexaphyrins. *Eur. J. Org. Chem.* **2020**, 736-743. **DOI:** https://doi.org/10.1002/ejoc.201901766

2. **Rawat, N.**; Sinha, A.; Prasannan; D.; Ravikanth, M*. Synthesis and Studies of Stable Nonaromatic Dithia Pyribenzihexaphyrins. *J. Org. Chem.* **2021**, 86, 6665-6673. **DOI:** https://doi.org/10.1021/acs.joc.1c00439

3. **Rawat, N.**; Sinha, A.; Ravikanth, M*. Synthesis and Structural Properties of NIR-Absorbing Pyridine-Containing Heptaphyrins. *Chem Asian J.* **2022**, 17, e202101141. **DOI:** https://doi.org/10.1002/asia.202101141

4. **Rawat, N.**; Ojha, B.; Sinha, A.; Ravikanth, M*. Synthesis of Pyridine-Containing Crowned Fused Expanded Porphyrins. *Chem Asian J.* **2022**, *17*, e202101425. **DOI:** https://doi.org/10.1002/asia.202101425

5. Ojha, B.; Laxman, K†.; **Rawat, N†.**; Ravikanth, M*. Synthesis of Expanded Crowned Macrocycles Containing Two Pyrrolo[1,2-a]indole Units. *Asian. J. Org. Chem.* **2022**, *11*, e202200112. **DOI:** https://doi.org/10.1002/ajoc.202200112

6. **Rawat, N.**; Ojha, B.; Ravikanth, M*. Synthesis and Properties of Nonaromatic *Meta*-Benziheptaphyrins and Aromatic *Para*-Benziheptaphyrins. *Chem Asian J.* **2022**, *17*, e202200715. **DOI:** https://doi.org/10.1002/asia.202200715

7. Yadav, B†.; **Rawat, N†.**; Ravikanth, M*. Synthesis and Studies of Di(*p*-Benzi)Decaphyrin and Di(9,10-Anthracenyl)Decaphyrin. *Chem Asian J.* **2022**, *17*, e202200943. **DOI:** https://doi.org/10.1002/asia.202200943

8. Kaur, G†.; **Rawat, N†.**; Ravikanth, M*. Dibenzothiophene-Containing Thiacarbaporphyrinoids. *J. Org. Chem.* **2023**, 88, 14989–14997. **DOI:** https://doi.org/10.1021/acs.joc.3c01448

9. **Rawat, N.**; Singh, T.; Singh, A*. Photocatalyst Free Visible-Light-Induced Difluoroalkylative Oximation of Aryl Olefins. (Manuscript under preparation)

(†*Equal contribution*, **Corresponding author*)

Photocatalytic, *α*-Aminoalkyl Radical Mediated, Methylene Extrusive Ring Closing Transformation of *o*-Alkynyl and *o*-Cyano Acrylamides

Ganesh Chandra Upreti, Tavinder Singh, Kirti Khanna, Debasish Sahoo and Anand Singh*
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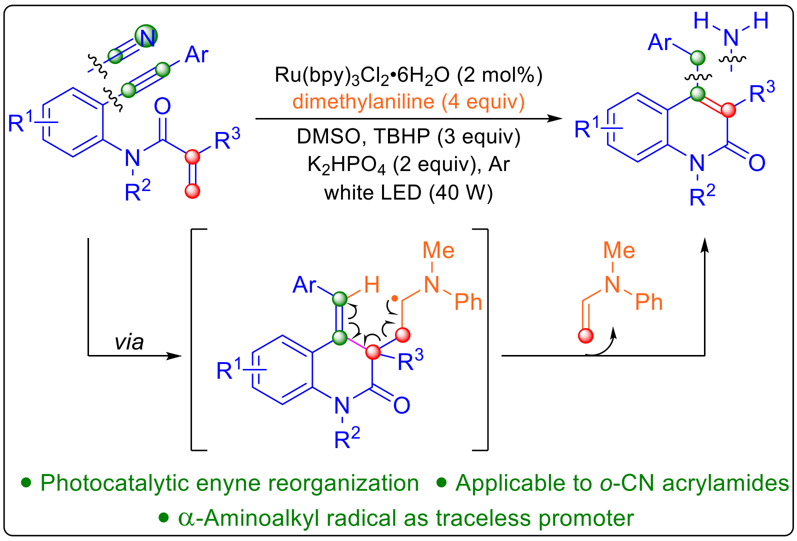
Abstract: Herein we report a visible-light-induced, α-aminoalkyl radical-mediated cascade reaction of 1,7-enynes that establishes a unique ring-closing enyne transformation pathway which occurs with concomitant loss of a methylene moiety. The α-aminoalkyl radical derived from *N*,*N*-dimethylaniline was demonstrated to be a traceless promoter of enyne reorganization leading to 4-alkylquinolinones. The reaction can also be extended to nitrile-substituted acrylamide systems, leading to carbostyrils. Experiments with deuterated *N*,*N*-dimethylaniline-*d6* ($PhN(CD_3)_2$) established the involvement of 1,5-H atom transfer in the mechanism.



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2. Upreti, G. C.; Singh, T.; Khanna, K.; Sahoo, D; Singh, A.; *Org*. *Lett*. **2024**, *26*, 17, 3652–3656.
3. Upreti, G. C.; Singh, T.; Chaudhary, D.; Singh, A.; J. *Org*. *Chem*. **2023**, *88*, 16, 11801–11808.
4. Upreti, G. C.; Singh, T.; Khanna, K.; Singh, A.; *J. Org*. *Chem*. **2023**, *88*, 4422−4433.
5. Upreti, G. C.; Singh, T.; Ranjan, S.; Gupta, R. K.; Singh, A.; *ACS Omega* **2022**, *7*, 29728−29733.
6. Singh, T.; Upreti, G. C.; Arora, S.; Chauhan, H.; Singh, A. *J. Org*. *Chem*. **2023**, *88*, 5, 2784–2791.

Bio-sketch

Profile

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Biosketch:
Ph.D.: Indian Institute of Technology Kanpur, Supervisor: Dr. Anand Singh (July 2018-May 2024)
M.Sc.: Kumaun University Nainital, Uttarakhand (2017)
B.Sc.: Kumaun University Nainital, Uttarakhand (2015)

Awards/achievements
Outstanding PhD thesis award (June 2024)
INSPIRE Fellowship (2018)
INSPIRE Scholarship (2012)
INSPIRE Award (2011)
GATE (2018)
NET (2018)
National means-cum Merit Scholarship" (NMMS) 2008-2012

Representative Publications:

1. Upreti, G.C.; Singh, T.; Khanna, K.; Sahoo, D.; and Singh, A. *Org. Lett*. **2024**, *26*, 17, 3652–3656.
2. Upreti, G.C.; Sahoo, D., and Singh, A. *Eur. J. Org. Chem*. **2024**, e202400640, doi.org/10.1002/ejoc.202400640 (Just accepted).
3. Upreti, G.C., Singh, T., Chaudhary, D. and Singh, A. *J. Org. Chem.* **2023**, *88*, 11801-11808.
4. Upreti, G.C., Singh, T., Khanna, K. and Singh, A. *J. Org. Chem*. **2023**, *88*, *7*, 4422–4433.
5. Upreti, G.C., Singh, T., Ranjan, S., Gupta, R.K. and Singh, A. *ACS Omega*, **2022**, *7*, 29728−29733.

6. S. R. Nasireddy, Upreti, G.C, A. Singh, Eur. J. Org. Chem. 2024, 27, e202400114. https://doi.org/10.1002/ejoc.202400114
7. Singh, T., Upreti, G.C., Arora, S., Chauhan, H. and Singh, A. *Org. Biomol. Chem.*, **2023,** DOI: 10.1039/d3ob00923h.
8. Singh, T., Nasireddy, S.R., Upreti, G.C., Arora, S. and Singh, A. *Org. Lett*. **2023**, *25*, *30*, 5558–5562.
9. Singh, T., Upreti, G.C., Arora, S., Chauhan, H. and Singh, A. *J. Org. Chem*. **2023**, *88*, *5*, 2784–2791.
10. Garg, P., Upreti, G.C. and Singh, A. *J. Org. Chem.* **2022**, *87*, 7219−7228.
11. Singh, T., Panday, P., Upreti, G.C., Ranjan, S., Gupta, R.K. and Singh, A. *Org. Biomol. Chem.*, **2022**, *20*, 4522–4525.

Title: Multifunctional surfactants derived from amino acids and their interactions with Bovine Serum Albumin (BSA)

Name: Sumedha Gupta
Indian Institute of Technology, Kanpur
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Abstract:

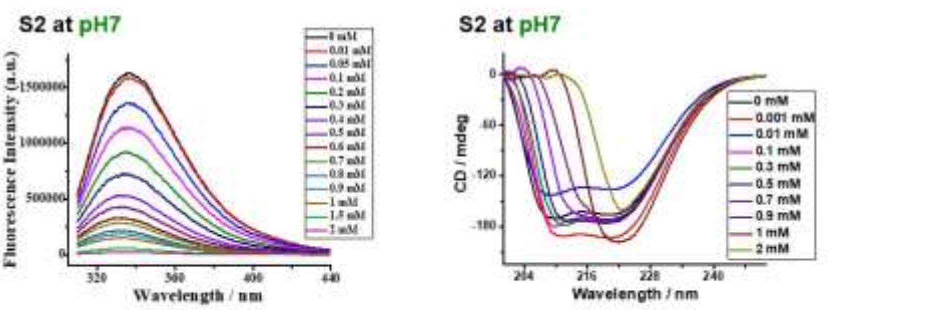
Amino acid-based surfactants are considered to be greener alternatives to traditional surfactants. However, multifunctional amino acid-based surfactants have never been reported in the past. They have numerous applications in food, pharmaceutical and cosmetic industries world-wide. When a protein is treated with a surfactant, it can either stabilize or destabilize the protein by largely affecting its dynamics.

Inspired by the results obtained from the studies of various amino acid-based surfactants with BSA, we have designed two anionic surfactants (**S1** and **S2**) and four bolaamphiphilic surfactants (**S3**, **S4**, **S5** and **S6**) and studied their interactions with BSA. So far, amino acid-based surfactants containing only one carboxylic acid as a head group have been studied. Our studies are aimed at understanding the effect of multiple anionic head groups on the surfactants and to study the effect of pH and temperature on the surfactants containing multiple oppositely charged functional groups.

Figure/Scheme (if any):

Quenching of fluorescence intensity of BSA by the surfactant **S2** at different concentrations

Conformational changes in secondary structure of BSA by the surfactant **S2** at varying concentrations



References and Notes:

1. Ghosh *et al., J. Phys. Chem. B.* **2015,** *119*, 7804–7815
2. Halder *et al., J. Photochem. Photobiol. B. Biol.* **2021,** *225*, 112351

Bio-sketch

Profile

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Biosketch:
I am a fourth year PhD student pursuing PhD (Chemistry) from Indian Institute of Technology, Kanpur under the supervision of Prof. Ramesh Ramapanicker. I have completed my M.Sc. Chemistry from Kurukshetra University, Kurukshetra with a CGPA of 9.18. I have qualified GATE 2021 with a GATE score of 684 and have secured AIR 239. I am currently working on the design and development of amino acid-based surfactants containing multifunctional head groups and studying their interactions with the protein. My research work also includes tuning the properties of sugar molecules attached to a peptide sequence in order to study their gelation behaviour by varying the hydrophilicity.

Representative Publications:

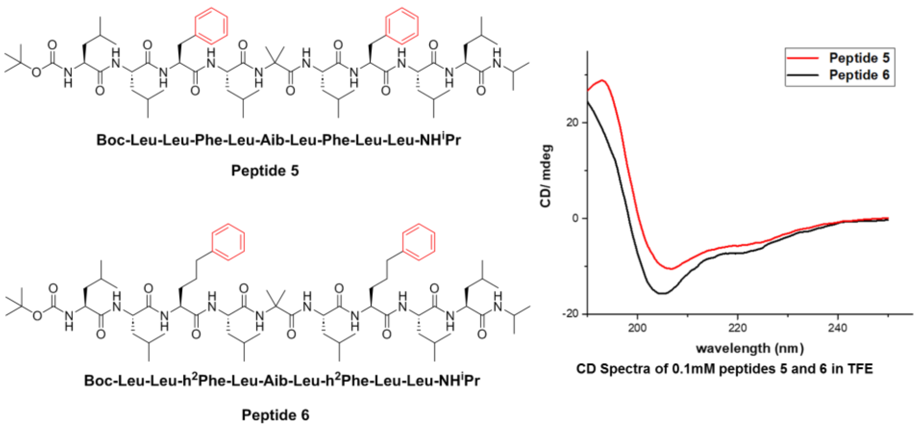
1.

Title: Use of homologated phenylalanine residues to control folding of oligopeptides

Name: Vikrant Vini
Institution: Indian Institute of Technology Kanpur
(Email: vikrantv21@iitk.ac.in)

Abstract: Interactions between aromatic side chains of amino acids are known to stabilize the fold and assembly of short peptides. The aromatic π…π and C-H…π interactions have been widely explored in the design of short peptides with specific folding and aggregation patterns. Different set of peptides containing homologs of phenylalanine were designed to study the effect of lengthening of the aromatic side-chains on inducing intra or intermolecular aromatic ring interactions and thus stabilizing the secondary structure of helices.

Figure/Scheme (if any):



CD Spectra of 0.1mM peptides 5 and 6 in TFE

References and Notes:

1. Chacko *et al*., *Eur. J. Org. Chem.* **2012**, 7120–7128
2. Mahalakshmi *et al*., *J. Peptide Res*. **2005**, *65*, 113-129

Bio-sketch

Profile

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Biosketch:
I am a fourth year PhD student (Chemistry) from Indian Institute of Technology, Kanpur under the supervision of Prof. Ramesh Ramapanicker. I completed my M.Sc. in Chemistry from Indian Institute of Technology Jodhpur with a CGPA of 8.69. During my M.Sc. I did a one-year project in developing [3+2] cycloaddition reactions for synthesis of heterocycles.
I am currently working on designing oligopeptides containing side-chain modified amino acid residues with specific folding and aggregation patterns.

Representative Publications:

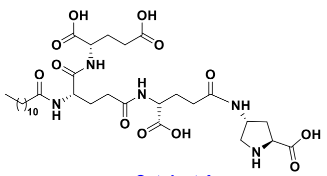
1. A. Chauhan, V. Vini, A. Kumar and R. D. Erande, *Org. Bimol. Chem.*, 2024, **22**, 6690-6694.

Title: "Surfactant Like Water Soluble Molecules" for Asymmetric Organocatalysts.

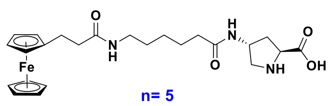
Name: Sruthi Manoharan, Susanta Kumar Behera and Ramesh Ramapanicker*
Institution: Indian Institute of Technology Kanpur.
(Email: sruthi22@iitk.ac.in)

Abstract: Asymmetric organocatalysis has received a lot of attention in the recent past and is seen as a relatively environmentally benign method of catalysis. Several attempts have been made to use water-soluble organocatalysts with the possibility of recovering the catalyst. However, barring a few isolated examples, most of the reactions performed in aqueous media result in reduced selectivity. The use of water-soluble organocatalysts is still not a viable option for large-scale synthesis. In light of this, we have designed surfactant-like organocatalysts that are expected to form micelles in an aqueous solution and would isolate the organic reactants from an aqueous environment which may result in increased selectivity and yield. The project's expected outcome is the development of water-soluble catalysts that are effective in various asymmetric reactions and are environmentally friendly.

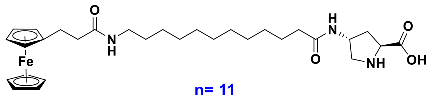
Figure/Scheme (if any):



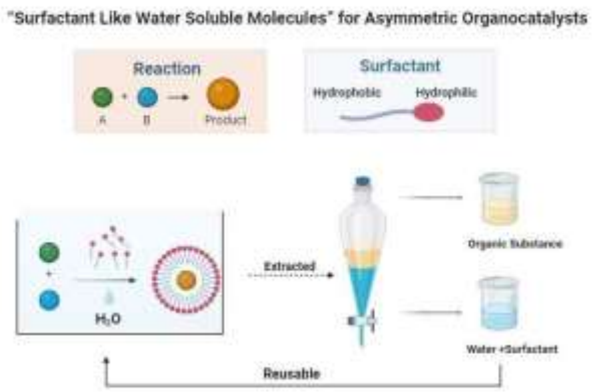
Catalyst A



n= 5
Catalyst B



n= 11
Catalyst C



References and Notes:

1. Hayashi, Angew. Chemie - Int. Ed. 2006, 45 (6), 958–961.
2. Mase, N.; Nakai, Y.; Ohara, N.; Yoda, H.; Takabe, K.; Tanaka, F.; Barbas, C. F. J. Am. Chem. Soc. 2006, 128 (3), 734–735.
3. Al-Momani, L.; Lataifeh, A. Ind. Eng. Chem. Res. 2022, 61 (6), 2417–2424.

Bio-sketch

Profile

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Biosketch:

I am pursuing my PhD at IIT Kanpur as a PMRF Fellow under the supervision of Prof. Ramesh Ramapanicker, specialising in peptide chemistry. My research focuses on the design, synthesis, and application of peptides in advanced chemical systems, with an emphasis on developing surfactant-like organocatalysts for asymmetric reactions. I completed my MSc in Applied Chemistry at Calicut University in 2018, where I secured the first rank and received several academic awards, including the INSPIRE Fellowship (2020) and GATE (2022). Prior to joining IIT Kanpur in 2022, I gained professional experience as a quality controller at Ernad Pigments, where I conducted chemical and physical testing of cement in accordance with BIS standards. My current work aims to develop eco-friendly, water-soluble catalysts that improve selectivity for large-scale applications in asymmetric synthesis.

Title: Asymmetric Counteranion-Directed Catalysis: A Powerful Concept in Organic Synthesis*

*[Post-doctoral research work: *The research was conducted at Max-Planck-Institut für Kohlenforschung, Department of Homogeneous Catalysis, Germany, under the supervision of Prof. Benjamin List*]

Santanu Ghosh

Current Affilation: Assistant Professor, Department of Chemistry, Shiv Nadar Institution of Eminence, Delhi NCR, NH-91, Dadri, Gautam Buddha Nagar, Uttar Pradesh-201314, India
Email: santanu.ghosh@snu.edu.in

Abstract:

Asymmetric counteranion-directed catalysis (ACDC), also known as chiral anion catalysis, induces enantioselectivity through the ion pairing or weak coordination of a chiral, enantiomerically pure anion provided by the catalyst with the cationic intermediate in a reaction.[1] The term asymmetric counteranion-directed catalysis was coined in 2006 by List, and since then, this theory has been extensively utilized for many challenging asymmetric transformations.[2] Herein, we showcase our recent achievements in challenging asymmetric cycloaddition and protolactonization reactions utilizing the ACDC concept. Our established method enables the creation of multiple stereocenters in a single step, producing several advanced enantiopure intermediates for the synthesis of bioactive molecules and fragrance ingredients.[3] This strategy allows us to bypass multistep synthesis, eliminate the use of toxic metals in catalysis through a greener organocatalytic approach, and make the process more environmentally friendly and atom-economical.

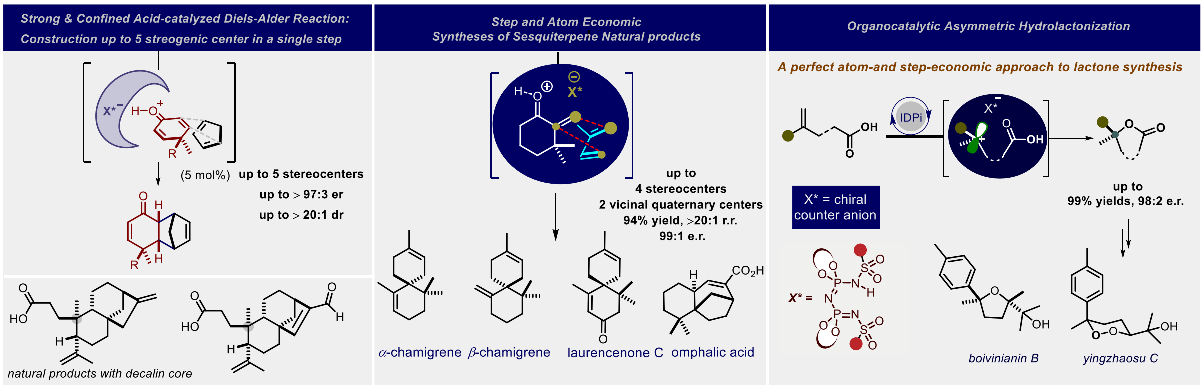

Figure 1: ACDC in Asymmetric Cycloaddition and Protolactonization Reaction.

References and Notes:

1. Mahlau, M.; List, B. *Angew. Chem. Int. Ed*. **2013**, *52*, 518–533.
2. Mayer, S.; List, B. *Angew. Chem. Int. Ed.* **2006**, *45*, 4193–4195.
3. (a) Ghosh, S.; Das, S.; De, C. K.; Yepes, D.; Neese, F.; Bistoni, G.; Leutzsch, M.; List, B. *Angew. Chem. Int. Ed.* **2020**, *59*, 12347–12351. (b) Ghosh, S.; Erchinger, J. E.; Maji, R.; List, B. *J. Am. Chem. Soc.* **2022**, *144*, 6703–6708. (c) Maji, R.; Ghosh, S.; Grossmann, O.; Zhang, P.; Leutzsch, M.; Tsuji, N.; List, B. *J. Am. Chem. Soc.* **2023**, *145*, 8788−8793.

Bio-sketch

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Biosketch:
Dr. Santanu Ghosh completed his Ph.D. in 2015 from the Indian Institute of Science Education and Research (IISER) Bhopal, India, under the supervision of Prof. Alakesh Bisai. His research focused on the catalytic enantioselective construction of vicinal all-carbon quaternary stereogenic centers and the total synthesis of dimeric cyclotryptamine alkaloids. He then moved to the University of California, Santa Barbara, as a SERB Indo-US Postdoctoral Fellow, where he conducted postdoctoral research under Prof. Armen Zakarian. There, he worked on the enantioselective alkylation of 2-alkylpyridines controlled by organolithium aggregation. In 2018, Dr. Ghosh joined the Max-Planck-Institut für Kohlenforschung, Germany, as a Max-Planck Postdoctoral Fellow in the Department of Homogeneous Catalysis. Under the mentorship of Prof. Benjamin List (Nobel Laureate in Chemistry, 2021), he gained expertise in using chiral weakly coordinating and highly confined anions in asymmetric organocatalysis. In 2023, he joined Shiv Nadar Institution of Eminence as an Assistant Professor, where he began his independent career. His research interests include natural product synthesis, asymmetric catalysis, and new reaction discovery. Dr. Ghosh values collaboration and knowledge exchange as essential tools for advancing skills and innovation in his field.

Representative Publications:

1. Maji, R.; Ghosh, S.; Grossmann, O.; Zhang, P.; Leutzsch, M.; Tsuji, N.; List, B.* *J. Am. Chem. Soc.* 2023, 145, 8788−8793.
2. Ghosh, S.; Erchinger, J. E.; Maji, R.; List, B.* *J. Am. Chem. Soc.* **2022**, *144*, 6703–6708.
3. Ghosh, S.; Das, S.; De, C. K.; Yepes, D.; Neese, F.; Bistoni, G.; Leutzsch, M.; List, B.* *Angew. Chem. Int. Ed.* **2020**, *59*, 12347–12351.
4. Gladfelder, J.; Ghosh, S.; Podunavac, M.; Cook, A. W.; Ma, Y.; Woltornist, R. A.; Keresztes, I.; Hayton, T. W.; Collum, D. B.; Zakarian, A.* *J. Am. Chem. Soc.* **2019**, *141*, 15024−15028.
5. Ghosh, S.; Chaudhuri, S.; Bisai, A.* *Org. Lett.* **2015**, *17*, 1373–1376.
6. Ghosh, S.; Bhunia, S.; Kakde B. N.; De, S.; Bisai, A.* *Chem. Commun.* **2014**, ***50***, 2434–2437.
7. Ghosh, S.; De, S.; Kakde B, N.; Bhunia, S.; Adhikary, A.; Bisai, A.* *Org. Lett.* **2012**, *14*, 5864–5867.
8. Ghosh, S.; Kinthada, L. K.; Bhunia, S.; Bisai, A.* *Chem. Commun.* **2012**, *48*, 10132–10134.

Dispirocyclic Orthoester via an Acetal Oxo-Carbenium Ion: Total Syntheses of Aculeatins A, B, D, and 6-*epi*-D

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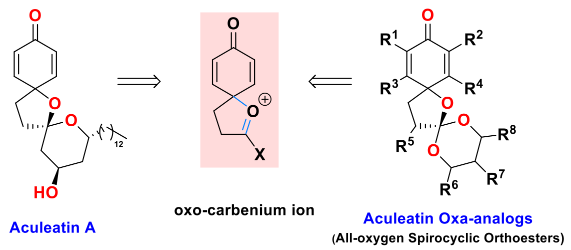
Abstract: Hypervalent iodine chemistry[1] has long been proven to be a valuable tool for the synthesis of cyclohexadienone-based spirocyclic lactone and ethers. However, the synthesis of spirocyclic orthoesters using hypervalent iodine chemistry is unknown thus far. Further, cyclohexadienone-spirocycles represent intricate synthetic targets, a fascinating category of compounds featuring two or more rings interconnected through a single atom commonly present in Aculeatin-type natural products. On the other hand, orthoesters are compounds having a sp^3-hybridized carbon atom bonded to three alkoxy groups known for their sensitivity toward acid and heat. We have developed a spiroacetal-oxacarbenium ion-based cascade methodology that accesses diversified skeletons having cyclohexadienone-linked all-oxygen dispirocyclic orthoesters. Further, this developed method has also been utilized as a key transformation for accomplishing a unified total synthesis of Aculeatin A, B, and D.[2,3] Aculeatin natural products showed high cytotoxicity against the KB cell line (IC_{50}=1.7 μM; IC_{50}=2.0 μM; IC_{50}=1.6 μM and IC_{50} of 0.9 μM respectively) and also antiprotozoal activity against some *Plasmodium* and *Trypanosoma* species alongside the antimalarial activity. Our design and synthesis of Oxa-Aculeatin analogs and the total synthesis of Aculeatin natural products will be discussed.



References and Notes:

1. Singh, F. V.; Kole, P. B.; Mangaonkar, S. R.; Shetgaonkar, S. E. *Beilstein J. Org. Chem.* **2018**, *14*, 1778–1805.
2. Heilmann, J.; Mayr, S.; Brun, R.; Rali, T.; Sticher, O. *Helv. Chim. Acta* **2000**, *83*, 2939–2945.
3. Heilmann, J.; Brun, R.; Mayr, S.; Rali, T.; Sticher, O. *Phytochemistry* **2001**, *57*, 1281–1285.

Bio-sketch

Profile

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Biosketch: Manoj Kumar was born in Adooka, Jhunjhunu, Rajasthan, India in 1998. After completing his B.Sc. in Chemistry (Hons.) at Delhi University, Delhi, India, in 2018, he moved to IIT Roorkee, Uttarakhand, India, for his M.Sc., where he spent two significant years learning about synthesis in detail. Upon completing his M.Sc., he joined Dr. Parthasarthi Subramanian at the Department of Chemistry, IIT Kanpur, Uttar Pradesh, where he is currently pursuing his Ph.D. His research interest mainly involves developing cascade reactions and utilizing these developed reactions in the Total synthesis of complex natural and unnatural molecules. Apart from developing cascade methodology, he is currently involved in the Total synthesis of the Aspidospera alkaloids.

Representative Publications:

1. Parammal, A.; Singh, S.; **Kumar, M**.; Xavier, J. S.; Subramanian, P. Robust Synthesis of Terpenoid Scaffolds under Mn(I)-Catalysis. *J. Org. Chem.* **2023**, *88*, 10761–10771.
2. Singh, S.; Parammal, A.; **Kumar, M.**; X, J. S.; Subramanian, P. Iso -Pentadienyl Carbonate as a Five Carbon Synthon in Manganese(I)-Catalyzed Selective Linear 1,3-Dienylation. *Chem. – A Eur. J.* **2023**, *29*, e202301632.
3. Parammal, A.; **Kumar, M.**; Singh, S.; Xavier, J. S.; Subramanian, P. The Total Synthesis of Aspidofractinine and Related Alkaloids. *European J. Org. Chem.* **2023**, *202300960*.
4. **Kumar, M.**; Singh, S.; Subramanian, P. Synthesis of Dispiro-Orthoester via an Acetal Oxo-Carbenium Ion. *Chem. Commun.* **2024**. https://doi.org/10.1039/D4CC03031A. (Just accepted)

Bio-Sketches – Session Chairs

FORCE-IICS 2024 Conference
October 3 – 6, 2024

@Uday Samudra Backwater Resort,
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Bio - Sketch

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PhD @ IIT Kanpur, UP, INDIA (Supervisor: Prof. Vinod K. Singh)
Postdoc @ University of California, Berkeley, CA, USA (Mentor: Prof. Richmond Sarpong)

Independent Career:
@IISER Bhopal (2009 – 2019)
@IISER Kolkata (2019 – till date)

PhD Guided: **25** Current PhD Students: **15** BS-MS Guided: **18** Project Assistant: ~**65**
Extramural Funding: 14 Extramural Fundings (**11** completed & **3** ongoing)

Research Focus: Strategies/Methodologies for Structurally Intriguing Natural Product of Biological Relevance

Representative Publications:
Chem. Sci. **2022**, 13, 11666; *ACS Catal.* **2023**, 13, 2118; *Chem. Sci.* **2023**, 14, 8047; *Chem. Sci.* **2024**, 15, 9164; *Chem. Sci.* **2024**, 15, 14946;

Position held:
- Professor (May 2019 - till date): Dept. of Chemical Sciences, IISER Kolkata
- Professor (2018 - 2020): Dept. of Chemistry, IISER Bhopal; Associate Professor (2013 – 2018); Assistant Professor (2009 – 2013)
- Post-Doctoral (2006 –2009): Dept. of Chemistry, UC Berkeley, CA, USA.

Awards & Recognitions:
- Fellow, Royal Society of Chemistry (FRSC), (March 2023)
- STARS-MoE 2023 Grant
- Prof. A. Srikrishna Memorial Lecture 2023 (UoH)
- ‘CDRI Award’ 2022 for Excellence in Drug Research (2022)
- SERB Special Call on 'Reagentless Chemistry' 2022
- Prof. Dhananjay Nasipuri Memorial Award 2021 (ICS)
- Silver Medal, Chintan Rasayan Sanstha (CRS) 2021 (June 2021)
- ‘SERB-STAR Award’ (2021-2024)
- ‘Bronze Medal’, CRSI, India (July 2020)
- Fellow, Indian Chemical Society (FICS), (July 2020)
- Young Scientist Award by CRSI, India (July, 2018)
- Young Scientist Award by the BRNS, DAE (2011-2014) through a research grant
- DST Fast-Track Research Project (March, 2013-February, 2016) for Young Scientist
- GRC Travel Grant, 17th GRC on Stereochemistry (2008), RI, USA

Bio-Sketch

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Career Profile:

2015-present	*Senior Professor*, IACS
2010-2015	*Professor*, IACS.
2006-2010	*Associate Professor*, IACS
2005-2006	*Assistant Professor*, IACS
2002-2005	*Senior Lecturer*, IACS
2000-2002	*Post-Doctoral Research*, Massachusetts Institute of Technology (MIT), USA
1995-1999	*PhD*, CSIR-Indian Institute of Chemical Technology/Osmania University, Hyderabad

Awards/Achievements and Fellowships:

- Fellow of the Royal Society of Chemistry (FRSC) – 2022
- Featured in *'75 under 50'* Scientists Shaping Today's India - 2021
- Fellow, Indian Academy of Sciences (FASc) - 2017
- Materials Research Society of India (MRSI) Medal - 2017
- CRSI (Chemical Research Society of India) Bronze Medal – 2011
- Fellow, West Bengal Academy of Science & Technology (FAScT) – 2008
- Ramanna Fellowship Award of DST, India – 2006-2009
- B. M. Birla Science Prize in Chemistry – 2006

Publications:

1. *ACS Medicinal Chemistry Letters* 2024.
2. *ACS Applied Nano Materials* 2024, *7*, 4946-4959.
3. *Chem. Eur. J.* 2023, *29*, e202300928.
4. *Langmuir* 2023, *39*, 15690–15704.
5. *Anal. Chem*. 2023, *95*, 13638-13648.
6. *Chem. Commun.* 2018, *54*, 9929-9932.
7. *Angew. Chem. Int. Ed.* 2011, 5*0*, 11243-11247.

Bio-sketch

Profile

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Biosketch: Geetharani was born and raised in Madurai, Tamilnadu, India. She began her independent research career as an Assistant Professor at department of inorganic and physical chemistry, Indian Institute of Science Bangalore, India in 2016. She was promoted to an Associate professor in 2022. She is a recipient of DST-Inspire Faculty Award. She has been elected as Young Scientist/Affiliate by all three Science Academies in India. She received the SERB-Women Excellence Award from the President of India. She is also an Editorial member of Chemistry – An Asian Journal and a member of the Early Career Advisory Board of the European Journal of Inorganic Chemistry. Her research interests are in the areas of catalysis, main group and organometallic chemistry.

Representative Publications:

1. Keerthika, K.; Bazil Muhammed, S.;Geetharani, K.* Synthesis of Trifluoromethylated Ketones from ,-Unsaturated Ketones via Catecholboron Enolates, **J. Org. Chem., 2024**.
2. Meher, N.; Suryavansi, M.; Geetharani, K.* Regioselective Hydroboration of Unsymmetrical Internal Alkynes Catalyzed by Cobalt Pincer-NHC Complex, **Org. Lett., 2024**, *26*, 5862-5867.
3. Keerthika, K.; Bazil Muhammed, S.;Geetharani, K.* A Metal-free and Operationally Simple Radical Trifluoromethylative Borylation of Unactivated Alkenes, **Chem. Eur.J., 2023, e202303468.**
4. Paul, S.; Verma, P. K.; Kashyap, A.; Mondal, R.; Geetharani, K.* Approach to the Synthesis of gem-Thiolated Alkylboronates via Cobalt-Catalyzed Diboration of Aldehydes, **Org. Lett., 2023**, 25, 2901-2906.
5. Meher, N. K.; Verma, P. K.; Geetharani, K.* Cobalt-Catalyzed Regioselective 1,2-Hydroboration of N-Heteroarenes, **Org. Lett., 2023, 25, 87-92**
6. Verma, P. K.; Meher, N. K.; Geetharani, K.* Homolytic Cleavage of Diboron(4) Compounds by Diazabutadienes. *Chem Commun.* **2021**, *57*, 7886 – 7889. Highlighted on the Cover Page of the Article.
7. Verma, P. K.; Souvik, M.; Geetharani, K.,* Efficient Synthesis of Aryl Boronates via Cobalt-Catalyzed Boryla-tion of Aryl Chlorides and Bromides. *ACS Catal.* **2018**, *8*, 4049-4054. Highlighted in Synfacts 2018, 14(07), 0746.

Bio-sketch

Profile

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Biosketch:

Ph.D. (2006), Indian Institute of Science, Bangalore, India.
Postdoctoral Research Fellow (2006-2008), Department of Chemistry and Institute of Theoretical Science, University of Oregon, Eugene, United States.
Alexander von Humboldt Research Fellow (2008-2009) and subsequently Postdoctoral Research Associate, Max Planck Institute of Colloids and Interfaces, Potsdam, Germany.
Postdoctoral Fellow (2010-2011), Institute of Physics, Bhubaneswar, India.
Assistant Professor (2011), Department of Chemistry, IIT Roorkee.
Associate Professor (Present), Department of Chemistry, IIT Roorkee.

Representative Publications:

1. Borah, R.; Debnath, P. *Soft Matter* **2016**, *12*, 4406-4417.
2. Ahamad, N.; Debnath, P. *Phys. A (Amsterdam, Neth.)* **2020**, *549*, 124335.
3. Shukla, P.; Ahamad, N.; Debnath, P. *Macromol. Theory Simul.* **2022**, *31*, 2100056.
4. Shukla, P.; Pathak, N.; Debnath, P. *Phys. Scr.* **2024**, *99*, 035946.

Bio-sketch

Profile

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Prof. Anuj Sharma obtained his Ph.D. in Organic Chemistry from CSIR-IHBT, Palampur in 2006. Afterwards, he held a post doc at Katholeik University, Leuven Belgium with Prof. Erik Van der Eycken and later, a NIH post doc at the University of Arizona, USA under Prof. Laurence Hurley till 2011. He joining IIT Roorkee as an Assistant Professor thereafter and currently a Professor in the Department of Chemistry, IIT Roorkee. His research interest is broadly in the field of synthetic organic chemistry, specifically radical mediated environmentally benign organic transformations, visible light photoredox catalysis and mechanochemistry based organic synthesis.

Representative Publications:

1. R. I. Patel, B. Saxena, and **A. Sharma***, "General electron-donor-acceptor complex mediated thioesterification reaction via site-selective C-H functionalization using aryl sulfonium salts" *Green Chem.* **2024**, advance article, DOI: 10.1039/d4gc03768e.
2. R. Kumar, A. Sharma and **A. Sharma***, "Mechanochemically induced Thianthrenium Salts-Based Arylation of Diverse Heterocyclic Scaffolds" *ASC Sustainable Chem. Eng.* **2024**, *12*, 12808-12818.
3. N. Singh, A. Sharma, J. Singh, A. P. Pandey, and **A. Sharma ***, "Visible Light-induced EDA-Mediated C-3 Coupling of Quinoxalin-2(1H)-ones with Unactivated Aryl Iodides" *Org. Lett.* **2024**, *26*, 6471-6476.
4. A. Sharma, J. Singh, and **A. Sharma***, "Synthesis of Quinazolinones and Benzothiazoles Using α-Keto Acids under Ball Milling" *J. Org. Chem.* **2024**, *89*, 5229-5238.
5. B. Saxena, R. I. Patel, S. Sharma and **A. Sharma***, "Mechanochemical-assisted decarboxylative sulfonylation of α,β-unsaturated carboxylic acids with sodium sulfinate salts" *Green Chem.* **2024**, *26*, 2721-2729.

Bio-sketch

Profile

Dr. Rambabu Chegondi

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Rambabu Chegondi received his M.Sc. (2003) degree from University of Hyderabad and completed Ph.D. (2009) in Organic Synthesis from Indian Institute of Chemical Technology (CSIR-IICT), Hyderabad under the supervision of Dr. S. Chandrasekhar. In 2009, he moved to The University of Kansas, USA to work with Prof. Paul R. Hanson as a postdoctoral researcher. He joined CSIR-IICT, Hyderabad as CSIR-Pool-Scientist (SRA) in 2014 as an independent researcher. He is currently a Principal Scientist at the OS&PC department, CSIR-IICT, focusing on the development of new enantioselective desymmetrization methodologies and new process development of key APIs. He has received the Eli Lilly Asia Best Thesis Award 2009, AVRA-Young Scientist Award-2019, Thieme Chemistry Journals Award, and SERB-STAR Award. He is an FRSC and currently an Editorial Advisory Board Member of Organic Letters.

Representative Publications:

1. 1. Jadhav, S. B.; Dash, S. R.; Maurya, S.; Nanubolu, J. B.; Vanka, K.; Chegondi, R. *Nat. Commun.* **2022**, *13*, 854.
2. 2. Gollapelli, K. K.; Patil, V. B.; Vinaykumar, A.; Chegondi, R. *Chem. Sci.* **2021**, *12*, 1544.
3. 3. Thopate, S.B.; Jadhav, S.B.; Nanubolu, J. B.; Chegondi, R. *ACS Catal.* **2019**, *9*, 10012.
4. 4. Gollapelli, K. K.; Donikela, S.; Manjula, N.; Chegondi, R. *ACS Catal.* **2018**, *8*, 1440.
5. 5. Gollapelli, K. K.; Kallepu, S.; Govindappa, N.; Nanubolu, J. B.; Chegondi, R. *Chem. Sci.* **2016**, *7*, 4748.

Bio-sketch

Profile

Name Aparna Ganguly, PhD

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Biosketch:

Dr Aparna Ganguly completed her graduation and post- graduation in Chemistry from University of Delhi and subsequently obtained her PhD in Materials Chemistry under the supervision of Professor A. K. Ganguli at IIT Delhi. After a short stint at teaching Physical Chemistry at Central University of Rajasthan, she moved back to the Nanoscale Research Facility, IIT Delhi as a scientist where she worked extensively on porous materials and their applications. In 2014, she joined the Royal Society of Chemistry where she is currently the Editorial Development Manager and manages the journal portfolio and their growth in India. As a part of her role, she works quite extensively with the scientific community, various Indian chemical societies, and researchers across various disciplines of Chemical Sciences and support the journal teams.

Bio-sketch

Profile

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Biosketch: Dr. Badsara obtained M.Sc. degree from Banaras Hindu University in 2006 and Ph.D. degree from the University of Hyderabad, India in 2013 (with Professor Deevi Basavaiah). During 2013-14, he was a postdoctoral fellow with Prof. Chin-Fa Lee at National Chung Hsing University, Taiwan. Since 2014, he is working as Assistant Professor at the University of Rajasthan, Jaipur India. His research interest mainly includes Electro-organic synthesis, transition metal-free approaches for organic synthesis and Baylis-Hillman chemistry.

Awards and Achievements

- Selected for the Chemical Research Society of India (CRSI) Bronze Medal -2025.
- ISCB Young Scientist Award-2019 in Chemical Sciences by Indian Society of Chemists and Biologists, India.
- DST INSPIRE Faculty Award-2015

Representative Recent Publications:

1. P. Jat, S. S. Badsara*, *J. Org. Chem.* **2024**, *89*, 12263-12276.
2. K. Ucheniya, P. Jat, A. Chouhan, L. Yadav, S. S. Badsara*, *Org. Biomol. Chem.*, **2024**, *22*, 3220-3224.
3. P. K. Jat, L. Yadav, A. Chouhan, K. Ucheniya, S. S. Badsara*, *Chem. Commun.*, **2023**, 59, 5415-5418.
4. K. Ucheniya, A. Chouhan, L. Yadav, P. K. Jat, S. S. Badsara*, *J. Org. Chem.*, **2023**, *88*, 6096.
5. A. Chouhan, K. Ucheniya, L. Yadav, P. Jat, A. Gurjar, S. S. Badsara*, *Org. Biomol. Chem.*, **2023**, *21*, 7643-7653.
6. P. K. Jat, K. K. Dabaria, R. Bai, L. Yadav, S. S. Badsara*, *J. Org. Chem.*, **2022**, *87*, 12975-12985.
7. Z-W. Chen, R. Bai, P. Annamalai, S. S. Badsara*, C-F. Lee*, *Chem. Asian J.* **2024**, Accepted article, doi.org/10.1002/asia.202400780

Bio-sketch

Profile

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Gangwal School of Medical Sciences and Technology
Chemistry/Nanoscience/Center for Engg in Medicine/
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Prof. Sandeep Verma has been working at the Department of Chemistry and as an affiliated faculty at Center for Nanoscience and Mehta Family Center for Engineering in Medicine, Indian Institute of Technology Kanpur. He is also an Honorary Adjunct Professor at School of Science, Royal Melbourne Institute of Technology University, Melbourne, and School of Agriculture, Biomedicine and Environment, La Trobe University, Melbourne, Australia. Affiliated Faculty. His research interests include chemical neuroscience, new antibiotics, and microfluidic devices. With over 250 publications and several patents, his work has been recognized by Shanti Swarup Bhatnagar Prize, Distinguished Alumnus Award of Banaras Hindu University, Society of Materials Chemistry Gold Medal, CRSI Silver Medal, and Swarnajayanti Fellowship, to name a few. He is an elected Fellow of Indian National Science Academy, Indian Academy of Sciences, National Academy of Sciences, and Indian National Academy of Engineering. He is an Associate Editor of Chemical Communications (RSC, UK). He served as Secretary, Science and Engineering Research Board, Department of Science and Technology (2019-2022). At present, Prof. Verma is leading Gangwal School of Medical Sciences and Technology, at IIT Kanpur.

Representative Publications:

1. Synthesis of a highly thermostable insulin by phenylalanine conjugation at B29 Lysine. *Commun. Chem. 161*, (**2024**) (https://doi.org/10.1038/s42004-024-01241-z)
2. Membrane-targeting, ultrashort lipopeptide acts as an antibiotic adjuvant and sensitizes MDR Gram-negative pathogens toward narrow-spectrum antibiotics. *Biomed. Pharmacother. 176*, 116810 (**2024**) (https://doi.org/10.1016/j.biopha.2024.116810)
3. Amyloid mimicking assemblies formed by glutamine, glutamic acid, and aspartic acid. *ACS Chem. Neurosci.*, **2024**, *15*, 2253-2264.
4. Peptide-triggered IL-12 and IFN-γ mediated immune response in $CD4^+$ T-cells against *Leishmania donovani* infection. *Chem. Commun.*, **2024**, *60*, 4092-4095.
5. Anti-proliferative, -migratory and -clonogenic effects of long-lasting nitric oxide release in HepG2 cells. *Chem. Commun.*, **2024**, *60*, 3527-3530.

6. Machine learning approaches for antibiotic development and prediction of microbial resistance. *Chem. Asian J.* (**2024**) (https://doi.org/10.1002/asia.202400102) (Review).

Bio-sketch

Profile

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Harinath Chakrapani completed his undergraduate and post-graduate studies in Chemistry from Loyola College (1994-97) and Indian Institute of Technology Madras (1997-99), respectively. In the fall of 1999, he moved to Duke University, USA to pursue his doctoral studies, which he completed in Dec. 2005. After a brief stint as a postdoctoral research associate at Wake Forest University, USA, he moved to the Center for Cancer Research, National Cancer Institute USA as a Visiting Fellow in Aug 2006. He joined Indian Institute of Science Education and Research Pune in July 2009 and is currently Professor. His primary research interests are in the area of physical and mechanistic organic chemistry, with applications in understanding biological responses to stress, circumventing mechanisms of antimicrobial resistance, and prodrug design and delivery.

Recent Publications

1. Manna, S.; Agrawal, R.; Yadav, T. Anand Kumar, T.; Kumari, P. Dalai, A.; Kanade, S. Balasubramanian, N. Singh, A.; **Chakrapani, H.** "Orthogonal Persulfide Generation through Precision Tools Provides Insights into Mitochondrial Sulfane Sulfur" *Angewandte Chemie International Edition* **2024**, in press https://doi.org/10.1002/anie.202411133
2. Chaudhary, B.S.; Anand Kumar, T.; Vashishta, A.; Tejasri, S.; Kumar, A. S.; Agarwal, R.; **Chakrapani, H.** "An Esterase-Cleavable Persulfide Donor with No Electrophilic Byproducts and a Fluorescence Reporter" *Chemical Communications*, **2024**, 60, 1727-1730.
3. Sawase, L.; Anand Kumar, T.; Mathew, A. B.; Khodade, V. S.; Toscano, J. P.; Saini, D. K.; **Chakrapani, H "**β-Galactosidase-activated nitroxyl (HNO) donors provide insights into redox cross-talk in senescent cells" *Chemical Communications*, **2023**, *59*, 12751-12754.
4. Sawase, L.; Jishnu, C.V.; Manna, S..; **Chakrapani, H.** "A modular scaffold for triggerable and tunable nitroxyl (HNO) generation with a fluorescence reporter" *Chemical Communications*, **2023**, *59*, 3415-3418.
5. Bora, P.; Sathian, M.B.; **Chakrapani, H.** "Enhancing Cellular Sulfane Sulfur Through β-glycosidase-Activated Persulfide Donors: Mechanistic Insights and Oxidative Stress Mitigation" *Chemical Communications*, **2022**, *58*, 2987–2990.
6. Bora, P.; Manna, S.; Nair, M.; Sathe, R.M.S.; Singh, S.; Adury, V.S.S.; Gupta, K.; Mukherjee, A.; Saini, D. K.; Kamat, S.S.; Hazra, A. B.; **Chakrapani, H.** "Leveraging an Enzyme/ Artificial Substrate System to Enhance Cellular Persulfides and Mitigate Neuroinflammation" *Chemical Science*, **2021**, *12*, 12939-12949.

Bio-sketch

Profile

Dr. Vishal Rai
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Dr. Vishal Rai obtained his Ph.D. in Chemistry from IIT Bombay under Prof. I. N. N. Namboothiri (2003-2008). He subsequently held a postdoctoral position and MITACS-Elevate fellow position in Prof. Andrei Yudin's group at the University of Toronto, Canada (2008-2011). His contributions to peptide macrocycles created the platform for Encycle Therapeutics. Later, he joined the Department of Chemistry at IISER Bhopal in 2011.

His research group is leading the development of chemical technologies for the *precision engineering of proteins*. They are also involved in synthesizing homogeneous antibody-conjugates, protein immobilization, and analytical tools for peptides and proteins. His research team wants to contribute to Society through homogeneous bioconjugates for directed cancer chemotherapeutics and surgical oncology. Besides, they are investing efforts to make small-molecule precision therapeutics possible in the future.

He is the Founder and Director of *Plabeltech Private Limited* (https://plabeltech.com). The state-of-the-art protein and antibody engineering technologies such as LDM®, Gly-Tag®, and Maspecter® empower the company. His team established the Precision Antibody Engineering CEnter (*SERB-PACE*) to meet India's technological demands in biologics. Also, he is the recipient of the Rashtriya Vigyan Puraskar: Shanti Swarup Bhatnagar, Swarnajayanti Fellowship, Ramanujan Fellowship, CRSI Bronze Medal, CDRI Award for excellence in drug research, SERB Technology Translation Award, RSC-WIS Young Scientist Award, DAE Young Scientist Award, among others.

He has received distinguished teacher awards, a G. D. Gokhale fellowship, and has been recognized as a pioneering investigator by Chemical Society Reviews (RSC, UK) and AsiaChem. He has served on the Editor-in-Chief search committee member for ACS publications. He is an advisory board member of *Chemical Science* and an ECB member of *ACS Chemical Biology*. He has been involved in scientific outreach activities as a NOST council member, ICBS national co-chair, and Asia representative in Commonwealth Chemistry. Also, he is an invited Fellow of the Royal Society of Chemistry (FRSC), UK.

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Profile

Name **Kiran Kumar Pulukuri**

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Biosketch:

Dr. Kiran earned his B.Sc in 2005 and M.Sc (Chemical Sciences) in 2007 from Pondicherry University. He subsequently joined the CSIR-IICT for his Ph.D. program, focusing on synthesis of complex natural products and glycopeptides under the guidance of Dr. T. K. Chakraborty. In 2013, he completed and submitted his thesis at CDRI-Lucknow, before proceeding to the Rice University for post-doctoral studies. There, he spent six years in the lab of Prof. K. C. Nicolaou as postdoctoral fellow and research scientist.

In 2019, Dr. Kiran started his independent career as an assistant professor in the Department of Chemistry at IISER-Tirupati. His research interests encompass a diverse range of topics, including Total Synthesis of Natural Products, Synthetic Methodology, Asymmetric Catalysis, Electro Organic Synthesis, and Natural Product-based Drug Discovery.

Representative Publications:

1. Asuthosh Panigrahy and Kiran Kumar Pulukuri*, *ChemRXIV*. **2023**, DOI: 10.26434/chemrxiv-2023-3fldg-v2.

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Profile

Abhijit Patra
Professor

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Abhijit Patra, earned his Ph.D. in 2009 from the University of Hyderabad, focusing on molecular nano/microcrystals. Following post-doctoral research at PPSM, ENS Paris-Saclay on photo-switchable materials, and at the University of Wuppertal as an Alexander von Humboldt fellow on conjugated polymer nanoparticles, he initiated his independent research career at the Indian Institute of Science Education and Research Bhopal in 2012. Currently serving as a Professor in the Department of Chemistry at IISERB, his research interests encompass multifunctional porous organic polymers and optical materials, leveraging fluorescent molecular and polymeric assemblies at nano/microscale.

Research Interests:

- Porous organic polymers for energy storage and environmental remediation
- Fluorescent optical materials based on molecular and polymeric assemblies

Awards and Honours:

- 2023: Fellow of The National Academy of Sciences, India, FNASc
- 2023: Chemical Research Society of India (CRSI) Bronze Medal
- 2018: Emerging Investigator: Journal of Material Chemistry C (Royal Society of Chemistry)
- Sept 2010 - June 2012: Alexander von Humboldt Fellowship awarded in Materials Science

Selected Recent Publications:

1. Das, S.; Batra, A.; Kundu, S.; Sharma, R.; Patra, A. *Chem. Sci.* **2024**, *15*, 102.
2. Dutta, T. K.; Das, S.; Sarkar, M.; Bhattacharjee, M.; Patra, A. *Chem. Mater.* **2024**, *36*, 8027.
3. Sarkar, S.; Dutta, T. K.; Mandal, B. P.; Patra, A. *Chem. Commun.* **2024**, *60*, 5010.
4. Giri, A.; Shreeraj, G.; Dutta, T. K.; Patra, A. *Angew. Chem. Int. Ed.* **2023**, e202219083.
5. Jaiswal, S.; Giri, A.; Mandal, D.; Sarkar, M.; Patra, A. *Angew. Chem. Int. Ed.* **2023**, *62*, e202312910.
6. Sarkar, M.; Patra, A. *Chem. Commun.* **2023**, *59*, 2584.
7. Kundu, S.; Chowdhury, A.; Nandi, S.; Bhattacharyya, K.; Patra, A. *Chem. Sci.* **2021**, *12*, 5874.
8. Hussain, M. W.; Bhardwaj, V.; Giri, A.; Chande, A.; Patra, A. *Chem. Sci.* **2020**, *11*, 7910.

Bio-sketch

Ramesh Ramapanicker
Professor

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Dr. Ramesh Ramapanicker received his PhD degree in 2007 from the Department of Organic Chemistry at the Indian Institute of Science Bangalore. He then worked as a postdoctoral researcher in the Department of Organic Chemistry and Biochemistry at the Uppsala University Sweden till 2010. In 2010, he joined the Department of Chemistry, Indian Institute of Technology Kanpur as an Assistant Professor and he was promoted to a Professor in July 2021. His research group works on the design and synthesis of oligopeptides containing unusual amino acids. The group is actively involved in introducing new functional and structural features to synthetic oligopeptides by careful design.

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Profile

Name **Khushbu Kushwaha**

Designation *Managar, Research Publishing*

Institution Wiley

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Homepage:

Biosketch:
Khushbu Kushwaha obtained her PhD in Organic Chemistry from the University of Delhi (India) in 2012. The topic of her research was the synthesis of azaphenothiazine-derived pharmacophores and their anticancer activity. She then relocated to Belgium and joined the organic synthesis group at the University of Antwerp (UA) as a postdoctoral research associate. At UA her work mainly focused on developing alternative and convenient methodologies for the synthesis of small and medium-sized nitrogen heterocycles. Further, she spent two years at the Department of Chemistry and Molecular Biology of Gothenburg University as a Visiting Researcher and worked on developing liquid chromophores. Overall, she published 20 research papers in high-impact journals. She joined Wiley-VCH in August 2019 as an Associate Editor and was promoted to Senior Associate Editor in July 2024. She has recently been promoted to Manager, Research Publishing, and has been managing a team of Assistant editors. She works for high-impact journals such as *Advanced Functional Materials, Chemistry-An Asian Journal*, and specialized journals such as the *Asian Journal of Organic Chemistry*. She has also been actively involved in outreach activities including community engagement through author workshops, institute visits, and organizing special collections.

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Profile

Name **Dr. Swagata Banerjee**

Designation: Associate Editor, Wiley

Institution: Wiley

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Biosketch: Swagata obtained her Ph.D. in Chemistry from Trinity College Dublin, Ireland. During her postdoctoral tenure, she worked on semiconductor photocatalysis (Technical University-Dublin), polymer-based luminescent oxygen sensors (University College Cork), and use of multifunctional nanomaterials in sensing and environmental remediation (Osmania University, & ICMR-National Institute of Nutrition, Hyderabad, India). Swagata worked as a senior subject matter expert at Journal of Visualized Experiments (JoVE). She joined Wiley as an in-house editor in 2023 and currently associated with Small, Advanced Optical Materials and Advanced Electronic Materials journals

Representative Publications:

1. Swagata Banerjee, N. Pavan Kumar, Adiraj Srinivas, Shibsekhar Roy, 'Core-shell Fe_3O_4@Au nanocomposite as dual-functional optical probe and potential removal system for arsenic (III) from Water' Journal of Hazardous Materials 375 (2019), 216–223.
2. Swagata Banerjee, Olga V Arzhakova, Alla A Dolgova, Dmitri B Papkovsky, 'Phosphorescent oxygen sensors produced from polyolefin fibres by solvent-crazing method', Sensors and Actuators B: Chemical 230 (2016), 434-441.
3. Swagata Banerjee, Suresh C Pillai, Polycarpos Falaras, Kevin E O'Shea, John A Byrne, Dionysios D Dionysiou, 'New insights into the mechanism of visible light photocatalysis', J. Phys. Chem. Lett. 5 (2014), 2543–2554.
4. Swagata Banerjee, Jonathan A. Kitchen, Sandra A. Bright, John E. O'Brien, D. Clive Williams, John M. Kelly and Thorfinnur Gunnlaugsson, 'Synthesis, spectroscopic and biological studies of a fluorescent Pt(II) (terpy) based 1,8-naphthalimide conjugate as a DNA targeting agent', Chem. Commun., 49 (2013), 8522-8524.
5. Swagata Banerjee, Emma B. Veale, Caroline M. Phelan, Samantha A. Murphy, Gillian M. Tocci, Lisa J. Gillespie, Daniel O. Frimannsson, John M. Kelly and Thorfinnur Gunnlaugsson, 'Recent Advances in the Developments of 1,8-Naphthalimide Based DNA Targeting Binders, Anticancer and Fluorescent Cellular Imaging Agents' Chem. Soc. Rev., 42 (2013), 1601-1618.

INTERDISCIPLINARY INITIATIVE IN CHEMICAL SCIENCES (IICS)

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