XXIII NOST - Organic Chemistry Conference

February 29th – March 3rd, 2024

Program & Abstracts

Venue: Welcome ITC Hotel, Bhubaneswar

NOST TRUSTEES

Prof. Ganesh Pandey (Chairman)
Distinguished Professor
Dept. of Chemistry, Institute of Science
BHU, Varanasi - 221 005

Prof. S. Chandrasekaran
Department of Organic Chemistry
IISc Bangalore
Bangalore - 560 012

Prof. Sukh Dev
1Ashirwaad, 120, ISKON Mega City
Bhavnagar - 364 001
Gujarat

Prof. S.V. Kessar
Department of Chemistry
Panjab University
Chandigarh - 160 014

Prof. Goverdhan Mehta
Distinguished and Prof. Kallam Anji Reddy
Chair Professor, School of Chemistry
University of Hyderabad, Hyderabad

Prof. Vinod K Singh (Secretary)
Department of Chemistry
IIT Kanpur
Kanpur

Dr. J. S. Yadav
Former Director (CSIR-IICT)
Provost & Director (Research)
Indrashil University

Program Schedule

XXIII NOST-Organic Chemistry Conference
Venue: Welcome ITC Hotel, Bhubaneswar
February 29th-March 3rd, 2024

Day 1, Thursday	**February 29, 2024**
14.00 to 16.00 h	**Arrival, Check-In, Lunch and Registration**

16.00 to 16.05 h	**Welcome Remarks by Chair-NOST Council** Krishna P Kaliappan (IIT Bombay)
16.05 to 16.15 h	**NOST-A Brief Overview by President-NOST** Ganesh Pandey (BHU, Varanasi)

Trustees & DST-SERB Session	
Session I **(16.15 to 19.35 h)**	**Chairpersons:** **Vinod Singh/Jerome Lacour/Harinath Chakrapani**
16.15 to 16.45 h	**Hidetoshi Tokuyama (Tohoku University, Japan)** '*Total Synthesis of Structurally Complex Alkaloids via Late-Stage Oxidative Transformations'*
16.45 to 17.15 h	**Andrew Lawrence (University of Edinburgh, UK)** *'Rethinking Enantiocovergent Reactions'*
17.15 to 17.45 h	**Nandita Madhavan (IIT Bombay)** '*Ready Access to Cyclic Peptides for Pharmaceutical Applications'*
17.45 to 18.15 h	**Prabha Ibrahim (ReRx Therapeutics, USA)** '*Role of Chemistry in Small Molecule Drug Disc & amp; Development'*
18.15 to 18.35 h	**P. Venkatakrishnan (IIT Madras)** '*Strained to Perform: Conformationally Locked m-Cyclophane Crown Cages C 60'*
18.35 to 18.55 h	**Anant Kapdi (ICT Mumbai)** '*Acceptor Caged Phosphine Ligands: Exploration of Novel Catalytic Reactivity and Mechanism'*
18.55 to 19.15 h	**Nadja Simeth (Goettingen University, Germany)** '*Opto-Bioinorganic Chemistry for Smart Biological Tools and Labeling Agents'*
19.15 to 19.35 h	**Rajesh Viswanathan (IISER Tirupati)** '*Biogenesis of Plant and Marine Natural Products –A Template for Biomimetic Synthesis'*
19.35 to 21.30 h	**Conference Mixer**

Day 2, Friday	**March 1, 2024**
Astra Zeneca Session	
Session II **(09.00 to 11.00 h)**	**Chairpersons** **Namrata Rastogi/Ravi P. Singh**
09.00 to 09.30 h	**Ramanarayanan Krishnamurthy (Scripps Research Institute, USA)** '*Organic Chemistry in the Pursuit of Chemical Origins of Life'*
09.30 to 10.00 h	**T. Punniyamurthy (IIT Guwahati)** '*Merging Strained Rings and C-H Functionalization: Efficient Synthetic Tool for Heterocyclic Compounds'*
10.00 to 10.20 h	**Garima Jindal (IISc, Bangalore)**

	'*Mechanistic Investigation of Ligand Enabled Dirhodium Catalyst Modification: Implication in Reactivity and Stereoselectivity*'
10.20 to 10.40 h	**Chandra M. Volla (IIT Bombay)** '*Allenes in Metal-Catalyzed C-H Activation Reactions*'
10.40 to 11.00 h	**Ch. Rambabu (CSIR-IICT, Hyderabad)** '*Copper-Catalyzed Asymmetric Hydrofunctionalization of Alkoxy-allenes*'
11.00 to 11.30 h	**Photo Session & TEA/COFFEE BREAK**

Cipla & Jubilant Life Sciences Session	
Session III **(11.30 to 13.00 h)**	**Chairpersons:** **N. Jayaraman/G. Sekar**
11.30 to 12.00 h	**Kana M. Sureshan (IISER, Thiruvananthapuram)** '*Two Structurally Different Polymers from a Monomer*'
12.00 to 12.30 h	**K. V. Radhakrishnan (NIIST, Thiruvananthapuram)** '*Harmonizing Tradition and Innovation: Unveiling Nature's Alchemy Through Multidisciplinary Scientific Exploration*'
12.30 to 13.00 h	**Vibha Tandon (CSIR-IICB, Kolkata)** *"Preclinical efficacy of Topoisomerase I targeting Small Molecule, PPEF and its in-situ nanosuspension against methicillin-resistant Staphylococcus aureus"*
13.00 to 14.00 h	**LUNCH BREAK**
14.00 to 19.30 h	**Sight Seeing Trip (Visit to Konark)**
20.00 to 22.00 h	**DINNER**

Day 3, Saturday	**March 2, 2024**
Panacea Biotech Session	
Session IV **(09.00 to 11.00 h)**	**Chairpersons** **S. Srivatsan/Vijaya Anand**
09.00 to 09.30 h	**Pritam Mukhopadhyay (JNU, New Delhi)** '*Molecular and Supramolecular Architectures for Applications in Singlet Fission and as Conductive and Piezoelectric Materials*'
09.30 to 10.00 h	**Hidehiro Sakurai (Osaka University, Japan)** *'Recent Progress in Sumanene Chemistry'*
10.00 to 10.20 h	**Amit Pawar (IIT Mandi)** *'Harnessing N-Chlorobenzamide as an Oxidizing Directing Group for Reverse Regioselective Annulation with Vinylsilanes: Synthesis and Applications of 4-Silylated Isoquinolones'*
10.20 to 10.40 h	**Biplab Maji (IISER Kolkata)** '*Dearomative Cycloaddition Reactions via Visible Light Energy Transfer Catalysis*'
10.40 to 11.00 h	**Beeraiah Baire (IIT Madras)** '*Exploring the Reactivity of (Indol-3/2-yl)pentyn-3-ols: Approaches to Natural carbazoles, Unnatural Dimeric-carbazoles and Cyclopenta[b]indoles*'
11.00 to 11.30 h	**TEA/COFFEE BREAK**

AVRA-IICT Session	
Session V **(11.30 to 13.10 h)**	**Chairpersons:** **D. Srinivasa Reddy/Raji Reddy**
11.30 to 12.00 h	**Viresh Rawal (University of Chicago, USA)** '*Methods and Strategies for the Synthesis of Intricate Molecules*'

12.00 to 12.30 h	**Saumen Hajra (CBMRI, Lucknow)** '*Asymmetric Total Syntheses of Complex Bioactive Natural Products'*
12.30 to 12.50 h	**Mrinmoy De (IISc, Bangalore)** '*Selective Antibacterial activity of Functionalized Nanomaterials'*
12.50 to 13.10 h	**Ishu Saraogi (IISER Bhopal)** '*Chemical Strategies to Address Protein Aggregation Diseases'*
13.10 to 14.00 h	**LUNCH BREAK**
Syngenta Session	
Session VI **(14.00 to 16.00 h)**	**Chairpersons:** **C. V. Ramana/N. Selvakumar**
14.00 to 14.30 h	**P. V. Ramachandran (Purdue University, USA)** '*Tapping the Potential of Borane-Amines'*
14.30 to 15.00 h	**Akhila Sahoo (University of Hyderabad)** '*Harnessing C(sp^3)-H Bonds with Bifunctional Reagents'*
15.00 to 15.20 h	**Praveen Kumar Vemula (ISTEM, Bengaluru)** '*Chemistry as a tool to develop biomedical technologies to solve unmet clinical needs'*
15.20 to 15.40 h	**S. Srinivasa Gopalan (National Institute of Immunology, New Delhi)** '*Chemical tools for unravelling the structure and function of glycoconjugates in living systems'*
15.40 to 16.00 h	**Nidhi Jain (IIT Delhi)** '*Visible light photoredox catalysis in organic transformations'*
16.00 to 16.30 h	**TEA/COFFEE BREAK**

PI Industries Session	
Session VII **(16.30 to 17.30 h)**	**(Flash Presentations)** **Chairpersons: S. Gharpure/P. Srihari/S. V. Ramasastry**
Flash presentations (5 minutes each)	
16.30 to 17.30 h	**Parthasarathi Subramaniam (IIT Kanpur)** *'Design and Synthesis of All-Oxygen Spirocyclic Orthoester: A Unified Total Synthesis of Aculeatin Natural Products'* **Utpal Bora (Tezpur University)** '*Studies on C-3 triaryl methylation of indoles and cyanation of arylhalides'* **Ramasamy Anandhan (University of Madras)** *'Photoredox/Electro-Catalysed Radical Cyclization Cascade of o-Alkynylated Benzamides'* **Sridhar Reddy (CSIR-IICT, Hyderabad)** *'Rollover cyclometallation of biarylamines/arylphenols for selective annulations with unsymmetrical alkynes'* **Guru B Ramani (IIT Jammu)** *'Practical Synthesis of Allenoates and Dihaloallenoates via Decomposition of Unprotected Alkynyl Hydrazones'* **Sukalyan Bhadra (CSIR-CSMCRI)** '*New Approaches for the Catalytic α-Functionalization of Ketones'* **Ganesh Venkataraman (IIT Kharagpur)** '*Nickel-Catalyzed Oxidative Cyclization of π-Systems* Over the Benchtop' **Ramesh Rasappan (IISER Thiruvananthapuram)** *'Organosilanes: Synthesis and Application of Solid TMSZnI in Cross-Coupling Reactions'*

Sun Pharma & BASF Session	
Session VIII (17.30 to 19.30 h)	**Chairpersons: Srinivas Oruganti/Diwan Rawat/Vishal Rai**
17.30 to 18.00 h	**Yong Rok Lee (Yeung Nam University, South Korea)** '*Construction of Biologically Interesting Aromatics via Benzannulation'*
18.00 to 18.20 h	**Parthasarathi Das (IIT-ISM, Dhanbad)** '*Expanding Discovery Chemistry Toolbox: From Concept to Practice'*
18.20 to 18.40 h	**Stellios Arseniyadis (Queen Mary University, London)** *"Revisiting Pd-AAA chemistry: Towards the development of active, selective, and stable single component chiral pre-catalysts"*
18.40 to 19.00 h	**Anil Kumar (BITS-Pilani)** *"Synthesis of N-Fused Polycyclic Heterocycles via Transition-Metal-Catalyzed Annulation Reactions"*
19.00 to 19.30 h	**Brian Stoltz (California Institute of Technology, USA)** '*Complex Natural Products as a Driving Force for Discovery in Organic Chemistry'*
19.30 to 19.40 h	**Concluding Remarks**
19.40 to 22.00 h	**Banquet Dinner**

Day 4, Sunday	**March 3, 2024, Breakfast and Departure**

ABSTRACTS

Trustees & DST-SERB Session

Chairpersons: Vinod Singh, Jerome Lacour & Harinath Chakrapani

Vinod K. Singh
Rahul & Namita Gautam Chair Professor
Department of Chemistry
IIT Kanpur- 208016
Email: vinodks@iitk.ac.in

Education:

M.Sc.	Banaras Hindu University, Varanasi	1980
Ph.D.	Malti-Chem Research Centre, Nandesari	1986
	(Degree: M.S. University, Supervisor: Dr Sukh Dev)	
Post-doctoral	University of Calgary, Canada	1985-1986
	University of British Columbia, Canada	1986-1987
	Harvard University, U.S.A.	1987-1990
	(Advisor: Professor E. J. Corey, Nobel laureate)	

Research Interests: Synthetic Organic Chemistry: Asymmetric Synthesis

Academic Positions:

Professor (HAG)	IIT Kanpur	18.08.2009 — Present
Professor	IIT Kanpur	13.09.2001 — 17.08.2009
Associate Professor	IIT Kanpur	24.05.1997 — 12.09.2001
Assistant Professor	IIT Kanpur	26.12.1990 — 23.05.1997
Senior Scientist	Neurogen, USA	01.03.1990 - 15.12.1990

Administrative Positions:

Founder Director	IISER Bhopal	12.06.2008 — 04.09.2018
Director *(additional charge)*	MANIT Bhopal	13.05.2017 — 24.07.2017
Mentor Director	IIIT Bhopal	13.05.2017 — 24.07.2017
Mentor Director	IISER Berhampur	12.11.2015 — 09.10.2017
Director *(additional charge)*	SPA Bhopal	28.07.2014 — 26.10.2015
Chairman, BoG	NITTTR Bhopal	01.05.2009 — 24.10.2009
Director *(additional charge)*	SPA Bhopal	06.10.2008 — 29.07.2009

Awards & Honors:

- Rahul and Namita Gautam Chair, IIT Kanpur (01.09.2019 — current)
- TWAS-CASAREP Award for Building Scientific Institutions (2020)
- Samman Patra by UP Government (2018)
- Padma Shri (2014)
- CRSI Silver Medal (2014)
- Distinguished Alumnus Award, BHU (2012)
- Goyal Prize (2011)
- J.C. Bose fellowship (2009-2023)

Jerome Lacour
Professor
University of Geneva,Sciences II Building
30 Quai Ernest Ansermet1211 Geneva 4
Email: jerome.lacour@unige.ch

Jérôme Lacour was educated at the École Normale Supérieure (Ulm, Paris). He holdsan *Agrégation* in Physical Sciences (major in Chemistry) and obtained in 1993 his Ph.D. in Chemistry at the University of Texas at Austin under the supervision of Prof. Philip D.Magnus. After post-doctoral studies in the laboratory of Prof. David A. Evans at Harvard University, he joined the Organic Chemistry Department of the University of Geneva in 1995.In 2001, he received the Sandoz Family Foundation professorship. Since 2004, he holds a fullprofessor position in the department. Currently, his primary research interests are in asymmetric synthesis and catalysis using organic, physical organic, organometallic and coordination chemistry tools.

Jérôme Lacour teaches general organic chemistry to 1st year biology and pharmacy students. He also lectures on physical organic chemistry to 3rd year and graduate students, and on current stereochemistry problems to graduate and postgraduate. He is a member of the Editorial Advisory Board of *Chemical Society Reviews*, *Chemical Science*, *Chem* and a Board member of *Chirality*. He is also a member of the International Scientific Committee of the *International Symposium on Chirality*.

Distinctions, Awards and Prizes:

- Faculty of Science, University of Geneva, Dean (2014-)
- Visiting Professorships: Nagoya (2018), Bordeaux (2013), Haifa (2012), École Centrale Marseille (2010), Strasbourg (2009), Angers and Dijon (2008), Lyon (2000)
- *EUCHEM "Bürgenstock" Conference on Stereochemistry*, Organizing Committee (2008-2017)
- Taiwan Chemistry Research Promotion Center, Visiting lectureship (2014)
- International Organic Chemistry Foundation (IOCF) lectureship, Japan (2014)
- Vice-Dean of the Faculty of Science, University of Geneva (2010-2014)
- *Chimia*, Editor-in Chief (2011-2014)
- Geneva Chemical Society, President (2010-2013)
- "Chirality 2008", the 20th International Symposium on Chirality, Chair
- COST Action D31, Vice-Chair (2007-2009)
- National Science Council, Taiwan, Visiting Lecturer (2007)
- 2006 Holger Erdtman Lecturer (KTH, Sweden)
- Grammaticakis-Neuman Prize, French Academy of Sciences (2005)
- Werner Prize and Medal, Swiss Chemical Society (2002)
- Sandoz Family Foundation Professorship (2001-2004)
- Synthélabo Postdoctoral Fellowship (1993-1994)

Harinath Chakrapani
Professor
Department of Chemistry
IISER Pune
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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 1999, he moved to Duke University, USA to pursue his doctoral studies, which he completed in 2005. His post-doctoral research work was carried out at Wake Forest University and the National Cancer Institute. He joined IISER Pune in July 2009 and is currently Professor.

Prof. Harinath Chakrapani's group designs, synthesizes and evaluates organic compounds that can produce redox-active species derived from sulfur, nitrogen and oxygen in a spatiotemporally controlled manner as tools for biochemical and cell biological studies. These biological reactive species are produced during normal metabolism but elevated levels can cause irreparable damage to cells. The tools developed in their lab provide insights into disease mechanisms as well as new leads in developing therapeutics. The focus is on infectious diseases, with a special focus on antimicrobial resistance as well as neurodegenerative disorders, which are frequently associated with dysfunction in redox homeostasis.

Selected Publications:

- Bora, P.; Manna, S.; Nair, M.; Satha, R.M.S.; Singh, S.; Adury, V.S.S.; Gupta, K.; Mukherjee, A.; Saini, D. K.; Kamat, S.S.; Hazra, A. B.; Chakrapani, H. *Chemical Science*, (2021) in press.
- Khandelwal, N.; Shaikh, M.; Mhetre, A.; Balaji, K. N.; Chakrapani, H.; Kamat, S. S. Fatty acid chain length drives lysophosphatidylserine-dependent immunological outputs (2021) *CellChemical Biology*, 28: 1169-1179.
- Kulkarni, A; Soni, I.; Kelkar, D.S. Dharmaraja, A. T.; Sankar, R. K.; Beniwal, G.; Rajendran,A.; Tamhankar, S.; Chopra,S.; Kamat, S. S.; Chakrapani, H.

Hidetoshi Tokuyama
Professor
Graduate School of Pharmaceutical Sciences
Tohoku University
Sendai, JAPAN
Email: tokyuama@mail.pharm.tohoku.ac.jp

Professor Hidetoshi Tokuyama obtained his Ph. D. in Organic Chemistry from Tokyo Institute of Technology in 1994. He subsequently moved to USA for a post-doctoral position with Prof. Amos B. Smith, III (1994-95). He joined the Tohru Fukuyama Group at the Graduate School of Pharmaceutical Sciences, the University of Tokyo as Assistant Professor in 1995 and grew upto the level of Associate Professor in 2003. Since 2006, he has been in his current position at Tohoku University. He is an associate member of the Science Academy Japan and a fellow of the Royal Society of Chemistry. He is currently a member of Editorial Board of *Organic Syntheses* and *Natural Products Reports*, RSC.

He has made significant contributions in areas organic chemistry with a special emphasis development synthetic methodologies and total synthesis of biologically active natural products. He has developed synthetic methodologies for nitrogen-containing heterocycles and applied to total syntheses of a number of alkaloids including (+)-halophytine, (–)-haouamine A, (–)-histrionicotoxin, (–)-rhaiznilam, (–)-acetylaranotine, and (+)-MPC1001B. He recently introduced phthalocyanine as highly chemoselective and environmentally benign catalysts for aerobic oxidation. He has more than 200 publications with more than 8200 citations. 30 students have been already awarded Ph. D. degree under his guidance. For his contributions in synthetic organic chemistry with focus on the synthesis of structurally complex natural products, he has received several awards including Katritzky Junior Award in Heterocyclic Chemistry from the International Society of Heterocyclic Chemistry, 2015, the Pharmaceutical Society of Japan Award for Divisional Scientific Promotion, 2015, and the Young Scientist's Prize: The Commendation for Science and Technology by the Minister of Education, Culture, Sports, Science and Technology, Japan, 2007.

Total Synthesis of Structurally Complex Alkaloids via Late-Stage Oxidative Transformations

Prof. Hidetoshi Tokuyama
Graduate School of Pharmaceutical Sciences, Tohoku University

Oxidative transformation of nitrogen containing polyfunctional compounds is difficult task because it generally gives a complex mixture due to the high reactivity of nitrogen functional groups to oxidizing agents. Recently, we have developed a biomimetic catalytic oxidation using an iron phthalocyanine complex (**1**), which was designed by mimicking cytochrome P450. The reaction proceeds with oxygen as a bulk oxidant and is effective for oxidative dimerization of tryptophan derivatives and unprotected tryptophan-containing peptides.[1] Taking advantage of the high functional group compatibility of the oxidation conditions, we have completed the first total synthesis of (+)-bipleiophylline (**2**) by featuring the oxidative coupling of the synthesized pleocarpamine (**3**) with pyrocatechuic acid at the final stage of the synthesis.[2] The late-stage oxidative transformation strategy was also effective for total synthesis of discorhabdin alkaloids. Discorhabdin B (**4**), H (**5**), K (**6**), and (–)-aleutianamine (**7**) were synthesized in a divergent manner via diastereoselective oxidative spirocyclization and a copper-mediated late-stage oxidative *N,S*-acetalization.

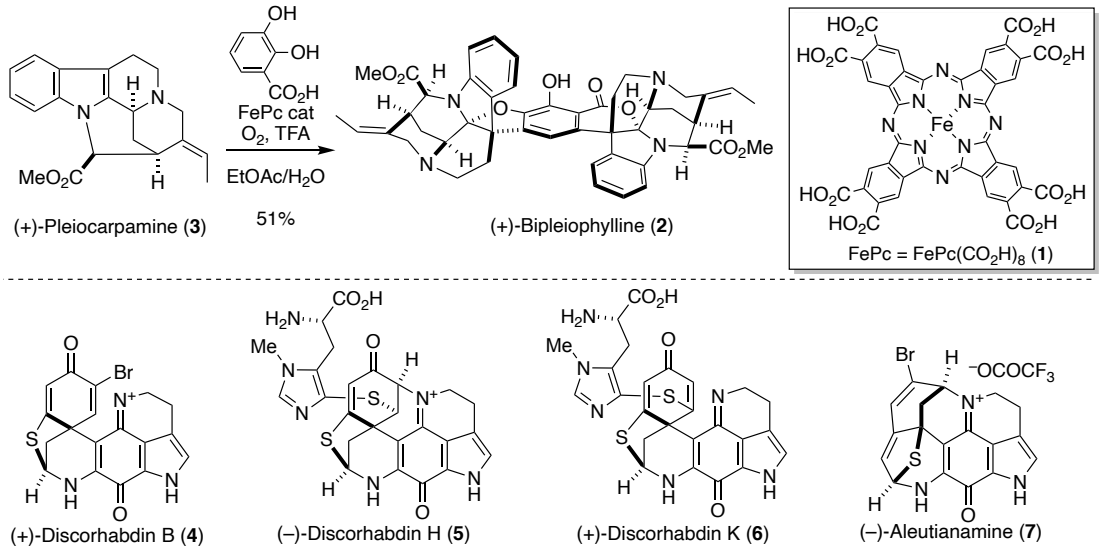

Figure 1: Structures of pleocarpamine (**3**), bipleiophylline (**2**), and discorhabdins.

1. H. Ueda, S. Sato, K. Noda, H. Hakamata, E. Kwon, N. Kobayashi, H. Tokuyama, *Angew. Chem. Int. Ed.* **2023**, *62*, e202302404.
2. K. Okada, K. Ojima, H. Ueda, H. Tokuyama, *J. Am. Chem. Soc.* **2023***, 145,* 16337-16343.
3. M. Shimomura, K. Ide, J. Sakata, H. Tokuyama, *J. Am. Chem. Soc.* **2023***, 145,* 18233-18239.

Andrew L. Lawrence
Professor
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University of Edinburgh
Edinburgh, U.K.
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Professional Appointments:
2020–present Professor – Personal Chair of Organic Synthesis, University of Edinburgh
2017–2020 Senior Lecturer – Organic Chemistry, University of Edinburgh
2013–2017 Lecturer – Organic Chemistry, University of Edinburgh
2012–2013 Australian Research Council DECRA Fellowship – Australian National University
2010–2011 Postdoctoral Researcher – Australian National University (Prof. Michael Sherburn)

Education:
2006–2010 DPhil, University of Oxford (Prof. Sir Jack Baldwin FRS and Dr Rob Adlington)
2002–2006 MChem (Hons) 1st Class, University of Oxford (St John's College)

Awards:
• Korea Advanced Institute of Science & Technology Lectureship Award 2024
• Science and Technology in Science (STS) Forum – Young Leader 2023
• Blavatnik Awards for Young Scientists in the UK Finalist 2023
• BMOS-RSC Young Investigator Distinction Award 2018
• RSC Hickinbottom Award 2017
• Thieme Chemistry Journals Award 2016
• Junior Science Programme Fellowship to attend the 49th Bürgenstock Conference 2014
• Australian National University, Research School of Chemistry Director's Prize 2012
• Australian National University, Postdoctoral Teaching Fellowship 2011
• The Oxford Society, Diamond Jubilee Award 2008

Funding (total equivalent to >£2.5 million):
• RSC – Research Enablement Grant, with Prof. Marcus Baumann (UCD, Dublin) (£10,000) 2022
• Leverhulme Trust – Research Grant (£293,670) 2021
• EPSRC – New Horizons (£200,000) 2020
• ERC – Starting Grant (€1.5 million) 2017
• EPSRC – First Grant (£125,000) 2016
• Royal Society – Research Grant (£15,000) 2015
• Marie Curie Actions – Career Integration Grant (€100,000) 2014
• ARC – Discovery Project (A$420,000) 2014
• ARC – DECRA Fellowship (3-year fellowship, A$375,000) 2012

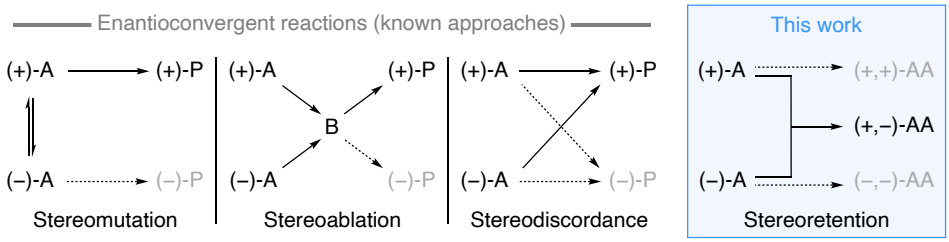
Summary of Publications, Invited Lectures, and Research Group:
• 33 publications in total; including, 3 Nat. Chem., 9 Angew. Chem. Int. Ed., 3 Chem. Sci., 5 Org. Lett., 1 J. Am. Chem. Soc., 1 Green Chem., 1 Nat. Rev. Chem.
• H-index: 17, All citations: 1089 (Google Scholar, January 2024)
• 86 invited lectures (45 conference lectures, 41 invited seminars)
• Current Group: 1 PDRA, 8 PhD, 2 MChem (Past Group Members: 8 PDRA, 9 PhD, 27 MChem)

Rethinking Enantioconvergent Reactions

Professor Andrew L. Lawrence

School of Chemistry, University of Edinburgh, Joseph Black Building, David Brewster Road, Edinburgh, EH9 3FJ, UK

Enantioconvergent reactions are preeminent in contemporary asymmetric synthesis as they convert both enantiomers of a racemic starting material into a single enantioenriched product, thus avoiding the maximum 50% yield associated with resolutions. All currently known enantioconvergent processes necessitate the loss or partial-loss of the racemic substrate's stereochemical information, thus limiting the potential substrate scope to molecules that contain labile stereogenic units. I will present an alternative approach to enantioconvergent reactions that can proceed with full retention of the racemic substrate's configuration. This uniquely stereo-economic approach is possible if the two enantiomers of a racemic starting material are joined together to form one enantiomer of a non-*meso* product. Experimental validation of this concept is presented using two distinct strategies; (1) a direct unsymmetrical coupling approach and (2) a multi-component approach, which exhibits statistical-amplification of enantiopurity. Thus, the established dogma that enantioconvergent reactions require substrates that contain labile stereogenic units is shown to be incorrect.



References:

[1] S. H. Bennett, J. S. Bestwick, V. P. Demertzidou, D. J. Jones, H. E. Jones, F. Richard, J. A. Homer, R. Street-Jeakings, A. F. Tiberia, and A. L. Lawrence, *Nat. Chem.* **2024**, accepted (*ChemRxiv* 10.26434/chemrxiv-2023-07jvx).

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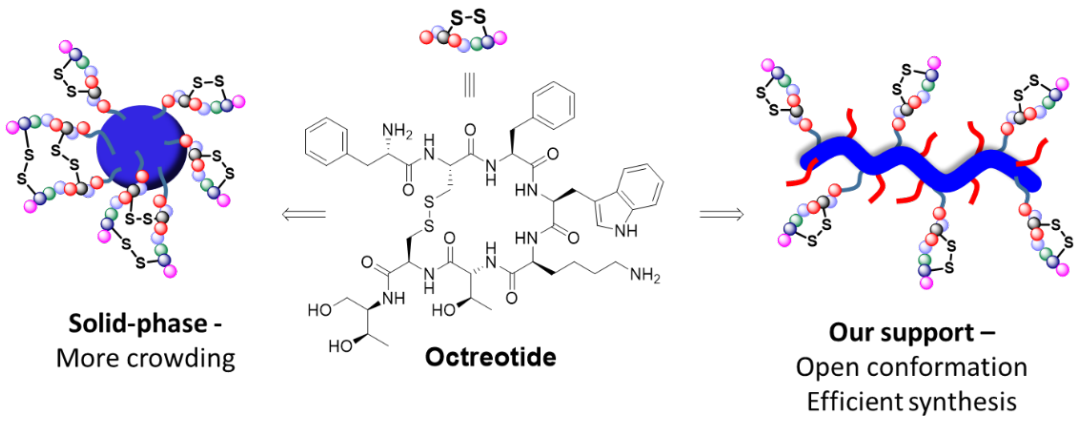
Nandita Madhavan got her bachelor's degree in chemistry from S.I.E.S. College (Mumbai University) and her master's degree from IIT Bombay. She joined the University of Illinois at Urbana-Champaign for her Ph.D., where her research focused on cyclodextrin derivatives for light activated ion transport. Her post-doctoral research at Georgia Institute of Technology involved supported catalysts for asymmetric organic synthesis. She started her independent research career in 2009 at IIT Madras and subsequently moved to IIT Bombay in 2016. Her research group mimics the activity of natural ion channel proteins using small peptides. Her group also develops cost-effective methods for peptide synthesis. She currently holds the position of the Dr. P. R. Sharadamani Chemistry Chair Professor. Nandita is also the co- P.I. of National Programme on Technology Enhanced Learning (NPTEL) IIT Bombay. She is on the editorial advisory board of Chemistry Select and Journal of Physical Organic Chemistry.

Ready Access to Cyclic Peptides for Pharmaceutical Applications

Nandita Madhavan
Department of Chemistry, Indian Institute of Technology Bombay

Peptide drugs are synthesized using solid phase peptide synthesis (SPPS)[1] for easy isolation of growing peptides. Excess coupling reagents and amino acids are added to overcome the reduced reactivity of amino acids on the support. Liquid phase peptide synthesis (LPPS) that utilizes supports that are soluble in the reaction medium are an attractive alternative to SPPS as support reactivity is improved.[2] The differential solubility of these supports in various solvents is exploited for peptide isolation *via* precipitation or extraction. Our group has developed polynorbornene supports with solubilizing groups that retain their solubility up to hexadecapeptide synthesis.[3] These polymers have an added advantage of being in an uncoiled form in the "good solvent" that solubilizes them. This conformational preference of soluble supports facilitates on-support cyclization to access drugs such as octreotide with an overall yield of 69% yield with high purity. Our group has also developed one-pot macrocyclization strategies to access macrocyclic amides/peptides as anion-transporters.[4]



References:

1. M. Muttenthaler, G. F. King, D. J. Adams and P. F. Alewood, *Nature Rev. Drug Discover*., **2021**, *20*, 309.
2. a) E. Bayer and M. Mutter, *Nature*, **1972**, *237*, 512; b) D. J. Gravert and K. D. Janda, *Chem. Rev*., **1997**, *97*, 489; c) A. Sharma, A. Kumar, B. G. de la Torre, F. Albericio, *Chem. Rev.* **2022**, *122*, 16, 13516.
3. a) N. Naganna and N. Madhavan, *J. Org. Chem.*, **2014**, *79*, 11549; b) B. Bisht, N. Naganna and N. Madhavan, *Org. Biomol. Chem.*, **2019**, *17*, 7238; c) B. Bisht and N. Madhavan, *J. Org. Chem.,* **2021**, *86*, 17667.
4. Behera, H.; Madhavan, N. *J. Am. Chem. Soc*., **2017**, *139*, 12919; b) Saha, P.; Madhavan, N. *Org. Lett.* **2020**, *22*, 5104-5108.

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Prabha Ibrahim, Ph.D. has worked in biopharmaceutical/pharma industry for nearly 30 years and has held leadership roles in drug discovery and development in multiple therapeutic areas with a track record of identifying NCEs and advancing them through pre-clinical and clinical development. Her record of success and scientific achievements includes inventor and co-inventor of more than 100 published patents, contributions to the nomination of multiple development candidates and filing of more than 20 INDs, and co-author of more than 40 scientific publications in peer-reviewed journals. She was instrumental in the discovery and development of multiple first-in-class medicines, including ZELBORAF® (vemurafenib), a BRAF inhibitor approved in 2011 for metastatic melanoma; TURALIO® (pexidartinib), a CSF-1R inhibitor approved in 2019 for symptomatic tenosynovial giant cell tumor; and LYFNUA (gefapixant), a P2X3 receptor antagonist approved in 2022 for chronic cough.

Prior to her role as CEO of ReRx Therapeutics, Prabha was a chief technology officer at Blade Therapeutics, a clinical-stage biopharmaceutical company dedicated to advancing novel anti-fibrotic therapies. She was a Chief Technology Officer of Afferent Pharmaceuticals, Inc. from November 2015 and continued her responsibility with Merck (NYSE: MRK) after acquisition of Afferent until March 2017. Prior to Afferent/Merck, she held multiple positions at Plexxikon for 14 years, with the last one being the Senior Vice President of Chemistry and Nonclinical Development. Prabha led multidisciplinary teams and held multiple project and program leadership roles. Prior to Plexxikon, Prabha was a Senior Research Scientist and Group Leader at CV Therapeutics (Nasdaq:CVTX), where she was a project co-leader for cell cycle project and a lead chemist for the second-generation ranolazine program. She started her career as medicinal chemist at Amgen (Nasdaq: AMGN), where she played an integral role in small-molecule drug discovery in inflammation.

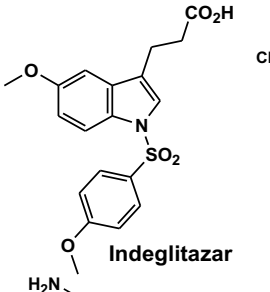
Prabha earned her Ph.D. at the University of Victoria, Canada, where she received the Distinguished Alumni Award in 2020 and is a member of the Dean of Science's Advisory Board. She was a Welch Foundation Fellow at Rice University, Houston, and received her M.Sc. Degree from The American College, Madurai, India, and B.Sc. degree from RDM College, Sivaganga, India. Prabha is a 2023 nominee for the Chemical Research Society of India's *CRSI Medal*.

Role of Chemistry in Small Molecule Drug Discovery & Development

Prabha Ibrahim
ReRx Therapeutics, Berkeley CA. USA

The underlying motivation driving the initiation of drug discovery and development efforts is the unmet clinical need to treat diseases or clinical conditions. Choosing a research area of interest is critical for anyone with aspirations for a professional research career, especially for industrial drug discovery and development programs. Although the role played by organic chemistry in the pharmaceutical industry is the main driver in the drug discovery process, the new scientific advances in synthetic techniques for rational drug design (computational chemistry), combinatorial chemistry, automated synthesis, compound purification and characterization opened a multiple area of opportunity to choose.

The talk will focus on the role of different aspects of chemistry in designing novel therapeutics using structural chemistry and structure activity relationship (SAR) in nominating the clinical candidate and the development road to the market.



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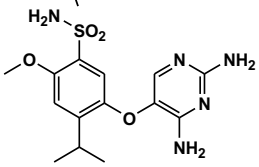
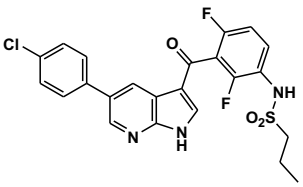
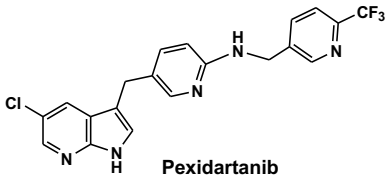


Gifapixant
(Lyfnua)



Vemurafenib
(Zerboraf)



Pexidartanib
(Turalio)

P. Venkatakrishnan,
Department of Chemistry
Indian Institute of Technology Madras
Chennai - 600036, INDIA
Email: pvenkat@iitm.ac.in

Education:

2007	PhD (Organic Chemistry): Indian Institute of Technology Kanpur, Uttar Pradesh, India
1999	MSc (Applied Chemistry): National Institute of Technology, Bharathidasan University, Tiruchirappalli
1997	BSc (Chemistry): The MDT Hindu College, Manonmaniam Sundaranar University, Tirunelveli, India

Professional Experience:

2024	Professor, Indian Institute of Technology Madras, India
2019 – 2023	Associate Professor, Indian Institute of Technology Madras, India
2013 – 2019	Assistant Professor, Indian Institute of Technology Madras, India
2010 – 2013	NIH Postdoctoral Research Fellow, National Institute for Nanotechnology, University of Alberta, Edmonton, AB, Canada
2008 – 2010	CEFIPRA Postdoctoral Researcher, Universite de Rennes1 (CNRS UMR 6510), Rennes, France
Sep 2007 – Jan 2008	Research Associate, Department of Chemistry, IIT Kanpur, India
Feb 2007 – Aug 2007	Visiting Researcher, Institute of Chemistry, Academia Sinica, Taipei, Taiwan
2000 – 2002	Project Assistant, Department of Chemistry, IIT Kanpur, India
1999 – 2000	Research Assistant, Department of Chemistry, NIT Tiruchirappalli

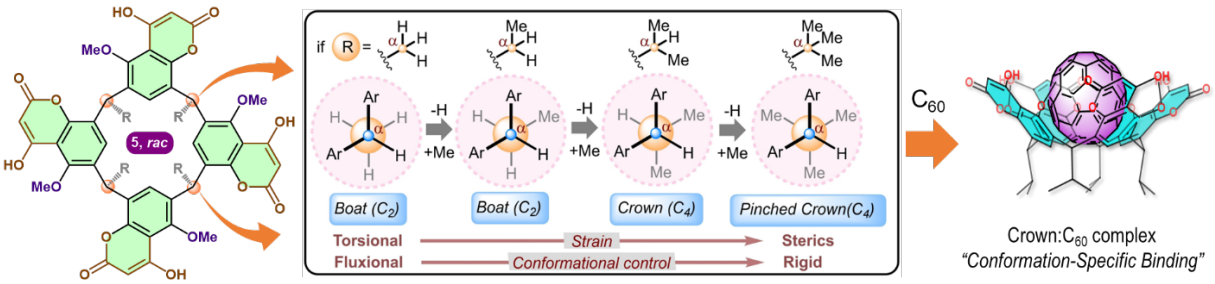
Research Interests:

Synthetic chemistry, Synthesis of novel functional organic (luminescent and electroactive) molecules for lighting, field-effect transistors, and photovoltaics, Engineering efficient organic dyes for bio-imaging, Nano-scale self-assembled architectures for functional devices.

Strained to Perform: Conformationally Locked *m*-Cyclophane Crown Cages C_{60}

Venkatakrishnan Parthasarathy
Department of Chemistry, Indian Institute of Technology Madras, Chennai - 600036

Resorcinarenes, a class of organic macrocycles (*m*-cyclophanes) known for their diverse applications, have captivated researchers for over five decades.[1] However, achieving conformational rigidity in resorcinarene crowns traditionally relies on covalent tethering or hydrogen bonding, sacrificing valuable upper-rim functionalities. In this presentation, I will showcase a novel premacrocyclization strategy that leverages torsional and steric strains imposed by α-substituents on the lower-rim *C*-alkyl chains to achieve well-defined crowns while preserving upper-rim accessibility.[2] This method affords the successful synthesis of conformationally rigid fluorescent *m*-cyclophane deep crowns.[3,4] X-ray crystallographic and computational analyses unequivocally demonstrate that α-branching in the *C*-alkyls is the key determinant of conformational rigidity. Notably, the pre-organized cavity within the locked deep crown exhibits remarkable selectivity towards spherical hydrophobic guests like C_{60} in both solution and solid states, enabling conformation-specific binding.[2]



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Institute of Chemical Technology
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Anant Kapdi was born in Mumbai, Maharashtra, India, in 1980, and studied chemistry at the University of Mumbai (MSc 2002) and York (MSc 2005; Dr. Ian J. S. Fairlamb). He completed his PhD in 2008 under the supervision of Dr. Fairlamb at The University of York (UK), before starting postdoctoral work in the research group of Prof. Lutz Ackermann at the Georg-August-University Gottingen as an Alexander von Humboldt Fellow. He returned to India in 2010 and was appointed as DST-SERC Fast Track Fellow (2011) and DST Inspire Faculty (2012) at the Institute of Chemical Technology, Mumbai before taking up UGC-FRP Assistant Professor position (2014) at the same institute. He has performed very well in his field of research, publishing more than 90 research publications in various reputed international journals and has 4 edited books in his name.

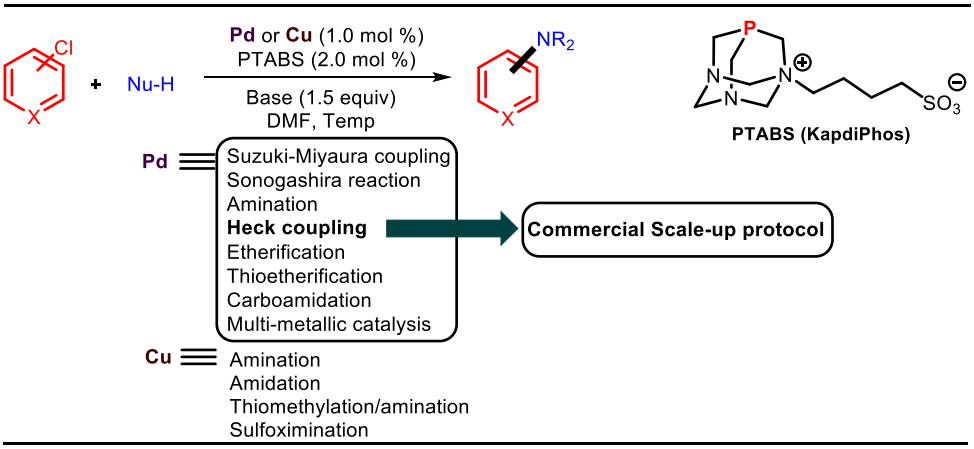
Anant has been instrumental in the formation of India's first-of-kind Scientific consortium (Innovation Sustainability Chemistry Consortium-ISSC) and is currently the founding Coordinator (India). Currently, he has been appointed as the Central Placement Coordinator for ICT, Mumbai, and looks after the training and placement for all the 3 campuses of ICT. Anant has received many recognitions for his scientific contributions as well as extensive administrative and outreach activities such as

a) Fellow of RSC under the Leader in Field category.
b) Fellow of Maharashtra Academy of Sciences
c) Prof. M. M. Sharma Science and Technology Award 2023 by Marathi Vidnyan Parishad
d) Was appointed an Associate Editor of the Royal Society of Chemistry journal, RSC Advances in 2015-2017
e) Appointed Associate Editor of Sustainability and Circularity Now, Thieme Publishers 2023-2027.
f) 2024 Thieme Chemistry Journal Awardee
g) C. B. Murarka Best Assistant Professor Award 2018-19
h) DAAD Fellowship for Scientists (not availed),
i) Alexander von Humboldt Return Fellowship (2013)
j) Prof. N. R. Kamath Book Award.

Acceptor Caged Phosphine Ligands: Exploration of Novel Catalytic Reactivity and Mechanism

Anant R. Kapdi
Institute of Chemical Technology

Phosphines as activating ligands have, in combination with transition metals, played an important role in the development of sustainable catalytic solutions for academia as well as industrial applications. Caged phosphines are a class of phosphines possessing three-dimensional scaffolds and capable of providing unique control over steric and electronic properties. The versatility of the caged phosphine ligands has been demonstrated elegantly by the groups of Verkade, Gonzalvi as well as Stradiotto.[1] Our contribution to this area comes in the form of the 1,3,5-triaza-7-phosphaadamantane-based caged ligands, especially PTABS (KapdiPhos) that has proved to be a revelation in promoting heteroarene functionalization in a highly efficient way. The talk will therefore be centered around the journey from the development of the ligand to the varied applications including scale-up possibilities, eventually culminating into its commercialization.[2] New catalytic reactivity and its mechanism has been explored along the way and will also be discussed.



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Nadja Simeth-Crespi
Professor
Organic and Biomolecular Chemistry
Göttingen University, Germany
Email: nadja.simeth@uni-goettingen.de

Qualifications and Career:

Stages	Periods and Details
Degree programme	Chemistry, 2009–2014, University of Regensburg, Germany
Doctorate	2014 – 2018, Prof. Dr. Burkhard König, Photochromic Small Molecular Tools: Altering Biological Function through Light, University of Regensburg, Germany
Stages of academic/professional career	Since 2021 W1-tt-W2 Professor for Molecular Labelling Chemistry, Georg-August-University Göttingen. 2018 – 2021 Postdoc as Feodor-Lynen Fellow (Alexander von Humboldt Foundation), University of Groningen, The Netherlands (Mentor: Prof. Dr. Ben L. Feringa)

Committee involvement & activities in the field of academic self-governance:

Since 2023	Member of the Managing Board of the Research Training Group 2455.
Since 2022	Member of the Board of the Multiscale Bioimaging Cluster of Excellence (MBExC)
Since 2021	Member of Steering Committee of the SBF initiative 1611 "Resource Economical Tools for Late-Stage Transformations"

Teaching, mentoring and supervision activities: Supervision of ten PhD and Master Students as well as four Bachelor Students since 2021.

Academic Distinctions:

Thieme Journal Awardee 2024, Cooperation Grant Lower Saxony-Israel, ESP Young Investigator Award 2023, Selected Representative for Germany at the 3rd EuChemS Life Science Division Young Investigator Workshop (2023), CAS Future Leader 2020-21 (2020), First runner-up FSE Postdoc Prize (2020), Armin-Buschauer PhD Prize for the best PhD thesis in Medicinal Chemistry at the University of Regensburg (2019), DAAD Travelling Grant to attend the 4th ERC-Grantee conference 2019 in Israel (2018), Collaborator in the High-Performance Computing (HPC) project code HP10C8U1NY granted by the Italian Consortium CINECA-SCAI (2017), PhD Fellowship of the Studienstiftung des Deutschen Volkes (2015-2018), Dr. Alphons Paulus Study Graduation Award (2015, Best Master's Degree in Chemistry 2014) Erasmus Fellowship for a 6-month research stay at the University of Gothenburg, Sweden (2014).

OPTO-BIOORGANIC CHEMISTRY FOR SMART BIOLOGICAL TOOLS AND LABELING AGENTS

Nadja A. Simeth[1,2]

[1]Institute for Organic and Biomolecular Chemistry, Department for Chemistry, University of Göttingen, Tammanstraße 2, 37077 Göttingen, Germany.

[2]Cluster of Excellence "Multiscale Bioimaging: from Molecular Machines to Networks of Excitable Cells" (MBExC), University of Göttingen, Germany.

In recent years, light has been employed as an external stimulus to photo-control diverse functional processes.[1] This approach relies on the use of small, light-responsive molecules that undergo a structural change upon irradiation, generating different functional states from a single molecule.[2] By attaching suitable substituents to such photoactuators, these molecules can be embedded in a system of choice to link their structural change to a change in the system's properties.[3] On the other hand, the sterical and electronic characteristics of the substituents influence the photophysical and photochemical properties of the core.[4] This mutual interaction needs to be finely balanced and studied in detail to rationally design probes and tools to study and modulate biological systems.

Here, we show different strategies to employ light-responsive building blocks to interact with and control biomacromolecules focusing on the 3D-structure of peptides and their supramolecular interaction. In this context, we will highlight how optimizing the substituents on different photoactuators allows us to tune several of their properties, such as their UV-Vis absorption profile and photoconversion quantum yield. We will demonstrate how these properties can be employed in various model systems. [5,6]

Eventually, we envision that deriving such design principles for an increasing number of light-responsive tools will pave the way to individually addressing a single photoactuator in a complex biologically relevant ensemble and thus, to the precise regulation of the biological machinery.

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6. N. A. Simeth et al. 2023 manuscript in preparation.
7. B. P. Corbet et al, Eur. J. Org. Chem. 2023, 26, e202201140.
8. I. Lace et al., ChemBioChem 2023, e202300270

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Prof. and Dean, Academics
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Rajesh Viswanathan received his master's degree in chemistry from Indian Institute of Technology, Kanpur in 1999. His MS-thesis project was on peptidomimetics with Prof. Javed Iqbal. His Ph. D. studies were in synthetic organic chemistry from Indiana Univ. in 2005 under the supervision of Prof. Jeffrey N. Johnston. His thesis work focused on strategies for total synthesis of cyanobacterial alkaloids. He was a postdoctoral fellow with Prof. Dale Poulter at the University of Utah, USA, where he developed prenyltransferase-based chemoenzymatic strategies to construct biosensors.

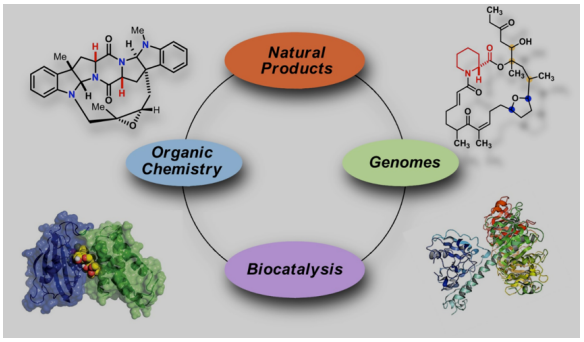
Subsequently, he joined Case Western Reserve University (Dept. of Chemistry) as an Assistant Professor. He was promoted to Frank Hovorka Assistant Professor and received Faculty Excellence Award (2014) and was the Gamma Sigma Alpha Outstanding Prof. awardee in 2016. He was the student invited speaker at the NIH-RISE program seminars held at the University of Puerto Rico (San Piedras Campus) in 2016. At Case Western, he served as the Board member for the Small Molecule Drug Discovery Core [SMDDC] and a Co-Investigator for a Program Project Grant, funded by the National Institutes of Aging (NIH P01). He serves as a consultant chemist for Gingko Bioworks, Boston – a synthetic biology firm interested in sustainable platforms for production of fine chemicals and perfumes.

He joined Indian Institute of Science Education and Research (IISER), Tirupati in 2018 and currently is an Associate Professor and the Dean, Academics. His research program has received SERB-CRG award (Organic Chemistry) and the National Science Foundation grant. His lab's research advances in the area of biocatalysis has led to a start-up, Avian Biovolatiles, as a joint venture between IISER and IIT Tirupati, where he holds the CSO position. He serves as an Editorial Board member of the *Journal of Biosciences* (Springer and IASc). His research interests are broadly in the areas of organic synthesis, natural product biosynthesis and the design and development of enzyme inhibitors as anticancer agents.

Biogenesis of Plant and Marine Natural Products – A Template for Biomimetic Synthesis

Rajesh Viswanathan*
Departments of Chemistry & Biology
Indian Institute of Science Education and Research Tirupati

Natural products consist of a significant portion of leads that effectively improve human health. A frequent hurdle in traditional natural product drug discovery is that commonly isolated product replicate the chemical space. With the advent of genomic tools that can expand the repertoire of natural product space, the community of biosynthetic experts have offered new set of strategies to elucidate new natural product chemical space. In this context, our group has delved into marine *Nocardiopsis & indigenous tribal plant species native to India*, in order to explore the biosynthetic chemistry. We have recently disclosed insights to understand the assembly mechanisms of marine natural products from *Nocardiopsis*.[1] This in turn inspired biomimetic chemistry, through which we create bioactive molecules, through total synthesis. We have reported bio-mimetic total synthesis of marine nocardioazine alkaloids that are anti-cancer natural products and their bioactive non-natural derivatives. As an application of our approach we have constructed endogenous amino acid-derived scaffolds as potentially non-toxic inhibitors of P-glycoprotein (PgP) mediated drug efflux pumps. Recently, results from our biosynthetic investigations reveal new pathways to antibbiotics in indigenous plant named *arogyapacha*, that has served traditional tribal medicine for a long time in India. In addition to spiroketal polyketides from this plant, we have identified several bioactive natural product pathways. These will be highlighted in the presentation.



Studies in the RV Lab

Biomimetic asymmetric synthesis of natural products

Elucidating unique enzymatic mechanisms

Developing non-toxic inhibitors of ribonucleotide reductase

References:

[1] (a) James & Viswanathan *et al. ACS Synthetic Biol.* **2016**, *5*, 547; & (b) Viswanathan and Lane *et al. ChemBioChem*, **2015,** *16*, 990-997.

[2] (a) Alqahtani, *et al. Org. Biomol. Chem.* **2015**, 13, 7177 & (b) Viswanathan and Lane *et al. Nature Communications*, **2023**, *14*, 2558.

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[4] Ajayan and Viswanathan *et al.* [unpublished recent results].

Astra Zeneca Session

Chairpersons: Namrata Rastogi & Ravi P. Singh

Namrata Rastogi
Principal Scientist
Central Drug Research Institute (CDRI)
Lucknow
Email: namrata.rastogi@cdri.res.in

Education:

Research Scholar (January 2001-July 2006) Indian Institute of Technology, Bombay, India
Supervisor: Professor Irishi N. N. Namboothiri

Postdoc:

Postdoctoral Research Associate (September 2006-March 2007) Indian Institute of Technology, Kanpur, India Supervisor: Professor Vinod K. Singh

Postdoctoral Research Associate (May 2007-April 2009) University of Minnesota, Minneapolis, USA Supervisor: Professor Ramaiah Muthyala

Positions:

Scientist (March 2011-March 2016) CSIR-Central Drug Research Institute (CSIR-CDRI), Lucknow, India

Senior Scientist (March 2016-till date) CSIR-Central Drug Research Institute (CSIR-CDRI), Lucknow, India

Senior Scientist, Jubilant Biosys Ltd, Bangalore (2009-2011)

Awards & fellowships:

Distinguished Woman Scientist-2019 in Chemical Sciences" by Indian Society of Chemists & Biologists

CSIR-CDRI's Incentive Award-2019

CSIR-CDRI's Incentive Award-2015

INSA-DFG fellowship, University of Regensburg, Germany (July-September, 2014)

Gregynog Young Organic Chemist-2015

Ravi P. Singh
Professor
Department of Chemistry
IIT Delhi
Email: ravips@chemistry.iitd.ac.in

Education:

Ph.D., Indian Institute of Technology, Kanpur, India. Supervisor: Professor Vinod K. Singh

Postdoc:

Post Doctoral Fellow: Harvard University, Prof. E. J. Corey (Nobel Laureate), 2005-2007
Post Doctoral Fellow: Brandeis University, Prof. Li Deng, 2007-2011

Positions:

Senior Scientist: National Chemical Laboratory, Pune, 2011–2013
Assistant Professor: Academy of Scientific and Innovative Research, New Delhi, 2011–2013
Assistant Professor: Indian Institute of Technology Delhi, 2013-2016
Associate Professor: Indian Institute of Technology Delhi, 2016-2021
Professor: Indian Institute of Technology Delhi, 2021-present

Selected Publications:

1. Yongwei Wu, Ravi P. Singh, Li Deng, Enantioselective Isomerisation of b,g-unsaturated butenolides in presence of cinchona alkaloid catalyst J. Am. Chem. Soc. 2011, **133**, 12458.
2. V. U. Bhaskara Rao, Amol P. Jadhav, Dnyaneshwar Garad, Ravi P. Singh, Asymmetric Vinylogous Mannich Reaction of Silyloxy Furans with N-tert-Butanesulfinyl Ketimines, Org. Lett., 2014, **16**, 648-651.
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Ramanarayanan Krishnamurthy was born in Mylapore (near Kapaleeswarar Temple) in Chennai, India. He received his B.Sc. in Chemistry from Vivekananda College (University of Madras), M.Sc. in chemistry from the Indian Institute of Technology, Mumbai, and Ph.D. from The Ohio State University, Columbus working with Professor David Hart. Captivated by a lecture given by Professor Albert Eschenmoser on the Chemical Etiology of Nucleic Acid Structure, he pursued his postdoctoral work at the Swiss Federal Institute (ETH) Zürich with Professor Eschenmoser. Following a NASA−NSCORT fellowship with Professor Gustaf Arrhenius at Scripps Institution of Oceanography, UCSD, La Jolla, he re-joined Professor Eschenmoser at the Skaggs Institute of Chemical Biology at The Scripps Research Institute (TSRI), La Jolla, resulting in a 13-year research collaboration. He is currently a Professor of Chemistry at Scripps Research, applying synthetic organic chemistry to understand the prebiotic chemical roots of life's biochemistry under early Earth scenarios.

Organic Chemistry in the Pursuit of Chemical Origins of Life

Ramanarayanan Krishnamurthy
Department of Chemistry
The Scripps Research Institute

Understanding the chemical origins of life can be viewed as primarily an organic chemistry undertaking within the geochemical constrains of early Earth. This approach has provided us with opportunities to discover 'alternative' chemistries that have, in turn, led to different insights and possibilities, with respect to chemical origins of -and chemical evolution leading to- life. The presentation will focus on the work from our laboratories exemplifying how employing organic chemistry in the pursuit of chemical origins of life can be a fertile endeavor.

"*The natural genesis of life on Earth is a hypothesis of evolutionary science; it is the task of synthetic organic chemistry to test this hypothesis experimentally. The aim of an experimental aetiological chemistry is not primarily to delineate the pathways along which our ('natural') life on Earth could have originated, but to provide decisive experimental evidence, through the realization of model systems ('artificial chemical life'), that life can arise as a result of the organization of organic matter*." Albert Eschenmoser, M. Volkan Kisakürek, *Helv. Chim. Acta*, **1996**, *79*, 1249-1259.

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Introduction: Chemical Evolution and the Origins of Life. Krishnamurthy, R.; Hud, N. *Chem. Rev.* **2020**, 120, 11, 4613–4615**.**

Systems Chemistry in the Chemical Origins of Life: The 18th Camel Paradigm. Krishnamurthy, R. *J. Systems Chem.* **2020**, *8*, 40-62.

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Punniyamurthy completed graduate studies at the Bharathidasan University and Ph.D. at the Indian Institute of Technology Kanpur (Prof. Javed Iqbal). He pursued postdoctoral research at the North Dakota State University (Prof. M P Sibi), Kyushu University (Prof. T Katsuki) and Montpellier University (Prof. A Vioux and Prof. J Moreau). In 2001, he joined at the Indian Institute of Technology Guwahati and his research interest is the sustainable Organic Synthesis focusing on site-selective C-H bond functionalization and stereospecific synthesis of medicinally important heterocyclic compounds. He is the fellow of the Indian Academy of Sciences, the National Academy of Sciences, the Indian National Science Academy and Royal Society of Chemistry, and recipient of J C Bose Fellowship, CRSI Silver medal and Distinguished Alumni Award of Bharathidasan University. He was also visiting Professor at the Oxford University, The Scripps Research Institute, San Diego, and Kyushu University.

Merging Strained Rings and C-H Functionalization: Efficient Synthetic Tool for Heterocyclic Compounds

Tharmalingam Punniyamurthy
Department of Chemistry, Indian Institute of Technology Guwahati, Guwahati -781039

Transition-metal-catalyzed directed C-H functionalization provides effective synthetic tool for the regioselective carbon-carbon and carbon-heteroatom bond formation. In addition, the cascade carbon-carbon and carbon-heteroatom of strained rings with suitable coupling partner can lead to formation of diverse heterocycles of medicinal interests, which are important in the development of sustainable organic synthesis. Our group has made a significant contribution for the past decade in these active topics and some of the recent results would be presented (Figure 1). The synthetic and mechanistic aspects of the potential transformations would be covered.

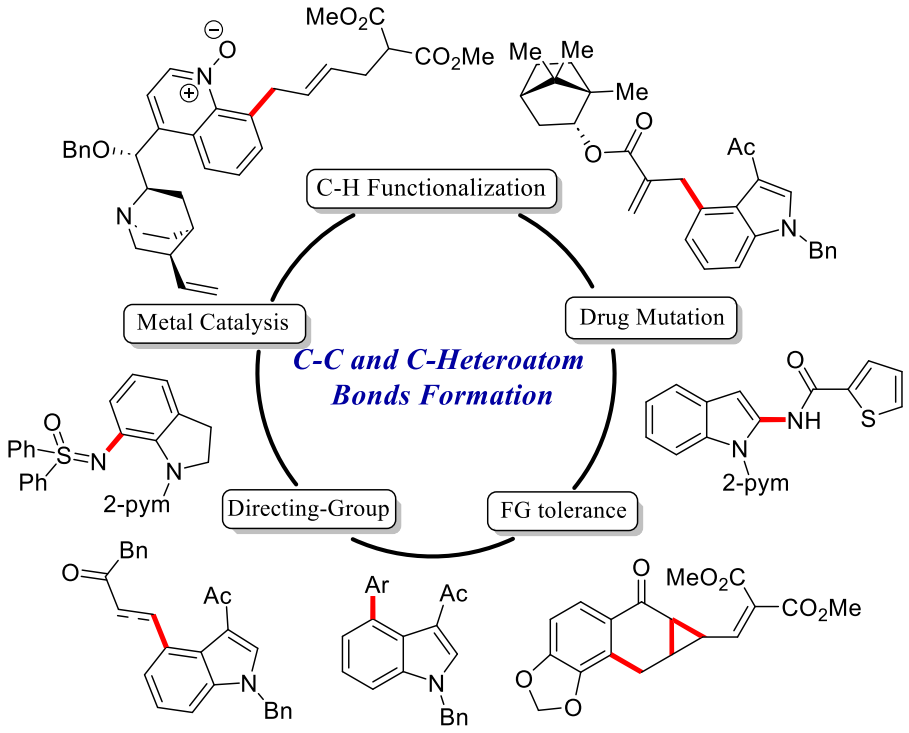

Figure 1. Representative works.

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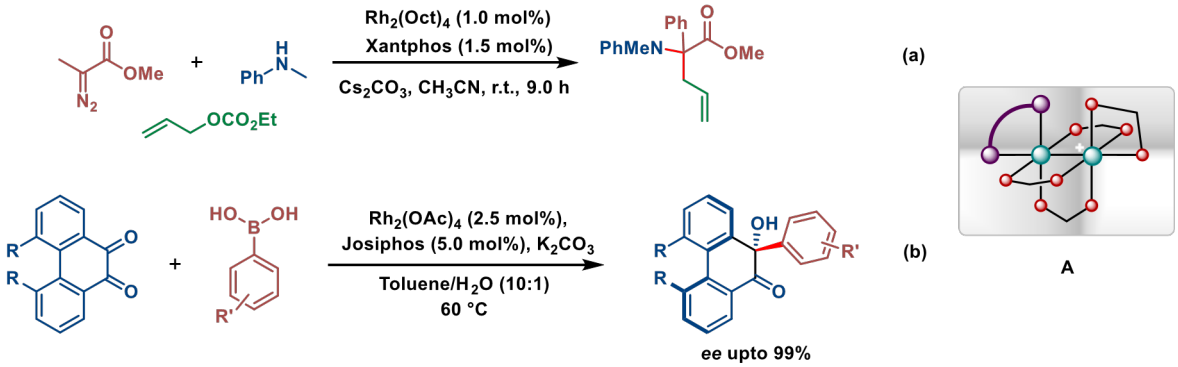
Garima Jindal is a computational chemist primarily interested in understanding the molecular level details of organic transformations catalyzed by small molecules and enzymes. She completed her undergraduate and postgraduate studies in Chemistry at the University of Delhi. Subsequently, she joined the group of Prof. R. B. Sunoj at IITB to pursue her graduate studies in computational chemistry. In 2015, she moved to the University of Southern California, Los Angeles, to work as a postdoctoral fellow with Prof. Arieh Warshel. She worked on enzymatic systems using molecular dynamics simulations. She started her independent research career as an assistant professor at IISc Bangalore in 2019. Her group is working on understanding the complex and intricate mechanism of carbene insertion reactions catalyzed by different metals and engineered heme proteins.

Mechanistic Investigation of Ligand Enabled Dirhodium Catalyst Modification: Implications in Reactivity and Stereoselectivity

Garima Jindal

Department of Organic Chemistry, Chemical Sciences Division, Indian Institute of Science, Bangalore560012

Dirhodium based paddlewheel catalysts display divergent and unique reactivities and are widely used in a multitude of reactions. The reactivity and selectivity can be tuned by either changing the bridging carboxylate ligands or anchoring external ligands at the axial site of the dimeric catalyst.[1] However, the shortcomings of both approaches necessitate the development of other catalysts, especially for stereoselective reactions. In a few recent studies, bisphosphine complexes have provided an alternative for catalyst modification (Scheme 1).[2] While newer reactivity is observed, the stereoselectivity for carbene insertion reactions still remains poor.[3] Interestingly, in another class of reactions involving the arylation of ketones, a specific set of ligands (Josiphos/Garphos) have shown excellent enantioselectivity (Scheme 1b).[2b] Irrespective of the reaction catalyzed, a commonly proposed active species involves an axial-equitorial coordination of the bisphosphine ligand with a concomitant dissociation of a carboxylate ligand (**A**). However, there is no evidence in favor of the active species, and therefore, the mechanism of such transformations remains unclear. In my talk, I will focus on our group's recent efforts using both computations and experiments to provide a mechanistic rationale behind the success of ligand modified Rh(II) catalysts. Our results show that the novel catalytic species and mechanisms proposed in literature do not hold good. Our study could pave the way for developing some challenging asymmetric transformations.



Scheme 1. Dirhodium catalyzed reactions with bisphosphines as ligands.

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Chandra was born in Parvathipuram (Andhra Pradesh, India). He received his M. Sc. in chemistry from University of Hyderabad in 2005 and graduated with a Ph. D. in organic chemistry from Ecole Polytechnique Federale de Lausanne (EPFL), Switzerland working under the guidance of Prof. Pierre Vogel in 2009. In 2010 he joined the group of Prof. Magnus Rueping at RWTH Aachen, Germany as a Swiss National Science Foundation Fellow. After two and half years in Germany, he moved to Stockholm University, Sweden for pursuing post-doctoral studies funded by Wenner-Gren Foundation with Prof. Jan.-E. Backvall. In October 2014, he returned to India to join as an assistant professor in the department of chemistry, IIT Bombay and in August 2023, he was promoted to full professor in the same department. His research interests include the study and development of different activation modes in metal and organocatalysis and their application in dual catalysis. He was awarded with INSA Medal for Young Scientist-2018, NASI-Young Scientist Platinum Jubilee Award-2018, Alkyl Amines Young Scientist Award-2018, IRCC Early Achiever Award-2017, Thieme Chemistry Journal Award-2021, AVRA Young Scientist Award-2020, Merck Young Scientist Award-2021 and OPPI Young Scientist Awards-2021.

Allenes in Metal-Catalyzed C-H Activation Reactions

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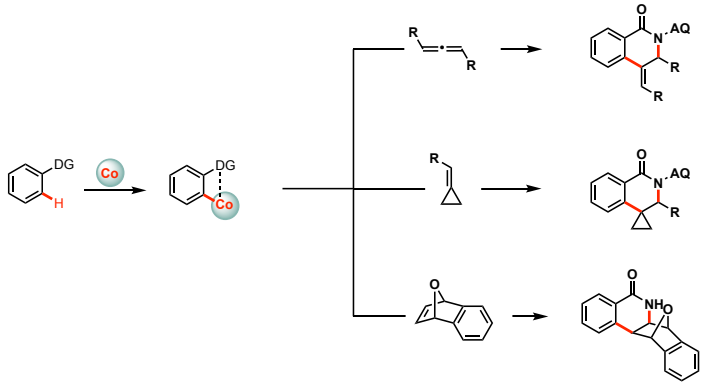
The invention of metal-catalyzed directing group assisted C-H activation has opened up new avenues for providing diverse array of decorated ring structures. Toward the development of sustainable earth-abundant metal catalysts, our research group has been investigating a series cobalt and nickel catalyzed C(sp^2)-H activation with under-utilized π-systems like allenes, methylenecyclopropanes and benzonorbornadienes. The key challenge in engaging these π-systems are the regiocontrol in the migratory insertion with organometallic species.



In this seminar, we will discuss our investigation of these less explored π-components in C-H activation, demonstrating the capacity of these scaffolds for achieving a variety of hetero-annulation and dienylation reactions. Key mechanistic implications in all these transformations will also be described.

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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 OSPC 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.

Selected publications:

1. Donthoju, A.; Phanindrudu, M.; Ellandula, S.; Ratan Lal M.; Nanubolu, J. B.; Chegondi, R. *Org. Lett.* **2023**, *25*, 7589–7594.
2. Jadhav, S. B.; Dash, S. R.; Maurya, S.; Nanubolu, J. B.; Vanka, K.; Chegondi, R. *Nat. Commun.* **2022**, *13*, 854.
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5. Gollapelli, K. K.; Donikela, S.; Manjula, N.; Chegondi, R. *ACS Catal.* **2018**, *8*, 1440.
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Copper-Catalyzed Asymmetric Hydrofunctionalization of Alkoxy-allenes

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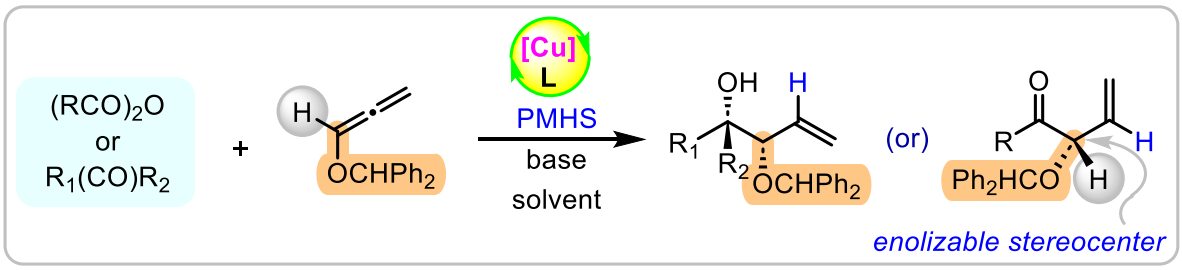
Organic Synthesis and Process Chemistry, CSIR-Indian Institute of Chemical Technology (CSIR-IICT), Hyderabad 500007, India

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 CuH-catalyzed enantioselective synthesis of complex 1,2-*syn-sec,tert*-diols and α-hydroxy ketones using hydrofunctionalization of alkoxy-allenes with carbonyl compounds.



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Cipla & Jubilant Life Sciences Session

Chairpersons: N. Jayaraman & G. Sekar

N. Jayaraman
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Dr. N. Jayaraman is a faculty member at the Department of Organic Chemistry, Indian Institute of Science, Bangalore, since 1999, and is currently a Professor and Chairperson of the Department. Completed early education at (i) Annamalai University (M.Sc., 1986-88); (ii) Indian Institute of Technology Kanpur (Ph.D. 1994, under the supervision of Professor S. Rangathan); (iii) University of Birmingham, UK (1994-1997) and University of California Los Angeles (1997-1999, under the mentorship of Professor Sir James Fraser Stoddart, Chemistry Nobel Laureate 2016), before joining IISc Bangalore.

Research areas of interest are in carbohydrate chemistry, dendrimer chemistry and liquid crystals. Synthesis of natural and unnatural carbohydrates, synthetic methods development, modifications of unsaturated monosaccharides, synthesis of tailor-made cyclic oligosaccharides, studies of the interaction of synthetic carbohydrates with proteins and lectins by biochemical, biophysical methods and biological studies of carbohydrate antigen-induced antibody generation are major emphasis. Studies of the carbohydrate liquid crystals, resulting from polarity segmentations, and identification of mesophase behavior of these non-ionic amphiphilic liquid crystals form major emphasis. Expanding the frontiers of synthetic macromolecules, namely, dendrimers, is another major research area. Syntheses of two new dendrimer series are established: poly(propyl ether imine) (PETIM) and poly(alkyl aryl ether) of up to six generations are synthesized, their chemical, biological and materials properties studied, relevant to organometallic catalysis, organocatalysis, self-assembly behavior, drug encapsulation, gene delivery and more.

Major awards, recognitions and services are: Institute of Chemical Technology, Univ. Mumbai Diamond Jubilee Distinguished Fellow (2008-9); Shanti Swarup Bhatnagar Award of the Govt. of India (2009); Fellow, Indian Academy of Sciences (2011); Associate Editor: Glycoconjugate Journal, Springer Nature Publications (2017 –); Associate Editor: Journal of Chemical Sciences, Indian Academy of Sciences Publication (2017 – 2023); Advisory Board Member: Carbohydrate Research, Elsevier; President, International Carbohydrate Organization (ICO) (2014 – 2016); Member, International Carbohydrate Organization; Rajib Goyal Prize, Kurukshetra University (2011); Secretary General, Chemical Research Society of India (2020 –).

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Prof. Sekar obtained his Ph.D. from IIT Kanpur in 1999 under the guidance of Padma Shri, Prof. Vinod K. Singh. He was a JSPS postdoctoral fellow at TUT, Japan, and an AvH postdoctoral fellow at Goettingen University, Germany. He also carried out postdoctoral research at Caltech, USA. Prof. Sekar's research on organic synthesis focuses on developing new synthetic methodologies that employ environmentally benign homogeneous catalysts, metal nanocatalysts, and halogen bonding catalysis. Prof. Sekar has more than 130 publications, graduated 25 Ph.D. students and presently guiding 12 Ph.D. students. He is the recipient of the Institute Research and Development Award (Mid-Career)-2017, JSPS, AvH postdoctoral fellowships, and CRSI bronze medal (2015). He is the Fellow National Academy of Sciences (FNASc, 2019), Fellow of Royal Society of Chemistry (FRSC), and Fellow of the Academy of Sciences, Chennai (FASCh). He is also a present council member of the National Organic Symposium Trust (NOST), Chemical Research Society of India (Joint Secretary, CRSI), and Academy of Sciences, Chennai.

Education:

- 1999 - Ph. D from IIT Kanpur
- 1995 - M. Sc from University of Madras
- 1993 - B. Sc from University of Madras

Representative Publications:

Copper-catalyzed domino synthesis of multisubstituted benzo[b]thiophene through radical cyclization using xanthate as a sulfur surrogate (N. Sundaravelu, Tushar Singha, Anuradha Nandy, and **Sekar**, *Chem. Commun.,* **2021***, 57*, 4512).

Selective oxidation of alkylarenes to aromatic acids/ketone in water by using reusable binaphthyl stabilized Pt nanoparticles (Pt-BNP) as a catalyst, Saha, R.; Sekar, G., *Applied Catalysis B: Environmental*, **2019**, 250, 325. (highlighted in "The Hindu" national English newspaper (31st March 2019)

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Kana M. Sureshan (born in 1973) received PhD from the University of Pune in 2002. He has carried out his post-doctoral research at Ehime University, Japan (2002-2004) availing JSPS fellowship, at the University of Bath (2004-2006) and at the Max Planck Institute for Molecular Physiology, Dortmund, Germany as an *Alexander von Humboldt* postdoctoral Fellow (2006-2008). In 2008, he joined the Institute of Life Sciences, Hyderabad as a senior scientist. In 2009, he moved to IISER Thiruvananthapuram as an Assistant Professor and from 2020 onwards he is a full professor and the Dean of Infrastructure & Planning. His research interests broadly lie in the fields of organic chemistry and supramolecular chemistry. He has published 120 research papers in international journals of high repute and has filed eight patents. He has given more than 250 invited talks and plenary lectures at various international conferences worldwide.

He received the innocentive award for designing the shortest and economic route for the tuberculosis drug, pretomanid. He received the Ramanujan fellowship (2010), Swarnajayanti fellowship (2014), Young Scientist award by YIM Boston, USA (2015), CRSI bronze medal from Chemical Research Society of India (2016), MRSI medal from Materials Research Society of India (2016), Bhagyatara Award instituted by the Panjab University (2019), Technology Innovation Award instituted by the Govt. of India (2020), Rajib Goyal Prize instituted by Kurukshetra University (2021), Excellence in Carbohydrate Research award by the Association of Carbohydrate Chemists and Technologists India (2022) and JC Bose National Fellowship (2024). Sureshan is a Fellow of the Royal Society of Chemistry, London, U. K. (2018) and Indian Academy of Sciences (2020). He is an International Advisory/Editorial Board member of journals, *Angewandte Chemie*, *Chemistry Europe*, *Chemical Society Reviews* and *ACS Applied Polymer Materials*.

Two Structurally Different Polymers from a Monomer

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The primary structure of a polymer has a huge influence on its properties. Tuning the primary structure of synthetic polymers necessitates the use of unique monomers for each polymer synthesis. But remarkably, nature often uses the same monomer to create structurally different polymers by varying regiochemistry, stereochemistry, etc. For example, cellulose and 1,3-β-D-glucan are regioisomeric polymers of D-glucose, starch and cellulose are polymers of D-glucose differing in stereochemistry and *cis*-1,4-polyisoprene (natural rubber) and *trans*-1,4-polyisoprene (*Gutta-percha)* are polymers of isoprene differing in the stereochemistry of the olefin. This remarkable ability of nature to tune the stereochemistry and regiochemistry to create different polymers having different properties from a single monomer is a motivation for researchers to synthesize structurally different polymers from a common monomer. Hybrid monomers possessing functionalities that can react differently to form two types of linkages under different conditions have been explored for synthesizing two structurally different polymers from a monomer.[1,2] Also, the synthesis of different polymers differing in stereochemistry from a common monomer could be achieved by using different catalysts or reaction conditions.[3] To date, there is no report on the chemical synthesis of regioisomeric polymers from a monomer. Topochemical azide-alkyne cycloaddition (TAAC) polymerization has emerged as a reliable method to synthesize various crystalline polymers.[4] By using this chemistry, we have shown that a single monomer can be used to make two structurally different polymers via the marriage of topochemistry and polymorphism.[5] These results will be discussed.

References:

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Education

BSc &MSc. Chemistry, Christ College, Irinjalakuda, Kerala, India (1986-1991) (University of Calicut).

Master of Human Resource Management (MHRM) from University of Kerala (2016)

Ph.D. in synthetic organic chemistry from University of Kerala under the supervision of Dr. Vijay Nair, CSIR-NIIST, Trivandrum

Post-Doctoral Fellowships

1. Tohoku University, Sendai, Japan with Professor Yoshinori Yamamoto,
2. Molecumetics Institute, Bellevue, Seattle, WA, USA with Professor Michael Kahn
3. NPG Research Institute, Raleigh, North Carolina, USA with Professor Bert Fraser-Reid. From 28 May 2002 onwards as Scientist at CSIR-NIIST, Trivandrum

Research interests

- Bio-prospecting of medicinal plants (Phytochemistry)
- Homogeneous and heterogeneous catalysis for industrially important molecules
- Synthetic carbohydrate chemistry
- Process innovation for crop protection chemicals
- Development of novel synthetic methodologies for sustainable chemistry

Awards & Fellowships

- Chemical Research Society of India (CRSI) Bronze medal for the year 2016
- First Rank in Master of Human Resource Management (MHRM) from University of Kerala in 2016
- Excellent rating for DST sponsored project in the area of palladium catalysis
- Excellent rating for Indo-French collaborative project with Université de Reims Champagne-Ardenne, Reims, France

Other assignments

1. Faculty, Academy of Scientific and Innovative Research, (AcSIR), New Delhi.
2. Visiting faculty in Department of Applied Chemistry, Cochin University of Science and Technology, Kochi
3. Visiting faculty, Indian Institute of Science Education and Research (IISER, Trivandrum)
4. Visiting Faculty, Université de Reims Champagne-Ardenne (URCA),Reims, France (Indo-French collaboration)
5. Indo-Finland collaboration with University of Jyvaskyla, Finland.

Harmonizing Tradition and Innovation: Unveiling Nature's Alchemy Through Multidisciplinary Scientific Exploration

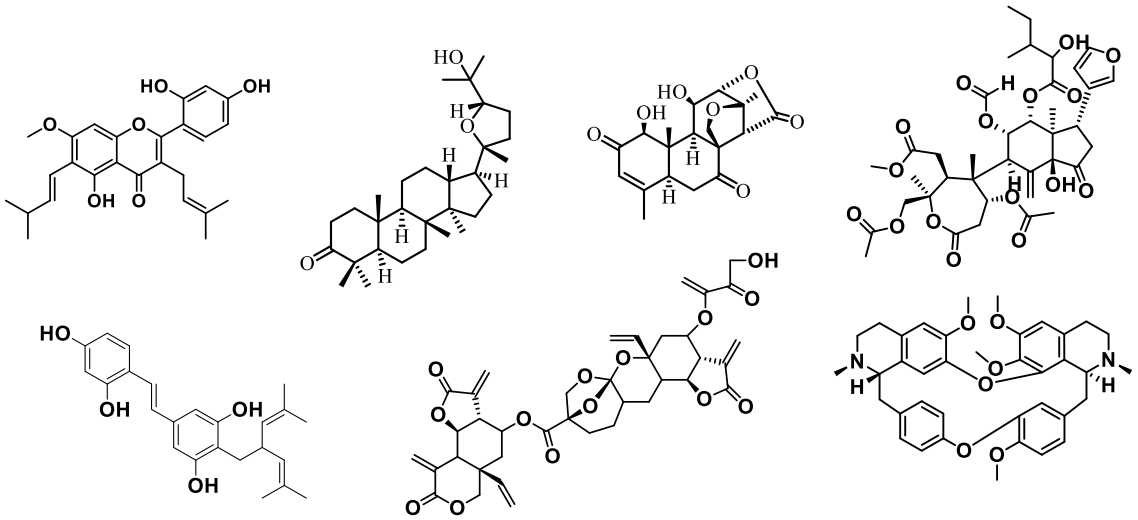
K. V. Radhakrishnan

Chemical Sciences & Technology Division,

National Institute for Interdisciplinary Science and Technology (CSIR-NIIST),

In the realm of pharmaceuticals, chemistry, and biology, the convergence of historical wisdom with contemporary scientific advancements holds immense promise. "Synergizing Ancient Wisdom and Modern Science: Exploring India's Traditional Knowledge for a Flourishing, Healthy Nation" delves into this captivating journey. India's vibrant biodiversity lies at the heart of discussions surrounding food and health security, yet a conspicuous void remains. This void pertains to the chemical intricacies, biochemical compound availability patterns, and ecological dynamics of vital plant species anchoring India's rich food and health biodiversity tapestry. Astonishingly, the treasure trove of small holder farms and untamed fields, housing invaluable health and food resources, has been sidelined, eluding scientific scrutiny.

Enter the collaborative force of botanists, social scientists, agricultural experts, natural product chemists, medicinal chemists, nutritionists, and biochemists - an interdisciplinary powerhouse. The objective: to illuminate the dormant potential within neglected biodiversity through evidence-based insights. Bridging the gap requires not only uniting expertise, but also forging deep connections with local communities. The aim is twofold: to harness fading biodiversity for groundbreaking strides in domains like food and health security and to embed traditional knowledge in the bedrock of a robust future. This symphony of collaboration aspires to compose a healthier and brighter prospect for India. Within these pages, the investigation unfurls, spotlighting the phytochemical profiles of select medicinal plants. Furthermore, it highlights the creation of potent molecules combating multi-drug-resistant strains of S. aureus and active anticancer agents combating SAS oral cancer. The discourse traverses uncharted territories, emphasizing the capability of this approach in tackling paramount health challenges. Embark on a voyage where ancient wisdom and modern science coalesce, envisaging a healthier, thriving India.



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Vibha Tandon obtained her Ph.D. degree in 1991. She published 93 papers in international journals, and have several patents to her credit. Prof. Tandon has mentored 25 Ph.D. students and around 70 students for six months project. She has been teaching Masters and Ph.D. students from last 25 years.

Recently she was awarded first A.V. Rama Rao Award of Women in Science, 2023. She is a NASI fellow. She was awarded Royal Society Fellowship (2007-08) to work at Prof. Michael J. Gait's laboratory, MRC Cambridge, UK. She has been on DAAD fellowship (2010-2011) and INSA visiting fellowship (2011-12) to work in the Radiation Biology laboratory of Prof. George Iliakis at Institute of Medical Radiation Biology at Essen, Germany; and Fulbright Senior Research fellowship (2012 -13) to visit Department of Cell Biology, Georgia State University, Atlanta USA.

Prof. Tandon's group is largely involved in translational research. Professor Tandon have two strong leads (novel molecule) in pipeline to be developed as drugs; a) PPEF, an antibacterial agent against MDR Bacterial strains and b) DMA, a radioprotector against radiation therapy in cancer patients. C) Identification of druggable targets in Head and Neck Cancer.

Her group shown that DMA a benzimidazole exerts radioprotection to normal cells during radiotherapy of tumor in patients. She deciphered that Akt/PKB/GSK3β/NFkB pathway is selectively activated in normal cells in tumor-bearing mice, but not in tumor cells. DMA confers protection against Xerostomia, reduce radioresistance and cause increased survival in HNSCC. The Intox Pvt. Ltd., Pune, and Eurofins–Advinus Pvt. Ltd., Bangalore are performing IND enabling studies on DMA. She is closely working with head and neck patients of Medanta Hospital, Gurgaon and GTB Hospital, Delhi.

Her group largely developed an antibiotic candidate PPEF targeting Topoisomerase IA and III protein selectively in bacteria, but safe in humans. Her group showed that PPEF efficiently kill 640 multi-drug resistant pathogenic strains of eleven gram-negative and positive bacterial strains identified by WHO as "Priority ESKAPE Pathogens".

Preclinical efficacy of Topoisomerase I targeting Small Molecule, PPEF and its in-situ nanosuspension against methicillin-resistant *Staphylococcus aureus*

Vibha Tandon[1,2]
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[2]Special Centre for Molecular Medicine, JNU,New Delhi

Recently, WHO declared antimicrobial resistance as the third greatest threat to human health. Absence of known cross-resistance, new class, new target, and a new mode of action are few major strategies being undertaken by researches to combat multidrug resistant pathogen. PPEF, a bisbenzimidazole was developed as highly potent antibacterial agent against ESKAPE pathogens, targeting topoisomerase IA. Accelerated molecular dynamics (MD) simulations were conducted to comprehend the molecular mechanisms underlying the inhibition of TopoIA and PPEF. The findings indicate that PPEF binds to and stabilizes the closed conformation of TopoIA, exhibiting a binding energy of -6 kcal/mol, while also destabilizing the binding of single-stranded DNA (ssDNA). We present a radical on-site generation of *In-situ* nanosuspension of PPEF (IsPPEF-NS) with enhanced efficacy against methicillin resistant *S. aureus* in septicemia model. The IsPPEF-NS showed precipitation efficiency of >90%, average particle size <500 nm, retained upto 5 h, a negative zeta potential and bi/trimodal particle size distribution. DSC, XRD confirmed partial amorphization and TEM revealed spherical particles. IsPPEF-NS was non-hemolytic and exhibited good stability in serum. More significantly, it exhibited a ~1.6-fold increase in macrophage uptake compared to free PPEF. Confocal microscopy revealed accumulation of IsPPEF-NS within the lysosomal compartment and cell cytosol, proposing high efficacy. In terms of antimicrobial efficacy, IsPPEF-NS outperforms free PPEF against clinical methicillin sensitive and resistant *S. aureus* strains. In a pivotal experiment, IsPPEF-NS exhibited over 83% survival at 8 mg/kg.bw and an impressive reduction of ~4-5 log-fold in bacterial load, primarily in the kidney, liver and spleen of septicemia mice. IsPPEF-NS prepared by the *in-situ* approach, coupled with enhanced intramacrophage delivery and superior efficacy, positions IsPPEF-NS as a pioneering and highly promising formulation in the battle against antimicrobial resistance.

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and Padma V. Devarajan . *J of Pharmaceutics* (IJPHARM-D-24-00268, Just Accepted)

Panacea Biotech Session

Chairpersons: S. Srivatsan & Vijaya Anand

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S. G. Srivatsan received his master's degree in chemistry from Indian Institute of Technology, Madras in 1995 and Ph. D. in Bioorganic Chemistry from Indian Institute of Technology, Kanpur in 2003 under the supervision of Prof. Sandeep Verma. He was an Alexander von Humboldt postdoctoral fellow with Prof. Michael Famulok at University of Bonn, Germany, where he developed catalytic RNAs and pharmacophores that target protein-RNA complexes and their enzyme activity. Subsequently, he joined Prof. Yitzhak Tor group as a postdoctoral fellow in University of California, San Diego. He joined Indian Institute of Science Education and Research (IISER), Pune in November 2008. He is currently a Professor and Wellcome Trust-DBT India Alliance Senior Fellow. He received the CDRI AWARDS–2019 for Excellence in Drug Research, Chemical Research Society of India Bronze medal (2020), National Prize for Research on Chemistry of Peptides and Nucleic Acids (sponsored by Professor CNR Rao Education Foundation) and Sun Pharma Research Award 2020. He also serves as an Editorial Advisory Board member of ACS Bioconjugate Chemistry. His research interests lie in the area of nucleic acid chemistry and biophysics, particularly in the development of nucleoside probes for studying nucleic acid structure and function, nucleoside-based self-assemblies, and nucleic acid labeling and imaging tools.

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Email: rvijayan@iisermohali.ac.in

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 a Professor at the Department of Chemical Sciences. He is also serving as the Dean of Research & Development at IISER Mohali. His research interests include organocatalytic enantioselective transformations and the synthesis of natural and unnatural biologically active compounds from *p*-QMs.

Pritam Mukhopadhyay
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Pritam obtained his Ph.D. from IIT Kanpur under the guidance of Prof. P. K. Bharadwaj. He then joined the group of Prof. L. Isaacs at the University of Maryland, College Park, USA, where he worked on the synthesis and studies of complex self-sorting systems. Later, he worked with Prof. S. Shinkai on the synthesis and studies of functional gels at the Kyushu University, Japan as a JSPS fellow. Pritam, subsequently joined the School of Physical Sciences, JNU, New Delhi. His group's research interests involve the synthesis and stabilization of organic radical ions, stabilization of highly electron-deficient and electron-rich systems and applications related to electron transfer reactions. The group is also interested in the design and synthesis of new supramolecular materials.

Research Interests:

- Organic and organometallic synthesis, Supramolecular Materials
- Design, Synthesis and Stabilization of Stable Organic Radicals and Radical Ions
- Green Synthetic Routes to Organic Open-Shell and Redox-Active Systems
- Electron Transfer Reactions and their Selectivity
- Organic Ferroelectrics, Pyroelectrics, Semiconductors
- Organic materials for Singlet Fission

Awards and Honours:

- CRSI Bronze Medal, 2023
- SwarnaJayanti Fellowship Award-2015, DST, India
- Associate member of the Indian Academy of Sciences, Bangalore, 2010
- JSPS Postdoctoral Fellowship-2005, Kyushu University, Japan
- ISCA Young Scientist Award in Chemistry, 2002
- DST-DAAD Exchange Research Fellow, 2000 at University of Saarlandes, Germany

Molecular and Supramolecular Architectures for Applications in Singlet Fission and as Conductive and Piezoelectric Materials

Pritam Mukhopadhyay

School of Physical Sciences, Jawaharlal Nehru University, New Delhi

Organic open-shell/closed-shell redox-active systems are intriguing building blocks for applications as spin-based materials and diverse energy-based applications.[1] In this lecture, I will briefly discuss our group's findings on the intriguing aspects of stabilization of organic radicals and how open-shell systems can provide access to interesting redox-active congeners that push the boundary of the electrochemical window.[2-4]

I will then deliberate on how these redox-active systems can be integrated into new supramolecular hosts. These hosts can enable access to multi-electron accumulation and proton conduction. We realized such multi-functional property by utilizing critical molecular and supramolecular elements in our design principle.[5]

We have also recently reported new push-pull type supramolecular hosts that can provide access to new singlet fission systems.[6] Singlet fission systems by virtue of their multi-excitonic properties are crucial as new generation of building blocks for energy-based applications as these can increase the current limit and efficiency of solar-cells. Finally, I will discuss on the design of a foldamer that crystallizes in polar space group and shows piezoelectricity in nano-domain as well in the bulk.[7]

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MEMBERSHIP OF SOCIETIES AND SERVICES:

Chemical Society of Japan: (Director, 2023-)
The Society of Synthetic Organic Chemistry, Catalysis Society of Japan, American Chemical Society, International Association of Colloid and Interface Scientists

EDUCATIONAL CAREER:

1985-1989 BSc. Department of Chemistry, The University of Tokyo
1989-1994 Ph.D: Graduate School of Science, The University of Tokyo

ACADEMIC CAREER;

1992-1994 JSPS doctoral fellow, The University of Tokyo
1994-1996, 1998-2000 Assistant Professor, The University of Tokyo
1996-1998 JSPS postdoctoral fellow, University of Wisconsin
2000-2004 Associate Professor, Osaka University
2004-2014 Associate Professor, Institute for Molecular Science
2007-2011 JST-PRESTO researcher
2012-2017 PI of ACT-C Project by JST
2014-present Professor, Osaka University

SERVICES AT OSAKA UNIVERSITY:

Head, Division of Applied Chemistry (2020-2022)
Head, Department of International Undergraduate Program (2017-2019)
Chair, Committee of International Affairs, Graduate School of Engineering (2020-)

AWARD:

2013 IUPAC Distinguished Award on Novel Materials and their Synthesis
2014 The CSJ Award for Creative Work
2015 NAGASE Science and Technology Award

CURRNT RESEARCH FIELD:

1. Synthesis and Properties of non-planar aromatic compounds “Buckybowls”
2. Development of metal nanocluster catalyst
3. Synthesis and reactions of organometallic compounds
4. Laser ablation in synthetic chemistry

Recent Progress in Sumanene Chemistry

Hidehiro Sakurai
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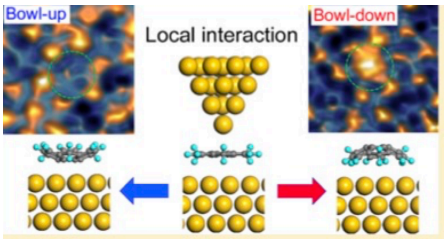
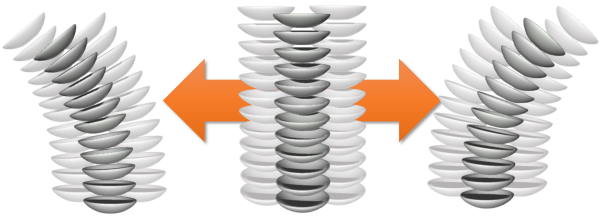
Sumanene is a C_{3v} symmetric pristine structure of buckybowl, a fragment of C_{60} [1]. Thanks to its structural features, it exhibits unique properties [2]. For example, it shows the characteristic dynamic behavior, such as bowl-to-bowl inversion, applicable to the molecular-scale memory device [3]. It favors forming a one-directional columnar assembly not only in the crystalline state[4,5] but also in the liquid-crystal [6] and in solutions, leading to unique "flexible" behaviors. In this presentation, I demonstrate the first synthesis of sumanene [7], and recent progress toward the general and facile synthetic method to construct various sumanene derivatives, including asymmetric synthesis [8] of nitrogen-doped heterabuckybowls [9,10] and supramolecular structure [11,12].





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12. Y. Yakiyama, T. Hasegawa, H. Sakurai, *J. Am. Chem. Soc.* **2019**, *141,* 18099.

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Dr. Amit B. Pawar completed his M.Sc. from the Savitribai Phule Pune University in 2007 with a specialization in Organic Chemistry. He obtained a Ph.D. from the Indian Institute of Science, Bangalore under the supervision of Prof. Kavirayani. R. Prasad in 2012, where he worked in the area of Total Synthesis of Natural Products. He was awarded the 1st prize from Eli-Lily for the "2012 Lilly Asia Outstanding Thesis Award." He carried out his post-doctoral work with Prof. Sukbok Chang at KAIST, South Korea in the area of C–H bond functionalizations (2013-2015). Later, he started his independent career as a DST-Inspire Faculty at CSIR-IICT, Hyderabad (2015-2019). Since November 2019, he has been working as an Assistant Professor in the School of Chemical Sciences at IIT Mandi, Himachal Pradesh, India.

His research is primarily focused on the development of Cp*Co(III)-catalyzed C–H functionalizations, Redox-neutral C–H functionalizations, and mild C–H activation reactions.

Harnessing *N*-Chlorobenzamide as an Oxidizing Directing Group for Reverse Regioselective Annulation with Vinylsilanes: Synthesis and Applications of 4-Silylated Isoquinolones

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Transition metal-catalyzed C–H annulation with π-components such as alkynes and olefins provide rapid access to important heterocycles such as isoquinolines and isoquinolones in a step-economic fashion. However, the majority of these transformations often lead to the formation of 3-substituted products while using terminal alkynes or alkenes. Therefore, the major challenge in such transformations is to tune the regioselectivity to form the 4-substituted product. This can be achieved by tailoring either the catalyst, directing group, or steric/electronic properties of the π-component. There are only a handful of examples known for accessing 4-substituted products. However, all of these transformations are restricted to Rh(III)-catalysis which is cost-intensive, and hence utilization of cost-efficient first-row transition metals in such transformations is of significant importance. In recent years, Cp*Co(III)-catalysis has provided a viable alternative for expensive catalysts based on precious metals for accessing various heterocyclic scaffolds under redox-neutral conditions utilizing oxidizing directing groups. In this lecture, we will discuss our efforts towards the synthesis of 4-silylated isoquinolones via Cp*Co(III)-catalyzed reverse regioselective [4 + 2] annulation of *N*-chloroamides with vinylsilanes and their applications in metal-free C-C bond forming reactions.

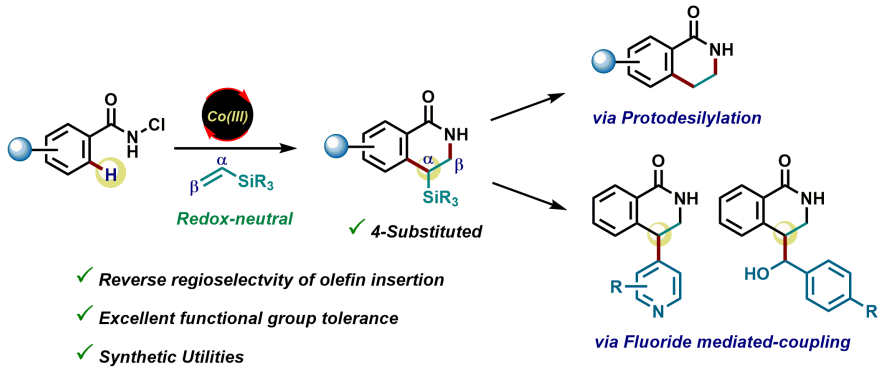

Figure 1: Cp*Co(III)-catalyzed reverse regioselective [4 + 2] annulation of *N*-chloroamides and vinylsilanes

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1987: Born, Howrah, India
2007: B.Sc. University of Calcutta (Chemistry Hons.)
2009: M.Sc. Indian Institute of Technology Kanpur (Chemistry)
2012: PhD Ludwig Maximillan Universität Munich, Supervisor: Prof. Herbert Mayr
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:
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:

- A.Palai, P.Rai, **B. Maji**, *Chem. Sci.*, **2023**,*14*, 12004.
- A. Jati, S. Dam, S. Kumar, K. Kumar, **B. Maji**, *Chem. Sci.* **2023**, *14*, 8624.
- 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.
- K. Das, S. Waiba, A. Jana, B. Maji, *Chem. Soc. Rev.* **2022**, *51*, 4386-4464.
- 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.
- K. Das, K. Sarkar, B. Maji, *ACS. Catal.* **2021**, *11*, 7060-7069.
- K. Sarkar, K. Das, A. Kundu, D. Adhikari, B. Maji, *ACS. Catal.* **2021**, *11*, 2786-2794.

Dearomative Cycloaddition Reactions via Visible Light Energy Transfer Catalysis

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Dearomative cycloaddition reaction is a blueprint for creating sp^3-rich three-dimensional molecular topology from flat-aromatic compounds. However, the reaction involving the arene system is highly challenging because of the high chemical stability inherent due to aromaticity. Further, severe reactivity, selectivity, and reversibility issues make this process arduous. One such process to overcome these challenges is the photochemical approach that induces the loss of aromaticity. Herein, we describe visible-light-induced triplet-triplet energy-transfer catalysis for the dearomative *meta*- and *para*-cycloaddition reaction of feedstock naphthalene molecules with tethered alkenes and vinyl benzenes. We performed DFT studies, photoluminescence, electrochemical, UV-VIS, and triplet energy quenching studies to understand the mechanism of those cycloaddition reactions. The developed protocol can be accessed for the cycloaddition reaction of feedstock naphthalene molecules with tethered alkenes and vinyl benzenes where structurally diverse 2-acyl naphthalenes with various functional groups could easily be converted to a diverse range of scaffolds in high yields and selectivities. The reaction can be scaled up to a gram scale and is also amicable for late-stage modification of various complex bioactive molecules. Furthermore, milder reaction conditions and substantially higher triplet energy of the dearomatized product prevent the reverse reaction, resulting in higher product yields. The research shed insight into visible light energy transfer catalysis, which is in the early stages of chemical synthesis.

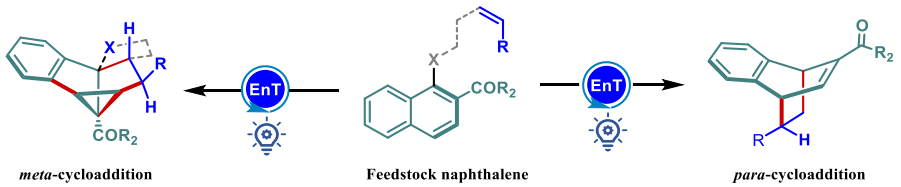

Figure 1. Visible light-induced triplet energy-transfer mediated *meta*- and *para*-cycloaddition of naphthalene derivatives.

References:

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Dr. Beeraiah Baire born in Choppadandi, Karimnagar of Telangana state. His initial schooling was done in Choppadandi. He has done his B. Sc in SRR Govt degree college, affiliated to Kakatiya University. He completed his M. Sc (Chemistry) from the University of Hyderabad in 2003. He obtained his Ph. D.in Organic Chemistry, from IISc, Bangalore, with (Late) Prof. Srikrishna in Nov 2007. Later he moved to University of Minnesota for his postdoctoral studies and worked in Prof. Thomas R Hoye's Lab from Dec 2009- Aug 2013. In September 2013, he joined the Department of Chemistry, IIT Madras as an Assistant Professor. Currently, he is working as a full Professor in the same department.

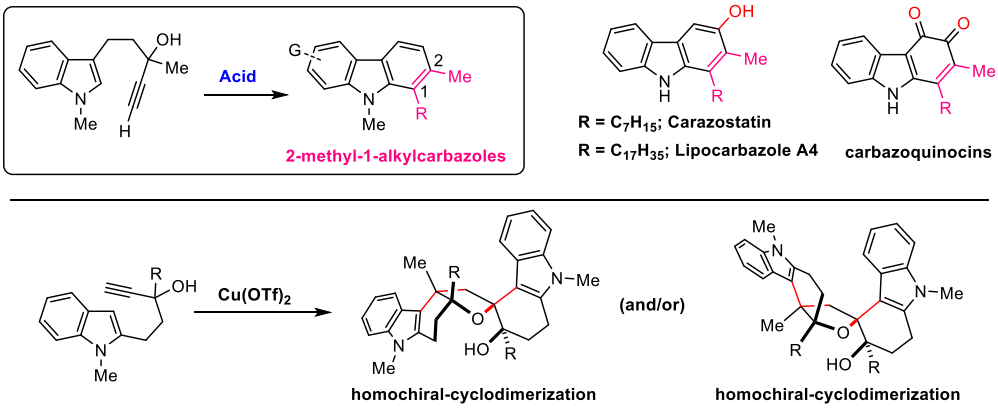
His research interests include the development of new synthetic methodologies by the exploration of unconventional reactivity of propargylic alcohols and their derivatives. His research group has also engaged in the total synthesis of bioactive natural products, and drug molecules. Some of the key developments of his research group include, a) The Z-enoate assisted Meyer-Schuster Rearrangement of propargylic alcohols; b) A new type of (*semi*)-Favorskii rearrangement; and c) Prototypical synthesis of bisindolylmethyl ethers.

He is an author of more than 75 research publications, 1-patent, and 2-book chapters. Under his supervision 7-Students have been awarded Ph.D. degree, and 9-students have been awarded their Master (M.Sc.) in Chemistry dissertation. Presently, 9-research scholars and 1-M.Sc. student are working under his guidance.

Exploring the Reactivity of (Indol-3/2-yl)pentyn-3-ols: Approaches to Natural carbazoles, Unnatural Dimeric-carbazoles and Cyclopenta[*b*]indoles

Beeraiah Baire
Professor, Department of Chemistry
Indian Institute of Technology Madras; Chennai-600036,

Propargylic alcohols have attracted immense attention as unique building blocks in organic synthesis.[1] Through the scientific endeavours of our research laboratory, we have been working on the reactivities of (indol-3/2-yl)pentyn-3-ols (indole appended propargylic alcohols) with a target of applying them towards the total synthesis of bioactive natural products and their derivatives. We have designed and developed a unified strategy for the rapid construction of 2-methyl-1-alkylcarbazole frameworks employing divergent 3-indolyl tethered propargylic alcohols under acid catalysis. Subsequently, total synthesis of *N*-methyl derivatives of various bioactive carbazole natural products like carbazomycins A-D, carazostatin, carbazoquinocin C and lipocarbazole A4 have also been achieved.[2] Similarly, we have also explored the reactivity of 2-indolyl tethered propargylic alcohols for the construction unnatural dimeric-carbazoles.[2c] The details will be discussed during the lecture.



Scheme: Acid promoted reactivity of 2-/3-indolyl tethered propargylic alcohols

References:

1) (a) J. Tsuji, T. Mandai, *Angew. Chem., Int. Ed. Engl*. **1996**, *34*, 2589; (b) R. Chinchilla, C.´ Najera, *Chem. Soc. Rev.* **2011**, *40*, 5084.

2) (a) P. Tharra, B. Baire, B. *Org. Lett.,* **2018***, 20,* 1118-1121; (b) D. Roy, P. Tharra, B. Baire, *Chem. Commun.,* **2022***, 95,* 10210-10213; (c) D. Roy, B. Baire, *Angew. Chem. Int. Edn.,* **2023**, e202304557, https://doi.org/10.1002/anie.202304557.

AVRA-IICT Session

Chairpersons: D. Srinivasa Reddy & Raji Reddy

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Director (additional charge)
CSIR-Indian Institute of Integrative Medicine, Jammu
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Background/Experineces:

- PhD, University of Hyderabad, 2000 (Advisor: Professor Goverdhan Mehta).
- Post-doctoral with Prof. Sergey A. Kozmin (University of Chicago, USA) and Prof. JeffreyAubé (University of Kansas, USA)
- 20+ Years of research experience (post-PhD) in total synthesis of natural products/ medicinalchemistry/ drug discovery
- 7 Years of experience in pharmaceutical industry (Dr.Reddy's & TATA Advinus), A moleculediscovered by his team at industry is currently in human phase-II clinical trials (Licogliflozin)
- Out-licensed patent/technology (two nos.) developed by team at CSIR-NCL
- Author of ~120 publications and an inventor in ~35 patents

Awards:

- J. C. Bose National Fellowship by SERB, DST, Govt. of India
- Shanti Swarup Bhatnagar Prize in chemical sciences
- Fellow of the Indian Academy of Sciences, India (FASc)
- Fellow of the National Academy of Sciences, India (FNASc)
- NASI-Reliance Industries Platinum Jubilee Award in the field of physical sciences
- Sun Pharma Research (Ranbaxy) Award in the field of pharmaceutical sciences
- Nominated member of the scientific body of Indian Pharmacopoeia, Govt. of India
- CRSI Bronze Medal in chemical science
- CDRI Award for Excellence in drug discovery research - chemical sciences
- Editor of Bioorganic & Medicinal Chemistry Letters (BMCL), an Elsevier journal

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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 fellow of National Academy of Sciences (FNASc) and Telangana Academy of Sciences.

He is an author of 165-publications, 10-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.

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Viresh Rawal was born in India and at a young age immigrated with his family to the United States, settling in Connecticut. He received his BS degree from the University of Connecticut (1980) and his PhD from the University of Pennsylvania (1986) under Professor Michael Cava. After postdoctoral work in the laboratories of Professor Gilbert Stork (Columbia University), he commenced his independent career at Ohio State University in 1988 and was promoted to Associate Professor in 1994. He relocated to the University of Chicago in 1995 and in 1998 was promoted to the rank of Professor. He served as the Chairman of the Chemistry Department from 2015-2018, and 2021-2013.

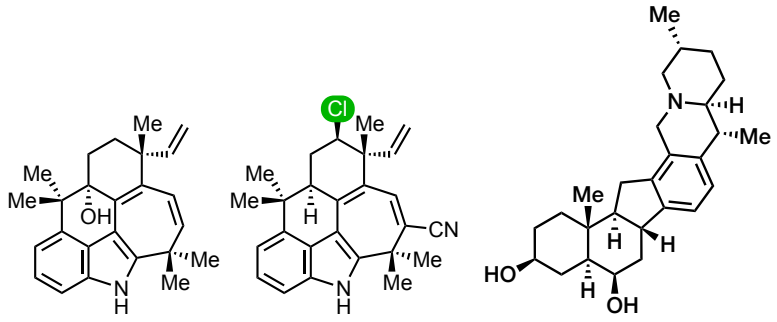
Rawal's research program covers a broad range of problems in organic synthesis, with an emphasis on the development of methods and strategies for complex molecule synthesis. The effort in total synthesis has culminated in the completion of numerous intricate targets, including (-)-isocomene, modhephene, silphiperfol-6-ene, (+)-tabersonine, (-)-quebrachamine, vindoline, arborescidines A-C, (+)-geissoschizine, dehydrotubifoline, akuammicine, zenkerene, elisapterosin B, elisabethin, mycalamides A and B, pederin, platencin, welwitindolinones B, C, and D, ambiguines G, P, Q, heilonine, hinckdentine A, and strychnine (two routes). Methodology development has played a central role in his work and considerable effort has been devoted to the development of transition metal catalysis of reactions, including enantioselective reactions. His group has also made pioneering contributions to organic catalysis using hydrogen bond donors, including the first demonstration of simple chiral alcohols serving as highly enantioselective catalysts. Their development of chiral squaramides, which are bifunctional hydrogen bond donor catalysts, represented a major advance in organocatalysis, and are among the most widely used catalysts for asymmetric synthesis.

Rawal has delivered over 300 plenary and invited lectures and his work has been recognized through many awards, including the ACS Award for Creative Work in Organic Synthesis (2024), International Society of Heterocyclic Chemistry, E.C. Taylor Award (2022), CRSI Medal (2019), Japan Society for the Promotion of Science Lectureship (2015), Novartis International Lectureship Award (2015), ACS Cope Scholar Award (2003), Swiss Chemical Society Lectureship Award (2002), and awards from Pfizer, Merck, and Eli Lilly (1995-1998). He has served on the editorial boards of *The Journal of Organic Chemistry* (2004-2008), *Organic Syntheses* (2007-2015), *Heterocycles* (2007-2023), *Organic & Biomolecular Chemistry* (2012-present), *Organic Chemistry Frontiers* and *Asian Journal of Organic Chemistry* (2012-2020), and *Tetrahedron* and *Tetrahedron Letters* (2015-present). He served as the Editor for *Science of Synthesis,* Volume 46, "Compounds with All-Carbon Functions, 1,3-dienes."

Methods and Strategies for the Synthesis of Intricate Molecules

Viresh H. Rawal
University of Chicago

The process of chemical synthesis involves a sequence of reactions that systematically elevate the complexity of a starting material until it ultimately morphs into the desired end product. While the specific reactions – or tactics – employed for each step are undeniably crucial for success, the underlying strategy is arguably of greater importance. The strategy should, ideally, not only address the primary structural challenges of a natural product, but it should also enable the synthesis of other members of that family of natural products. In this presentation, I will delve into the strategic and tactical considerations that shaped our work on the synthesis of indole alkaloid metabolites derived from cyanobacteria. Particular emphasis will be placed on the pentacyclic ambiguine group of compounds, which form a subset of the large hapalindole family of alkaloids. Time permitting, I will also discuss our approach for the synthesis of heilonine, a member of the *Veratrum* family of alkaloids.



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Professor
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Saumen Hajra has done his B.Sc. (Chem. Hons.) from RKM Vidyamandira, Belur Math and M.Sc. in Organic Chemistry from Calcutta University (Raja Bazar Science College). He obtained Ph.D. in Organic Chemistry (Photo-induced Electron Transfer Chemistry) under supervision of Dr. Ganesh Pandey from National Chemical Laboratory, Pune in 1997. He subsequently held postdoctoral positions at the North Dakota State University, USA with Prof. Mukund P. Sibi (1997-98) and Alexander von Humboldt Fellow with Prof. Waldemar Adam (1999-2000) at University of Wurzburg, Germany. In August 2000, he joined as an Assistant Professor of Chemistry at IIT Kharagpur and became Full Professor in 2011. After serving 14 years at IIT Kharagpur, he has moved to Centre of Biomedical Research (CBMR), Lucknow in 2014.

His research interests include development of new and modular strategies for the synthesis of biologically important molecules in optically pure form, and asymmetric catalysis.

Asymmetric Total Syntheses of Complex Bioactive Natural Products

Saumen Hajra
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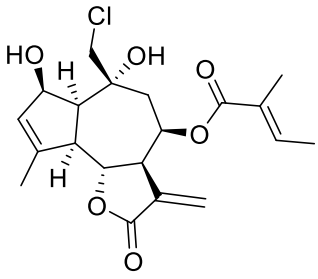
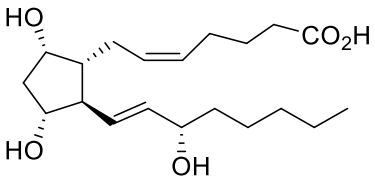
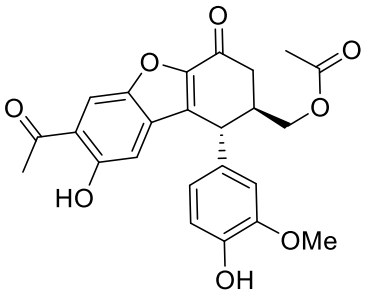
The natural products (NPs) are very attractive and biologically pre-validated starting points in medicinal chemistry. Even in recent time, about 50% of approved drugs are NPs and NP-derives. Thus, the development of efficient and cost-effective synthesis, in particular, of complex and multi-stereocenter bioactive natural product is always in demands. Highly abundant and inexpensive chiral terpenes are very attractive starting point for the synthesis of complex natural products. Scalable asymmetric total syntheses of eupalinilide E and prostaglandin PG_{F2a} from commercially abundant and inexpensive (*R*)-carvone will be presented in the symposium.[1,2] Further, recent accomplishment of first asymmetric total synthesis of propolishbenzofuran B isolated from Brazilian propolis (honey bees) will also be briefly discussed.[3]



Eupalinilide E



PG_{F2}



Propolisbenzofuran B

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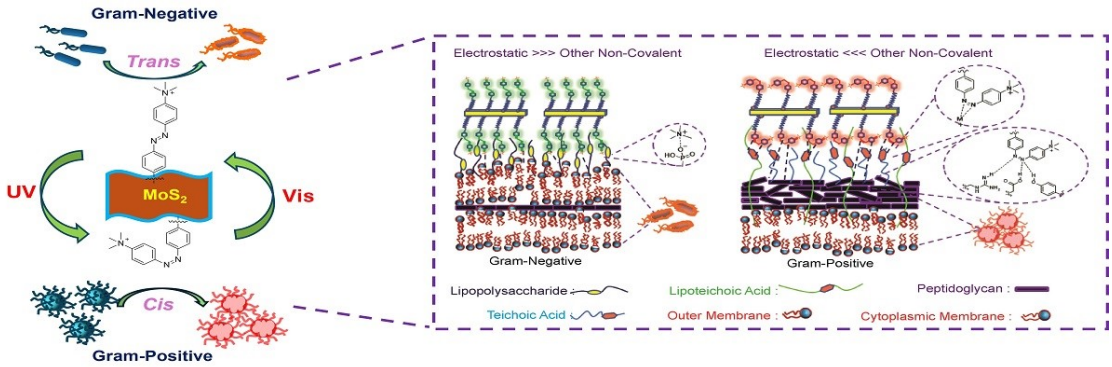
Indian Institute of Science
Email: md@iisc.ac.in

Mrinmoy De is an associate professor at the Department of Organic Chemistry at the Indian Institute of Science, Bangalore, India. He completed his BSc degree from Vidyasagar University with Gold medal. He received his M.Sc. from the Indian Institute of Technology, Bombay, and Ph.D. from the University of Massachusetts at Amherst under the supervision of Prof. Vincent M. Rotello. He was a CCNE (Center of Cancer Nanotechnology Excellence) and NSEC (Nanoscale Science and Engineering Center) postdoctoral fellow at Northwestern University. Since 2014, he has been at the Indian Institute of Science, Bangalore, where he is an associate professor in the department of organic chemistry. His research focuses on the preparation of various nanomaterials and their application toward the development of nanoantibiotics, nanozymes, sensors and photocatalysis. Mrinmoy De is the associate member of American Material Research Society (MRS), American Chemical Society (ACS), Material Research Scoiety of India (MRSI), Chemical Research Socety of India (CRSI) and Society Of Biological Chemists, India(SBCI). He is recipient of Ignite Life Science Foundation Grant, Young Scientist Award by Science and Engineering Research Board (SERB), Outstanding Researcher Award by NSF Nanoscale Science & Engineering Center and CRS Silver Medal.

Selective Antibacterial activity of Functionalized Nanomaterials

Mrinmoy De
Department of Organic Chemistry
Indian Institute of Science

Developing material-based antibiotics can be the most potent alternative due to the increasing resistance against conventional antibiotics. However, one of the important parameters in the development of antibacterial agents is Gram/strain selectivity, which is seldom explored in the case of nano-antibiotics. The multimodal action of surface-functionalized nanomaterials can exhibit strain-selective and enhanced antibacterial activity. Two-dimensional MoS_2 nanosheets (2D-MoS_2) have been widely used in many biological applications due to their distinctive physicochemical properties. In the past, it was theorized that chemically exfoliated MoS_2 can be modified using thiol chemistry. In this regard, we provided the first experimental evidence for this process using a facile solution-based method. By chemically engineering the ligands, we then showed the ability to modulate the surface of the MoS_2 sheets. In doing so, we have developed several strategies to demonstrated the ability to tune the surface of the conjugates for selective enzyme targeting, inhibition, and antibacterial activity. Those strategies are based on different proportions of positively and negatively charged functionalized ligands, tethered amino acids/peptides, conjugation of Ni-nanocluster, photo-controlled gating of selective bacterial membrane interaction, etc. Taken together, we have prepared simple and efficient Gram-selective 2D-MoS_2-based antibacterial agents, which can also be extended to other systems with antimicrobial properties.



Selective antibacterial activity of functionalized MoS_2.

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Ishu Saraogi obtained her BSc and MS in Chemistry, after which she moved to Yale University to pursue a PhD in bioorganic chemistry. Following a postdoctoral stint at Caltech, Dr. Saraogi joined IISER Bhopal in 2013, where her group works on developing chemical tools to modulate biomolecular interactions. Their research group focuses on the development of novel antibacterial and anti-amyloidogenic agents. She is a recipient of the Ramanujan Fellowship and POWER fellowship from the Science and Engineering Research Board (SERB). Their work was featured in the ChemBioTalents collection by the journal ChemBioChem (Wiley). 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. She serves on the editorial advisory boards of ChemBioChem (early career) and ACS Chemical Health & Safety.

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

Syngenta Session

Chairpersons: C. V. Ramana & N. Selvakumar

C. V. Ramana
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Dr. Ramana obtained his MSc. from Andhra University, Waltair (1991) and PhD from University of Hyderabad under the supervision of Professor M. Nagarajan (Synthetic Carbohydrate Chemistry). From 1998 to 2001 he was associated with Professor Andrea Vasella at ETH Zurich as a post-doctoral researcher (glycosidase inhibitors). From May 2001 onwards, he had been associated with National Chemical Laboratory (CSIR, India). At NCL, the focus of Ramana's group includes small molecules synthesis by employing transition metal complexes and developing new catalytic methods. The major focus of Dr. Ramana's group is the total synthesis of natural products and biologically important targets with a keen insight into developing new methods and extending the platform for the synthesis of pharmaceutically relevant small molecules. In general, his group is known decorating the total synthesis canvas with metal reagents and demonstrate designing of new synthetic tools involving the orchestration of sequential events in one-pot with one catalyst. In addition to this, his group also works in the areas of beta-peptides, C-saccharides synthesis, glyconanoparticles and application of C–H activation in non-infringing processes development.

He is a recipient CSIR Young Scientist award in Chemical Sciences (2003), NCL's Scientist of the Year award (2009), Professor D. K. Banerjee Memorial Lecture Award - IISc Bangalore (2011) and CRSI Bronze Medal in chemical sciences (2013) and Dr. A.V. Rama Rao Foundation Prize Lecture in Chemistry (2016) and CNR Rao National Prize in Chemical Sciences (2017). He is the fellow of Indian Academy of Sciences (2014, Bengalore). To his credit, he had about 150 publications, 17 patents and 27 students have been awarded PhD. degree under his supervision.

N. Selvakumar
Founder and CEO
DSK InnoSciences
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Graduated in Organic Chemistry from the Indian Institute of Science (IISc), Bangalore, India and with two subsequent post-doctoral studies at Iowa State University, USA (2 years) and University of Alberta, Canada (2 years), he had an illustrious career as medicinal chemist at Dr. Reddy's Laboratories, Hyderabad over a period of 9 years.

His noted contributions have been the discovery of DRF-8417, DRF-11057 and DRF-15248 for bacterial infection that have reached various phases of clinical trials. He is the author of over 30 research publications and about 10 patents.

Subsequently, he was part of the founding management team of Anthem Biosciences, Bangalore as Vice President Discovery where he was heading several project teams comprising of about 150 scientists in both Chemistry and Biology. During his tenure of three years, he played a pivotal role in establishing their early business.

In 2010, he promoted DSK InnoSciences with a vision to be a differentiating CRO in all areas of chemistry with its greenfield facility that commenced operations in the year 2014.

P. Veeraraghavan Ramachandran
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Purdue University
West Lafayette, IN 47907, USA
Email: chandran@purdue.edu

Professor P. V. Ramachandran received his BSc and MSc degrees from Calicut University, India and received his Ph.D. from the Indian Institute of Technology, Kanpur under the supervision of Professor Subramania Ranganathan before joining the laboratories of the late Professor Hebert C. Brown at Purdue University as a postdoctoral associate. Soon after, he joined the faculty of Purdue Chemistry Department and is currently a Professor of Chemistry. He is also the Director of the Hebert C. Brown Center for Borane Research at Purdue and the Chief Scientific Officer of Arta Therapeutics, a bio-tech company focusing on therapies for infectious diseases.

He has received several recognitions for his contributions to chemistry. He is a Fellow of the American Chemical Society (ACSF) and the Royal Society of Chemistry (FRSC). He is a Purdue University Faculty Scholar and has received Purdue University Undergraduate Mentoring Award (2012) and College of Science Team Award (2015). He is the recipient of the Boron in the Americas Award (2006). He was elected as the Chairman of the Fluorine Division of the ACS (2006) and has also chaired the ACS 19th Winter Fluorine Conference (2009). He was the Chair of the 13th Boron in the Americas Conference (2012). He received the Vikram Sarabhai Chair Award from the Indian National Science Academy for 2014-15.

Prof. Ramachandran's research focuses on the application of organoborane and fluoro-organic chemistry. His lab develops novel methods and reagents to facilitate the synthesis of a variety of complex molecular targets, particularly for the treatment of cancer, infectious diseases, and central nervous system disorders. He is a co-author of over 250 peer-reviewed publications, several book chapters, and reviews, and has several US patents to his credit. He has edited two books and is also an Associate Editor of Future Medicinal Chemistry. He has given keynote/plenary addresses in several international conferences.

Tapping the Potential of Borane-Amines

P. Veeraraghavan Ramachandran
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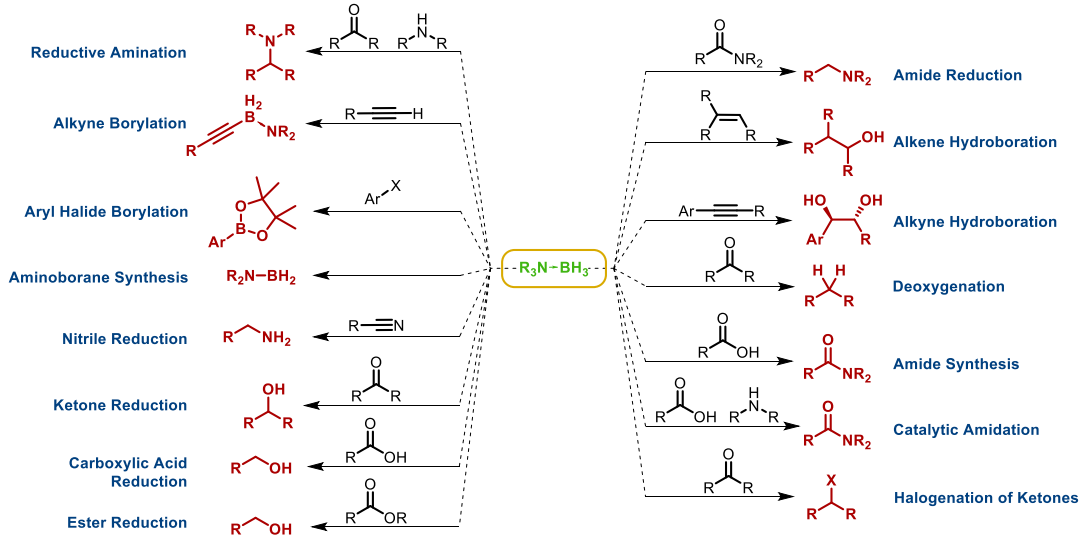
The pyrophoric, air- and moisture-sensitive organo-sulfur and -oxygen complexes of borane, such as borane-dimethyl sulfide and borane-THF, have become common reagents for organic transformations. However, the potential of the corresponding air-stable nitrogen complexes, borane-amines, has not been fully exploited, possibly due to the high cost and characteristic stability of these complexes. Recently, there has been considerable focus on borane-amines as hydrogen carriers, but their applications for organic transformations are still underdeveloped. We seized on this opportunity with the dual goals of designing facile, economical routes to borane-amines and to tap their full potential as synthetic reagents. With a little over a decade of attention on borane-amines, we have systematically developed several convenient syntheses[1] and demonstrated the utility of borane-amines, particularly borane-ammonia for materials and organic chemistry applications. The effect of borane-complexation of amines on their hypergolicity[2] and their applicability for nanoparticle synthesis[3] belong to the former class. The capacity of borane-ammonia for uncatalyzed[4] and catalyzed organic transformations (Scheme)[5] belongs to the latter class. A history of borane-amines, their new syntheses, and most recent applications will be discussed.

Scheme: Recent applications of borane-ammonia mediated reactions



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3. (a) *ACS Appl. Nano Mater.* **2019**, *2*, 5351-5355. (b) *ibid*. **2023**, *6*, 11070–11076.
4. *Chem. Comm.* **2016**, *52*, 11897-11900.
5. (a) *Org. Lett.* **2021**, *23*, 2938-2942. (b) *ibid.* **2022**, *24*, 8481-8486. (c) *ibid.* **2023**, *25*, 6902-6906.

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School of Chemistry
University of Hyderabad, Hyderabad
Email: akhilchemistry12@gmail.com

Education:

Postdoctoral Fellow, Kyoto University, Japan (with Prof. A. Osuka)	2004-2006
Postdoctoral Fellow-JSPS, Kyoto University, Japan (with Prof. T. Hiyama)	2002-2004
Postdoctoral Fellow, RWTH Aachen, Germany (with Prof. H-J. Gais)	2002-2002
Ph.D, National Chemical Laboratory, Pune, India (with Prof. G. Pandey)	2001
MSc (Organic Spl), Utkal University, Bhubaneswar, Odisha	1994

Career:

Professor, University of Hyderabad, India	2016-present
Associate Professor, University of Hyderabad, India,	2013-2016
Assistant Professor, University of Hyderabad, India,	2007-2012
Scientist, Sai Advantium Pharma Limited, Hyderabad, India,	2006-2007

Scientific activities:

-Published over 90 papers and 7 International Patents
-Delivered lectures over 75 seminars in the National Symposiums in India.
-Delivered 25 invited lectures in the International Conference.

Research topics:

-Development of novel synthetic methods for organic synthesis.
-Functionalizations of sp^2 and sp^3 C-H bonds. Stereoselective C-H functionalizations.
-Gold and silver-catalyzed organic transformations.
-Synthesis of fused-□-conjugated heterocycles.
-Synthesis of nitro and nitrogen-rich insensitive high energetic materials.

Awards:

Fellow of Indian Academy of Sciences (FASc)-2021
Fellow of Royal Society of Chemistry (FRSC)-2020
Fellow of National Academy of Sciences (FNASc)-2019
UGC-BSR-Mid Career Award-2020
Prof. D. K. Banerjee Memorial Lecture Award 2012, IISc, Bangalore.
Japan Society for the Promotion of Science (JSPS) Fellowship 2002.

Supervision and Guidance:

-PhD completed-**18**, -Currently supervising-**09** -Total Citations **4811**
[**h-Index = 42**; **i10 Index = 82;** Google Scholar as on 10/02/2024]

Recognition:

Associate Editor of the New Journal of Chemistry (RSC) from January 2017

Academia-Industry Collaboration:

Consultant to Sai Life Sciences (2007-2009); Adama Pvt. Ltd. (2015-2023).

Contribution to National /International Forum

• Prof. Angela Marinetti, CNRS-ICSN, GIIF-sur-Yvette, Paris under CEFIPRA.
• Member of School Board of Chemistry: Central University of Rajasthan, BHU
• Council Member of the National Organic Symposium Trust (NOST; 2019-2021; 2022-2025).
• Treasurer of CRSI-India; Member of the RSC, Member of the ACS-USA

Harnessing C(sp^3)-H Bonds with Bifunctional Reagents

A. K. Sahoo
School of Chemistry, University of Hyderabad

Aliphatic carboxylic acids are widely available and are ubiquitous. Therefore, development of expedient transformations of aliphatic carboxylic acids have drawn significant attention. The selective activation and functionalization of aliphatic carboxylic acids, however, poses formidable challenges due to the low reactivity of aliphatic C-H bonds. Over the past two decades, unique synthetic manifolds that uses directing groups and the transition metal catalysts, have been developed for C(sp^3)–H bond activation. Whereas two-fold C(sp^3)□H activation and sequential bond formations remains challenging. Herein we have successfully culminated this idea by showcasing the 2-pyridyl-methyl sulfoximine **(MPyS)** assisted two-fold C(sp^3)□H activation for the synthesis of benzo-fused caprolactones. In addition, multicomponent reactions via C(sp^3)–H bond activations for arene 1,2-difunctionalizations is also enumerated.

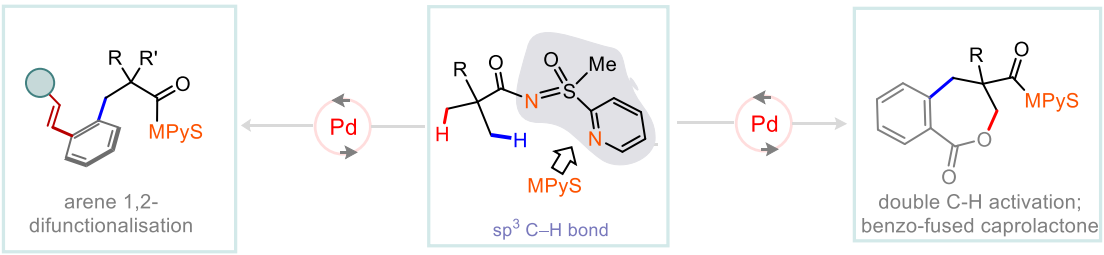

Figure 1: double C(sp^3)-H activation

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4. Ghosh, A.; Kondalarao, K.; Saha, A.; Gandon, V.; Sahoo, A. K. A Three-Component Arene Difunctionalization: Merger of C(sp^3)/(sp^2)□H Bond Addition. *Angew. Chem. Int. Ed*. **2023**, *62*, e202314362.

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Dr. Praveen Kumar Vemula is an Associate Professor at the Institute for Stem Cell Science and Regenerative Medicine (inStem), Bangalore. He has completed Masters in Chemistry from Osmania University (1998), and obtained PhD from Indian Institute of Science, Bangalore under supervision of Prof. Santanu Bhattacharya (2005). He did postdoc research at City College of New York. Subsequently, he has worked as Ewing Marion Kauffman Foundation Entrepreneurial Postdoc Fellow at Harvard Medical School. His expertise is developing chemical technologies for medical applications. His work spans the fields of biomaterials, drug discovery, drug delivery, medical devices, and chemical biology.

Vemula has published >90 peer-reviewed papers, has given >250 national and international invited lectures including two TEDx talks, and has >30 issued or pending national/international patents, which have been licensed to multiple biotech companies. Several technologies developed in his lab have formed the foundation for multiple products on the market, and currently under development. His technologies have led to the launch of 7 startup companies. Thus far, >25 products that are developed based on his technologies are in the market worldwide.

His work has been recognized by:
National Biotechnology Innovation Award-2023
DBT-Product, Process, Technology Development and Commercialization Award 2020
GYTI-SRISTI-BIRAC Award-2019

Chemistry as a tool to develop biomedical technologies to solve unmet clinical needs

Praveen Kumar Vemula
Institute for Stem Cell Science and Regenerative Medicine (DBT-inStem)

Our lab is focusing on clinical translational research through biomaterials and chemical biology programs. By using chemical design tools, we have been developing therapeutic and prophylactic biomaterials for medical applications. A wide range of technologies developed in the lab were used for multiple medical applications, such as treatment of inflammatory bowel diseases, arthritis and preventing rejection episodes in transplanted organs.[1-3] Additionally, prophylactic technologies were developed to prevent pesticide-induced toxicity and lethality. Additionally, we will discuss our efforts in translating these technologies into the clinic.

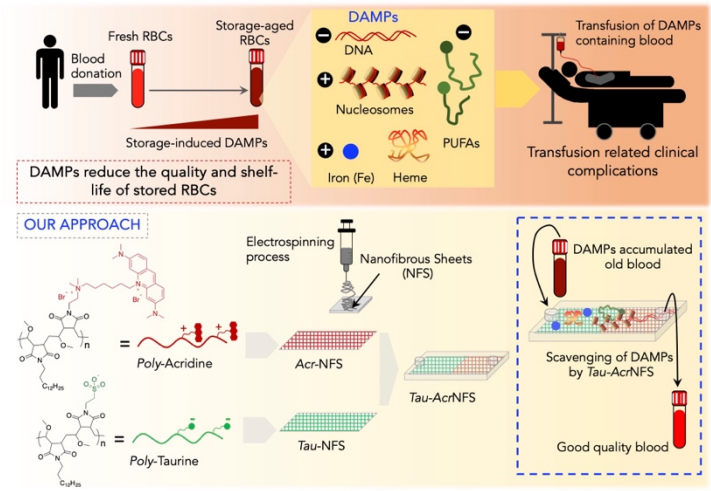

Figure 1: (Top panel) Stored blood produces DAMPs that cause oxidative stress and reduces the quality of stored blood. (Lower panel) Systematically designed polymers can be as nanofibrous sheets that can scavenge DAMPs using ionic interactions to improve the quality of stored blood.

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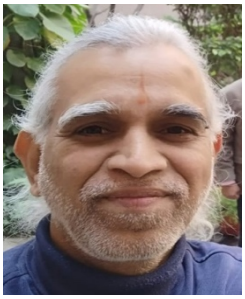

Gopalan received both B. Sc., and M. Sc., in Chemistry from RKM Vivekananda College, University of Madras, Chennai. He obtained his Ph. D., in Organic Chemistry, from the Indian Institute of Science (IISc), Bangalore, India, in 1998 under the supervision of Prof. Sosale Chandrasekhar. During 1998-99 as a post-doctoral fellow, he was introduced to carbohydrate chemistry and oligosaccharide synthesis with the mentorship of Prof. Dr. Andrea Vasella at the Laboratorium fur Organische Chemie, Eidgenössische Technische Hochschule (ETH), Zürich, Switzerland (1998-99).

During 2000-2003, he was a post-doctoral fellow in the project for synthetic carbohydrate conjugate vaccines under the mentorship of Dr. Vince Pozsgay, Dr. Rachel Schneerson, and Dr. John B. Robbins at the National Institute of Child Health and Human Development (NICHD), National Institutes of Health (NIH), Bethesda, MD, USA. During this stint, he learnt multi-gram scale synthesis of oligosaccharide fragments of *Shigella dysenteriae* type 1 *O*-antigen for conjugation to carrier proteins. During 2003-2007, he spent time as a post-doctoral research associate with Prof. Kevin J. Yarema at the Department of Biomedical Engineering, The Johns Hopkins University (JHU), Baltimore, MD, USA, whence he learnt metabolic glycan engineering in mammalian cells and techniques in biochemistry, molecular biology, cell biology, and immunology. The projects included metabolic engineering of human embryoid-body derived stem cells towards neural differentiation and application of conjugates of short-chain fatty acid (SCFA) and monosaccharides as anti-cancer agents.

Since 2007, he is a Scientist at the National Institute of Immunology and established the Laboratory of Chemical Glycobiology with the broad goal of research in glycobiology, glycoimmunology, and glyco-medicine. His research interests include the role of glycosylation in immune synapse formation, carbohydrate-based drug design, delivery systems for carbohydrates across the blood-brain barrier, glycomics and glycoproteomics, development of inhibitors for glycosylation, and the role of glycosylation in tumorigenesis, melanogenesis, and auto-immune disorders. He is a recipient of the Department of Biotechnology Ramalingaswami Fellowship (2008-2013).

Chemical tools for unravelling the structure and function of glycoconjugates in living systems

Srinivasa-Gopalan Sampathkumar

Laboratory of Chemical Glycobiology, National Institute of Immunology (NII), New Delhi 110067, India

Unlike the conserved fundamental building blocks for DNA, RNA, and proteins, the building blocks for carbohydrates vary widely between vertebrates, invertebrates, and bacteria. Monosaccharide building blocks are employed in complex carbohydrate metabolism to biosynthesize glycoproteins, glycolipids, and glycosaminoglycans – together known as the glycoconjugates. Compared to advances in genomics and proteomics, the progress in glycomics has been hampered due to their non-template driven biosynthesis and paucity of reliable tools. In this regard, the advent of metabolic glycan engineering and bioorthogonal ligation in living systems, pioneered by Reutter, Bertozzi, and others, provides a complementary approach to genetic methodologies. Our laboratory has been focused on the design, synthesis, and application of synthetic monosaccharide analogues for the interception and inhibition of glycoconjugate biosynthesis.

On the one hand, we developed the carbohydrate-neuroactive (CH-NA) hybrid strategy for non-invasive *in vivo* glycan engineering of sialoglycoproteins in the brain of mice using prodrug-like derivatives of *N*-acetyl-D-mannosamine[1]. CH-NA strategy enabled the manipulation of polysialic acid on neural cell adhesion molecule (NCAM) in brain in mice which is essential for neural development. On the other hand, we showed that the peracetyl *N*-thioglycolyl-D-galactosamine (Ac_5GalNTGc) is an efficient inhibitor of *O*-glycosylation[2,3]. Recently, we have identified a novel ManNAc analogue which enhanced the levels of sialyl-Lewis X (sLeX, also known as CD15s; **Fig. 1**) in lymphocytes and consequently enhanced cell adhesion to E-selectin coated surfaces. The ability to alter glycans while maintaining polypeptide levels *in vivo* has the potential to deconvolute the functions of glycans in health and disease.

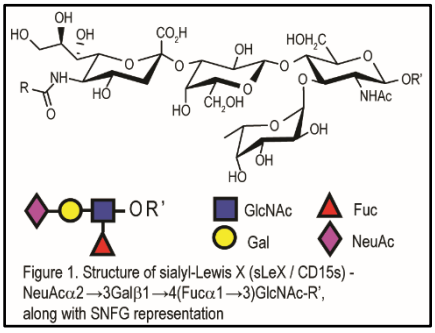

Figure 1. Structure of sialyl-Lewis X (sLeX / CD15s) - NeuAcα2→3Galβ1→4(Fucα1→3)GlcNAc-R', along with SNFG representation

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Dr. Nidhi Jain obtained her Ph.D. in Organic Synthesis from University of Delhi in 2005. She subsequently moved to USA for a post-doctoral position with Prof. Bongsup P. Cho (2005-08), and joined Indian Institute of Technology Delhi in 2010 as an Assistant Professor. She was the University topper in her graduation and is a recipient of T.R. Sheshadri Memorial Award by Delhi University, Teaching Excellence Award by IIT Delhi and CRSI Bronze Medal in 2022, as some of her academic accolades.

In the last 13 years of her independent research career at IITD, her group has contributed significantly to the field of C-H bond functionalization in organic synthesis and developed methods to engage them in late-stage functionalization. Economical and sustainable strategies for construction of C-C, C-N, C-O and C-S bonds assisted by palladium and copper catalysts, hypervalent iodine reagents and photocatalysis in visible light have been developed. All these methods allow access to molecules of high synthetic and commercial value. The scientific contributions have transpired into more than 70 research papers in international journals of repute (ACS, RSC, Wiley) with a total of more than 3600 citations and h-index 23. 10 PhD students have graduated from her research group, 8 are currently in progress and 40 masters students have been trained. She has been actively involved in institute building as Professor in charge-UQIDAR, coordinating with international academics and currently serving as Associate Dean Faculty.

Visible light photoredox catalysis in organic transformations

Nidhi Jain
Indian Institute of Technology Delhi

The area of visible light assisted C-H bond functionalization is developing swiftly with numerous research groups working to harness its complete potential. The lecture will discuss the advent and development of visible light photoredox catalysis for synthetic organic transformations. From regioselective C-H functionalizations like thiocyanation, halogenation and acylation to ring opening of heterocycles and radical addition on olefins; we have explored a diverse range of reactions. Photocatalyst-free generation of *para*-quinone methide in visible light for construction of tetrasubstituted carbon stereocenter and photocatalyzed dehydrogenation of aliphatic *N*-Heterocycles, linear amides, and carbamates will be demonstrated with key insights into their mechanism. All these techniques inspired by sustainable chemistry goals, allow access to molecules of high synthetic value, both in industrial and academic settings.

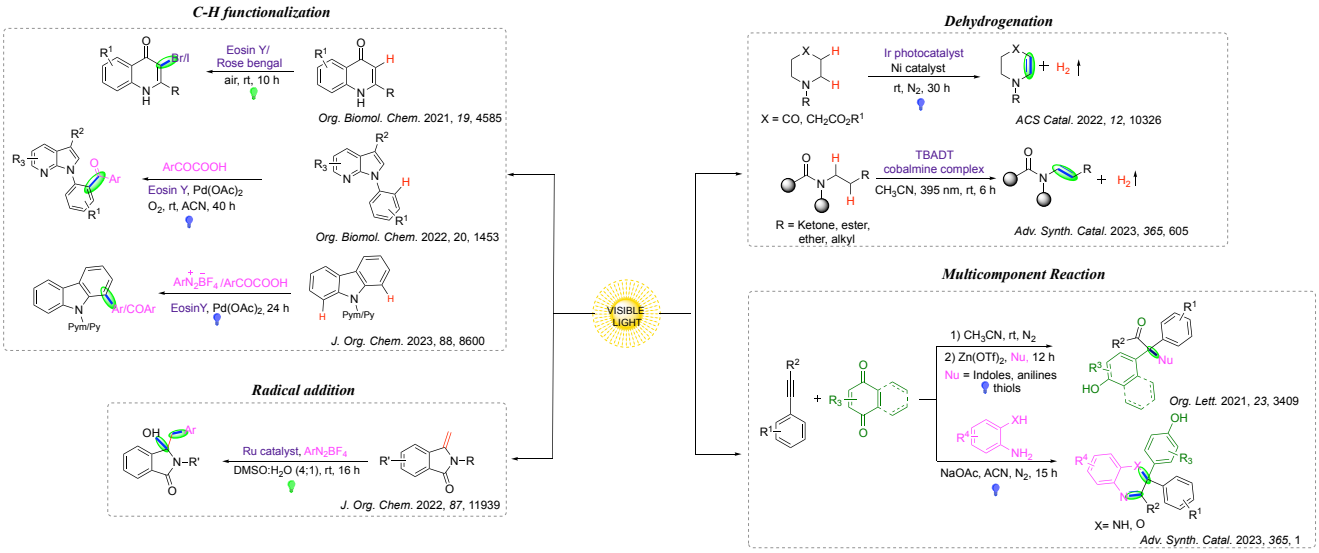

Figure 1: Visible light mediated organic transformations

PI Industries Session
(Flash Presentation)

Chairpersons: S. Gharpure, P. Srihari & S. V. Ramasastry

Santosh J. Gharpure
Professor In-Charge SINE & Rasiklal Hemani
Fragrance and Flavour Chair Professor
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Dr. Santosh J. Gharpure graduated with an M.Sc. degree in 1996, from Indian Institute of Technology Bombay, Powai. He obtained Ph.D. from Indian Institute of Science, Bangalore working with Late Prof. A. Srikrishna in 2001. He held a post-doctoral position with Prof. P. Andrew Evans at Indiana University, Bloomington, U.S.A. Subsequently, he joined the Department of Chemistry, IIT Madras, Chennai in the year 2004. In 2012, he moved to the Department of Chemistry, IIT Bombay, Powai, Mumbai as an Associate Professor and was promoted to Professor position in 2016. Currently, he holds the position of 'Rasiklal Hemani Fragrance and Flavour Chair Professor'. He is also Professor In-Charge of SINE, IIT Bombay's technology incubator. His research focuses on organic chemistry pertaining to natural and unnatural product synthesis and developing new synthetic methodologies. He is also working on problems relevant to industries from different domains.

Dr. Gharpure is a recipient of INSA Medal for Young Scientist. He was awarded IIT Madras Young Faculty Recognition Award (YFRA) for his contribution in teaching and research in 2010. He received B. M. Birla science Prize in Chemistry for the year 2011. He was selected as one of the Thieme Chemistry Journal Awardees for the year 2013. IIT Bombay conferred on him the Excellence in Teaching Award in the year 2015 and Departmental award for excellence in teaching in 2019. He was selected as Themis Medicare UICT Diamond Jubilee Distinguished Fellow in Pharmaceutical Science for the year 2015-16 of ICT, Mumbai. He was selected for the award of Chemical Research Society of India (CRSI) Bronze Medal in 2018. He is member of the International Advisory Board of European Journal of Organic Chemistry. He is a Fellow of Royal Society of Chemistry (FRSC). Recently, he was awarded INSA Teachers Award 2021 by Indian National Science Academy, New Delhi.

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Dr. P. Srihari born in Hyderabad, India (1974) completed his Masters from P. G. College of Science, Saifabad, Osmania University in 1997. After completing his M.Phil (1998) at University of Hyderabad, he has joined Dr. J. S. Yadav's group for his Ph.D programme (Nov 1998-Oct 2003). He moved to Rutgers, The state university of New Jersey, USA (Nov 2003) for his postdoctoral fellowship with Prof. Spencer Knapp and returned to CSIR-IICT, Hyderabad in July 2005 and joined as Quick Hire Research Fellow Scientist. Presently is working as Chief Scientist (previously designated as Scientist G) in the department of Organic Synthesis & Process Chemistry.

The main areas of research include Asymmetric synthesis, Synthesis of newly isolated potent natural products and their analogues, Medicinal Chemistry, Development of methodologies involving C-C / C-X bond formation reactions, Flow chemistry for API synthesis.

Dr. Srihari is a CSIR Young Scientist Awardee for the year 2009 in the field of Chemical Sciences and OPPI Young Scientist Awardee for the year 2009 in the field of Pharmaceutical Sciences, He is recipient of AVRA Young Scientist Award 2014, Dr. A.K.Singh Memorial Young Scientist Award for the year 2016 in Synthetic Organic Chemistry. CDRI Award of excellence in Drug Research in the area of Chemical Sciences for year 2018, CRSI Bronze medal in 2021 and Acharya P C Ray Flow Technology award in 2021.

He has published more than 140 publications in international Journals of repute and has 22 patent applications filed. Fifteen students have been awarded Ph.D doctorate under his guidance, 14 M.Sc. students and 6 M.Pharmacy students have completed their dissertation projects. Presently he is supervising 10 students for their Ph.D programme.

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Previous Positions Held:

2017 - till, Associate Professor
Department of Chemical Sciences, Indian Institute of Science Education and Research (IISER) Mohali, India
2011 - 2017, Assistant Professor
Department of Chemical Sciences, Indian Institute of Science Education and Research (IISER) Mohali, India
2010 - 2011, Senior Research Scientist Jubilant Biosys Ltd., Bangalore, India **2008 - 2010**, Senior Research Investigator
Bristol-Myers Squibb Biocon Research Center (BBRC), Syngene International Ltd., Bangalore, India
2005 - 2008, Postdoctoral fellow
The Scripps Research Institute, La Jolla, CA, USA (Advisor: Prof. Carlos F. Barbas, III)

Honours and Recognitions:

* Council member of the 'National Organic Symposium Trust (NOST)' for the period 2023-26
* Invited to become the 'Fellow of the Royal Society of Chemistry (FRSC)' under 'Leaders inthe Field (LITF)' scheme (2022)
* Recipient of the CDRI Award for Excellence in Drug Research 2022
* Editorial Board member of Organic & Biomolecular Chemistry from February 2022
* Awarded the 'RSC Research Fund' grant 2020
* Swarnajayanti Fellowship (2017-18) awarded by the Department of Science & Technology(DST), Govt. of India
* V. Rama Rao Research Foundation (AVRA) Young Scientist Award 2018
* Outstanding Reviewer for Organic & Biomolecular Chemistry in 2018
* Organisation of Pharmaceutical Producers of India (OPPI) Young Scientist award 2018
* Chemical Research Society of India (CRSI) Bronze Medal 2018
* Editorial Advisory Board member of Organic & Biomolecular Chemistry during 2017-2022
* Thieme Chemistry Journals Award 2017
* Young Scientist award from the organizing committee of 'Chemical Frontiers Goa' in 2016
* Admitted as a Member of the Royal Society of Chemistry (MRSC) in 2016
* Skaggs Postdoctoral Fellowship, The Scripps Research Institute, La Jolla, USA [2005-08]
* Awarded JRF and SRF (2001-05) by the CSIR-New Delhi

Parthasarathi Subramanian
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Dr. Parthasarathi Subramanian received his Bachelor's in 2004 and Master's in 2006 from Bharathidasan University and Madras University, respectively. After working as a senior chemist for a couple of years in GVK Biosciences, he joined Prof. Krishna P. Kaliappan at IIT Bombay for his doctoral degree. Immediately after his graduation, he associated as a postdoctoral researcher with Prof. Janine Cossy at ESPCI ParisTech (2016-2017). Subsequently, he worked with Prof. Lutz Ackermann at the University of Göttingen (2017-2018) and with Prof. K. C. Nicolaou at Rice University (2018-2020). He has been working as an assistant professor at IIT Kanpur since January 2020. Subramanian group focuses on developing new synthetic and catalytic methodologies to design novel strategic approaches to expedient total synthesis of bioactive natural and unnatural molecules.

Design and Synthesis of All-Oxygen Spirocyclic Orthoester: A Unified Total Synthesis of Aculeatin Natural Products

P. Subramanian
Indian Institute of Technology Kanpur

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. 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.

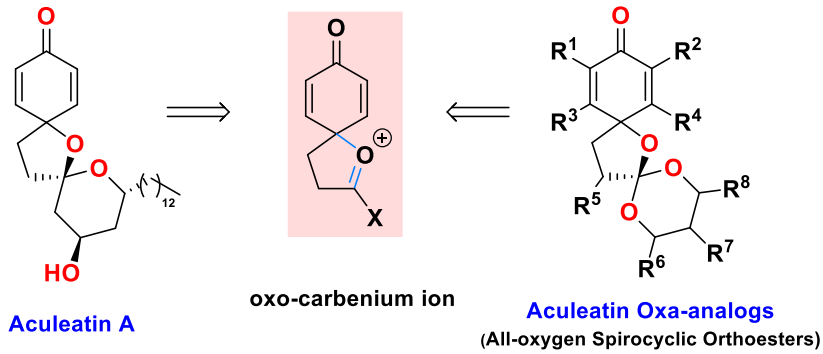

Figure 1: Structure of Spirocyclic natural and unnatural molecules.

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3. Heilmann, J.; Brun, R.; Mayr, S.; Rali, T.; Sticher, O. Minor Cytotoxic and Antibacterial Compounds from the Rhizomes of Amomum Aculeatum. *Phytochemistry* **2001**, *57*, 1281–1285.

Utpal Bora
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Professor Utpal Bora received his Ph.D. in 2005 under the guidance of Dr R. C. Boruah at CSIR-NEIST Jorhat. He was a recipient of a JSPS postdoctoral fellowship to work with Professor Hironao Sajiki at Gifu Pharmaceutical University, Gifu, Japan during 2005–07. In 2008, he joined Syngene International Limited, Bangalore as Associate Scientific manager and later moved to the Department of Chemistry, Dibrugarh University, Dibrugarh as Assistant Professor in 2008. In 2013 he joined the Department of Chemical Sciences, Tezpur University, Tezpur, where he is currently working as a Professor.

His research activity is focused on developing new environmentally friendly and efficient catalytic reaction methodologies of broad synthetic utility to construct various important organic molecules for their potential application in medicinal chemistry and in materials sciences. He has made significant contributions in the area of C-C cross coupling reaction such as Suzuki-Miyaura, Sonogashira cross-coupling reactions and C-N Chan-Lam cross coupling reactions. He is also engaged in development of effective catalytic methodology for synthesis and fictionalization of potential bioactive heterocyclic molecule of pharmaceutical importance via C-H activation. To achieve the target molecules via catalytic methods, his research group is focussing on development of Palladium and Copper based Homogeneous and Heterogeneous Catalyst. He has more than 110 publications and 10 students have been already awarded Ph.D. under his guidance and 2 post-doctoral associates have worked in his group.

Studies on C-3 triaryl methylation of indoles and cyanation of arylhalides

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Halogen bonding triggered by the Lewis basic nature of acetonitrile catalyzes the site-selective C-3 triaryl methylation of indoles and *N*-triaryl methylation of imidazoles with trityl chlorides under catalyst-, metal, and additive-free conditions at room temperature. UV-Vis and FT-IR analyses indicate the existence of halogen bonding which is the driving force of the reaction. This approach is suitable for a wide range of substrates, furnishing moderate to excellent yields (up to 100%) of triaryl methylated products under ambient reaction conditions. Equimolar amounts of reactants are sufficient to obtain the optimum yield and in some cases pure products can be obtained without column chromatography.[1]

Additionally facilitated by the dual role of Ceric Ammonium Nitrate (CAN), we have developed a methodology for the cyanation of aryl iodides/bromides with CAN–DMF as an addition to the existing pool of combined cyanation sources. In addition to being an oxidant, CAN acts as a source of nitrogen in our protocol. The reaction is catalyzed by a readily available Cu(II) salt and the ability of CAN to generate ammonia in the reaction medium is utilized to eliminate the additional requirement of a nitrogen source, ligand, additive or toxic reagents. The mechanistic study suggests an evolution of CN^- leading to the synthesis of a variety of aryl nitriles in moderate to good yields. The proposed mechanism is supported by a series of control reactions and labelling experiments.[2]

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1. D. Konwar, P. Sarma, J. C. Borah, and U. Bora, *Org. Biomol. Chem*., 2023, *21*, 6197–6204
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Ramasamy Anandhan
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Academic Career:

2014 – till date: **Assistant Professor**, Dept. of Organic Chemistry, UNOM, Chennai, INDIA.

Research Experience:

Aug 2012 – May 2014: **Postdoctoral fellow, Prof. Chen, Chien-Tien** group**,** Department of Chemistry,National Tsing-Hua University, Hsingchu, Taiwan

Education:

Oct 2006 – Aug 2011: **Ph.D in Organic Chemistry. Supervisor: Prof. P. Rajakumar**
Thesis title "*Synthesis of cyclophanes dendrimers*" University of Madras, India.

Academic Achievements and Awards:

* **Young Scientist Start up Research Grant (DST-SERB), 2015**
* **National Science Council Postdoctoral Fellowship (NSC)**, Taiwan
* **Thiru R.H. Ramachandra Rao gold medal Award** for the Best Ph.D thesis in University of Madras.
* **Council of Scientific and Industrial Research (CSIR) - JRF (NET)** in 2006
* **GATE (Graduate Aptitude Test in Engineering)** 2005 and 2006

During the last 10 years as an assistant Professor at University of Madras, Chennai, he has been an active researcher in Visible light mediated Organic transformations and electro organic synthesis. By distinction, his work has been recognized both nationally and internationally, as evidenced by his peer-reviewed and acclaimed publications of more than 30 in high-impact synthetic organic chemistry journals with 400 citations. 2 students have been already awarded Ph. D. degree under his able guidance. He has received many projects including DST-Young scientist grant, DST-CRG, RUSA and UGC etc.

Selected Publications:

1. Mandapati Bhargava Reddy, Sakthivel Prabhu, **Ramasamy Anandhan*** "Electrochemical reductive cascade cyclization of o-alkynylated derivatives for saturated amides/amines" ***Chemical Communications***, **2023**,**59**, 11125-11128.

1) Nalladhambi Neerathilingam, Kesavan Prasanth, **Ramasamy Anandhan*** "Substituent-controlled selective synthesis of 1,2-diketones and internal alkynes from terminal alkynes and arylboronic acids *via* α-stilbene radicals obtained from heteroleptic Cu(I) complexes under visible light" ***Green Chemistry***, **2022**,**24**, 8685-8690.

Photoredox/Electro-Catalysed Radical Cyclization Cascade of *o*-Alkynylated Benzamides

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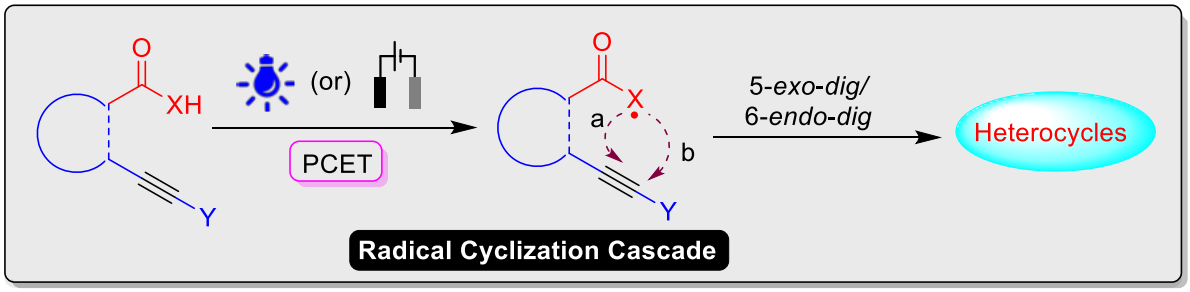
Visible light-mediated radical cyclization reaction is powerful and practical access to diverse carbocycles and heterocycles. Over the past decades, visible-light photoredox catalysis has been established as a powerful toolbox to generate a diverse range of radical intermediates via a single electron transfer process or energy transfer under mild reaction conditions. Compared with the popularity of carbon-centered radical cyclization, Nitrogen-centered radicals (NCRs) cyclization has gained significant interest for N-containing natural products, pharmaceuticals, and other biologically active molecules.[1] Recently, various synthetic methodologies have been developed for the generation of N-centered radicals from NCRs precursors (N−O, N-S, N−N, and N−halogen) by single-electron transfer (SET)-oxidation with an appropriate redox catalyst. However, the generation of NCRs from N-H bonds is challenging because of their high stability (N-H bond dissociation free energy [BDFE] ~ 100 kcal/mol).[2] In addition, the application of such photo redox-catalyzed NCRs to intramolecular addition to C-C unsaturated has been relatively less exploited. Our research studies towards the development of N-radical cyclization cascade via controlled intramolecular N-centered radical addition to C-C unsaturated bonds under photoredox and electrochemical conditions[3] will be described with a topical focus on the proton-coupled electron transfer (PCET) process.



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1. P, Wang.; Q, Zhao.; W, Xiao. *J. Chen. Green Synthesis and Catalysis* **2020**, *1*, 45.
2. (a) M, Bhargava Reddy.; K, Prasanth.; N, Neerathilingam.; R. Anandhan. *Org. Lett.,* **2022**, *24*, 8158; (b) M, Bhargava Reddy.; K, Prasanth.; R. Anandhan. *Org. Lett.,* **2022**, *24*, 20, 3674.
3. (a) P, Xiong.; H-C, Xu. *Acc. Chem. Res*., **2019**, *52*, 3339; (b) M, Bhargava Reddy.; S, Prabhu.; N, Neerathilingam.; R. Anandhan. *Chem. Commun.,* **2023**, *59*, 11125.

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Dr. Maddi Sridhar Reddy obtained his Ph. D. in Organic Synthesis from CSIR-IICT in 2006. He subsequently moved to Canada for a post-doctoral position with Prof. Pierre Deslongchamps (2007-10). He joined CSIR-CDRI as Senior Scientist in 2010 and later moved to CSIR-IICT in 2017 and is presently working as Senior Principal Scientist.

He has made significant contributions in the areas of organic and medicinal chemistries with a special emphasis on discovery of novel reactions through pi-activation of alkynes with alkynophilic transition metal catalysts, and use those methods to explore new chemical space towards novel bioactive molecules of therapeutic interest.
He has more than 70 publications with 2700 citations with h-index 34. 12 students have been awarded Ph. D. degree and several students have worked for their master degree under his able guidance. He is the recipient of Thieme Young researcher award 2015, AVRA young scientist award 2017 and SERB STAR award/research grant 2023 for his contributions.

Rollover cyclometallation of biarylamines/arylphenols for selective annulations with unsymmetrical alkynes

M. Sridhar Reddy
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Insertion of metal in to organic molecules proved to be immensely useful especially to sew new C-C bonds which enormously changed the fate of organic chemistry. Prefunctionalization at the requisite site (direct insertion) or nearby areas (directing group assisted insertion) usually facilitates the strategy. Recently, template directed C-H activation enabled the insertion of metal at distant sites. Rollover cyclometallation, the chelated heterocyclic ligand loses its bidentate coordination to undergo an internal rotation to reach a remote C–H bond, also allows insertion of metal at distant sites. Heterocyclic biaryl systems are known for such rollover cyclometallation. We disclosed recently our efforts of such rollover cyclometallations on biarylamines and arylphenols through some interesting reaction pathways.[1-3] We could even utilize a conjugate olefin to transport the metal center to the geometrically unreachable CH centers.[3] The annulation of such distantly activated sites with unsymmetrical alkynes could be achieved with high regioselectivity with the assistance of dual directing group strategy.

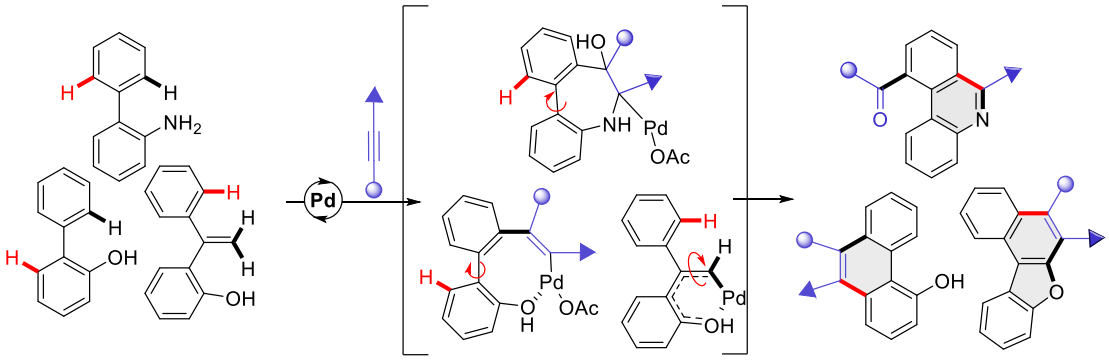

Figure 1: Pd-catalyzed rollover annulations of biphenylamines/arylphenols

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Dr. Guru Brahamam Ramani received his M.Sc. and Ph.D. (2013) from the School of Chemistry, University of Hyderabad, under the supervision of Prof. M. Periasamy. He pursued postdoctoral studies (September 2013 − January 2017) in the field of asymmetric organocatalysis at Prof. Kwunmin Chen's research group, Department of Chemistry, National Taiwan Normal University, Taipei, Taiwan. Then he moved to Prof. B. Olofsson's research group to work on the hypervalent iodine(III) reagents as a Wenner Gren postdoctoral fellow (March 2017 – February 2019) at the Dept. of Organic Chemistry, Stockholm University, Stockholm, Sweden. He spent a short time at Syngene International Ltd., Bangalore, in 2019. He has been working as an assistant professor at IIT Jammu since October 2019, and his research interests include asymmetric catalysis, alkyne/allene chemistry, hypervalent iodine chemistry, carbene and nitrene transfer reactions, and organoboranes.

Practical Synthesis of Allenoates and Dihaloallenoates *via* Decomposition of Unprotected Alkynyl Hydrazones

Guru Brahamam Ramani
Indian Institute of Technology Jammu, J&K.

Allenoates are versatile synthons for numerous synthetic transformations that include nucleophilic additions, electrophilic additions, rearrangement reactions, cycloaddition reactions, annulations, cyclization reactions, etc.[1] However, they have been mostly accessed through either Wittig olefination of ketenes or diazo coupling with alkynes.[2] Noticeably, both methods suffer from their own unique disadvantages. Herein, we have developed a practical route to allenoates by decomposition of operationally safe and bench-stable alkynyl hydrazones.[3] The environmentally benign and metal-free synthesis proceeds through a DABCO-promoted Wolff–Kishner reduction, followed by isomerization under mild conditions.[4] In addition, a reaction of alkynyl hydrazone with two equivalents of *N*-halosuccinimides captures electrophile in two-fold and delivers fully substituted dibromo-/diiodoallenoates. Whereas a similar reaction with three equivalents of N-halosuccinimides has provided 1,4-dicarbonyl 2,3-dihaloalkenes with complete *Z*-selectivity.[5] The 4-oxo-2,3-dihaloenoates are excellent synthons for target-oriented synthesis of valuable 5- and 6-membered heterocyclic scaffolds.

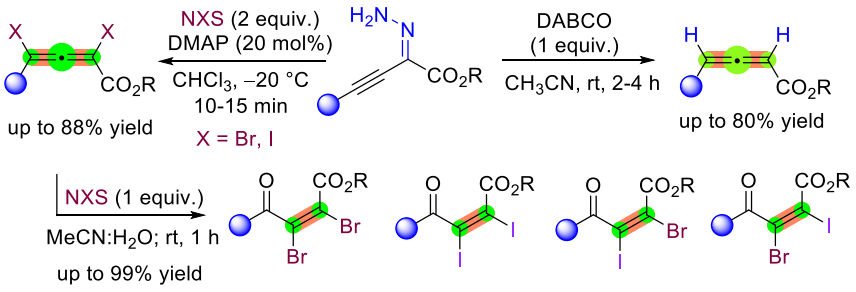

Figure 1: Synthesis of Allenoates and Dihaloallenoates

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Sukalyan Bhadra received both B.Sc. and M.Sc. degrees in Chemistry from the University of Calcutta, India and a Ph.D. degree in 2011 from Indian Association for the Cultivation of Science, India (Supervisor: Professor Brindaban C. Ranu). After two subsequent postdoctoral stints in TU Kaiserslautern, Germany (Advisor: Professor Lukas J. Goossen) and Chubu University, Japan (Advisor: Professor Hisashi Yamamoto), he began his independent career in 2016 at CSIR-CSMCRI Bhavnagar, India, where he currently works as a Senior Scientist. His research interest revolves around the development of synthetic methodologies towards metal promoted organic transformations, cooperative catalysis and asymmetric catalysis leading to the synthesis of fine chemicals, APIs and agrochemicals having marine significance. He has developed technologies for industrially important perfumery chemicals, such as Mefrosol and alpha-Campholenic aldehyde. He has published 45 research papers, 3 book chapters and filed 3 patents, on his credit. He is a recipient of Thieme Chemistry Journal Award 2023, DST-INSPIRE Faculty Award 2016, JSPS postdoctoral Fellowship 2013, Green Talent Award 2010, among others.

New Approaches for the Catalytic α-Functionalization of Ketones

Sukalyan Bhadra
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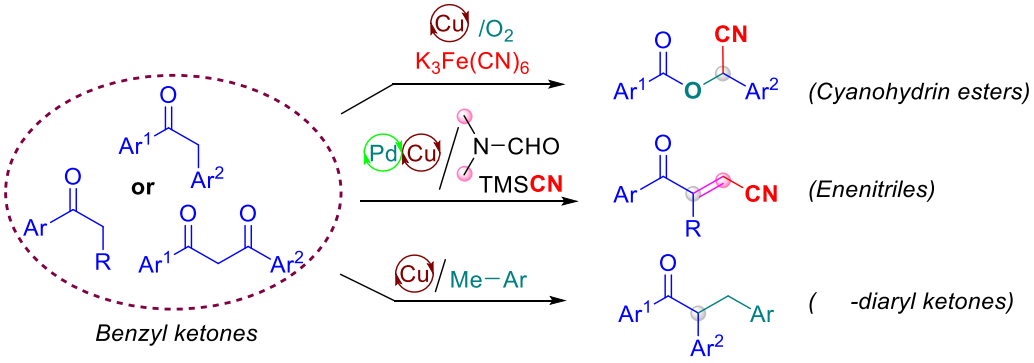
α-Functionalized ketones are common motifs in bioactive compounds, approved drugs, agrochemicals, functional materials etc. and serve as amendable building units for the synthesis of natural product-inspired compounds.[1] Conventional approaches primarily comprise the strong base mediated formation of a nucleophilic enolate from the ketone counterpart and subsequent coupling with an electrophilic partner to give the α-functionalized product.[2] However, addition of a strong base in excess quantity often leads to chemoselectivity issues, particularly for competing carbonyl groups present in the substrate and are not compatible with late stage derivatization of complex molecules. The step- and atom-economy of α-functionalization strategies can be improved, if conducted under single-step catalytic condition. In this context, we have introduced new approaches that allow for the metal-catalyzed regiospecific α-C–H bond transformation of abundant benzylic ketones giving expedient access to a variety of α-functionalized ketones. For instance, we have realized a copper-catalyzed cascade synthesis of cyanohydrin esters via α-functionalization of benzyl ketones using $K_3Fe(CN)_6$ as a sustainable cyanide source.[3] In this reaction, the copper-catalyzed α-oxygenation of aryl benzyl ketones is merged with a unique water/O_2-induced release of cyanide ions from $K_3Fe(CN)_6$ and a benzil-cyanide reaction. The cyanide release strategy was further integrated with a copper catalyzed oxygenation-decarbonylation sequence to produce cyanohydrin esters from 1,3-diketones. Likewise, we have achieved metal catalyzed strategies for the synthesis of α-cyanomethenylated ketones and α-benzylated ketones starting from broadly accessible benzyl ketones.[4-5]



Scheme 1. Catalytic α-Functionalization of Ketones

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Venkataraman Ganesh received his early education from Bishop Heber College Tiruchirapalli (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.

Nickel-Catalyzed Oxidative Cyclization of π-Systems Over the Benchtop

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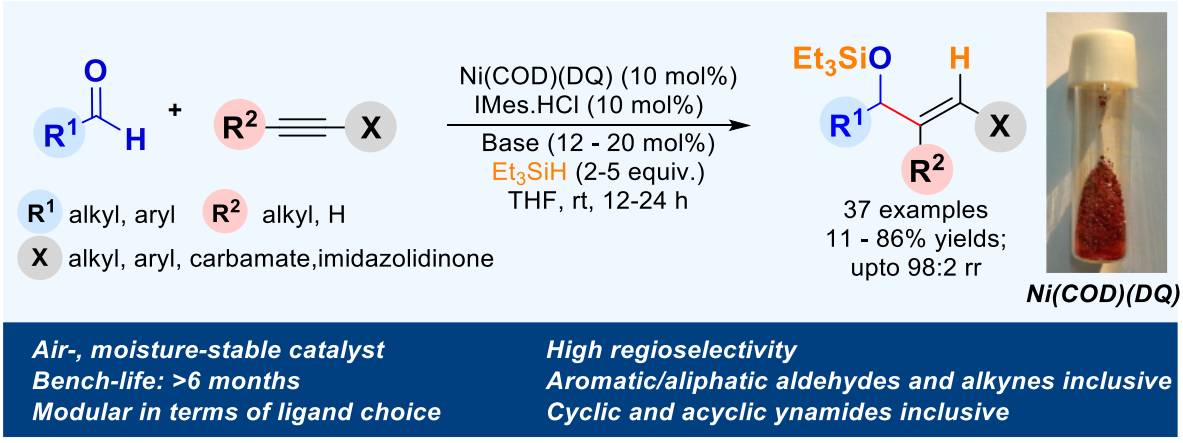
Nickel(0) complexes have been traditionally stored and used under highly controlled environments. Our research focuses on bringing sensitive nickel chemistry to the benchtop. We have demonstrated the potential of Schrauzer's Ni(COD)(Duroquinone),[1] an air-, and moisture-stable Ni0 complex as a catalyst for the reductive coupling of aldehydes and alkynes.[2] Control experiments revealed the exceptional bench stability of Ni(COD)(DQ) under ambient conditions for >200 days. The infrastructural cost associated with a glove box for storing and handling $Ni(COD)_2$ is avoided. A wide range of aromatic and aliphatic aldehydes/alkynes furnished the desired silyl allyl ethers in excellent yields and regioselectivities. Ynamides participate in the reductive coupling with aldehydes to give tri-substituted ene-carbamates as a single regioisomer. Downstream functionalizations like desilylation, hydrogenation, ring-opening of epoxide, and reductive cleavage of the ene-carbamate have been performed.



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Ramesh pursued his Ph.D with Dr. Oliver Reiser in University of Regensburg, Germany. Dr. Rasappan received the prestigious 'DAAD Fellowship' from Germany for his doctoral studies in Asymmetric Synthesis. Soon after his Ph.D (2009), he won the Alexander von Humboldt award and continued his work with Dr. Magnus Rueping in Aachen University, Germany. He subsequently did post-doctoral research with Dr. Corey Stephenson in Boston University, USA. Later, he joined the laboratory of Dr. Varinder Aggarwal, University of Bristol, England, shifting his research from photocatalysis to Lithiation-Borylation. Ramesh is also the receiver of the renowned Marie-Curie fellowship.

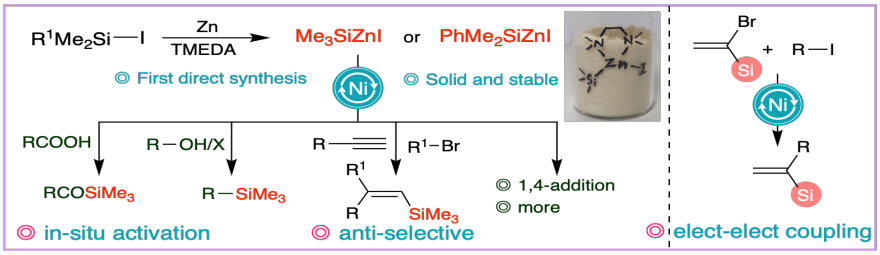
Ramesh joined IISER-TVM as an Assistant Professor in 2015 and promoted to associate professor in the year 2022. His area of expertise includes asymmetric catalysis especially the use chiral ligands like bis(oxazolines), organocatalysis (phosphoric acids & prolines), photocatalysis and short synthesis of natural products. Presently, his group is concentrating on cross-coupling reactions and photoredox catalysis, the majority of work focused on the synthesis and application of organosilanes.

Organosilanes: Synthesis and Application of Solid TMSZnI in Cross-Coupling Reactions

Ramesh Rasappan

The increased synthetic utility of organosilanes motivates researchers to develop a milder and more practical synthetic methods. Transition metal catalysis employing disilanes and silylboranes for synthesizing organosilanes circumvent the limitations of conventional hydrosilylations. While disilanes require special conditions, silylboranes have yet to be developed as TMS sources. Functional group compatibility renders silylzinc reagents highly desirable; however, their development is hindered by their synthesis using pyrophoric silyllithium and dissolved lithium salts. We described for the first time, the direct synthesis of PhMe2SiZnI and Me3SiZnI reagents by employing a coordinating TMEDA ligand. Importantly, they can be obtained as solid and stored for longer periods of time. We demonstrate their significance in cross-coupling of various free alkyl/aryl/alkenyl carboxylic acids with broader functional group tolerance.

The stereodefined and highly substituted vinylsilanes have unique reactivity, they undergo a broad range of transformations including stereospecific electrophilic substitution. Transition metal mediated syn-silylmetalation in which π-insertion of alkynes into Si−M takes place, represents the most efficient and atom economical process to synthesis highly substituted vinylsilanes. However, the cross-coupling of transient vinylmetal species to deliver trans-selectivity is nonetheless scarce. we developed a multi-component approach for the exclusive synthesis of Z-vinylsilanes via anti-selective addition of solid TMSZnI to terminal alkynes and the subsequent cross-coupling with activated alkyl halides.



Vinyltrialkoxysilanes are indispensable for organic synthesis, particularly cross-coupling reactions. We developed a protocol for the synthesis of α-vinyltrialkoxysilanes via cross-electrophile C(sp2)−C(sp2) coupling of bromoalkenes. The method has extensive compatibility with functional groups under milder reaction conditions. The C–O bonds are kinetically inert in cross-coupling reactions compared to those of carbon–halogen bonds. We developed a nickel mediated cross-coupling of carbamates with silylmagnesium reagents. In addition, we have also developed AgF assisted nickel catalysis in the enantiospecific silylation of benzylic ethers.

Sun Pharma & BASF Session

Chairpersons: Srinivas Oruganti, Diwan Rawat & Vishal Rai

Srinivas Oruganti
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Dr. Srinivas Oruganti is the whole-time Director of Dr. Reddy's Institute of Life Sciences since 2018. He also heads the Center for Process Research & Innovation, an industry-oriented chemistry research department of Dr. Reddy's Institute of Life Sciences. Dr. Oruganti received his Ph.D. in 2004 from the Indian Institute of Science, Bengaluru, in the area of photo switchable cluster glycosides, and did his postdoctoral research at the Centre de Biophysique Moléculaire, CNRS in the design and synthesis of glycocluster–tumor antigenic peptide conjugates for glycotargeting of dendritic cells. He has contributed significantly to various aspects of early stage process development of active pharmaceutical ingredients ranging from therapeutic areas like diabetes, cardio-vascular, multiple sclerosis and cancer. His pivotal contributions pertain to bringing an active pharmaceutical ingredient to market as a generic drug through innovation in chemical process development and offering a strategic vantage point to any pharmaceutical company in its efforts to carve out a niche for itself in ever challenging generic drug market. Recently, with support from Government of Telangana, Dr. Oruganti spearheaded the setting up of a multi-industry centric 'Flow Chemistry Technology Hub (FCT-Hub)' at DRILS to reiterate the commitment to chemical process development withguiding elements of sustainability and circular economy. He is an inventor in more than 100 patents and has published over 40 research papers in leading international journals.

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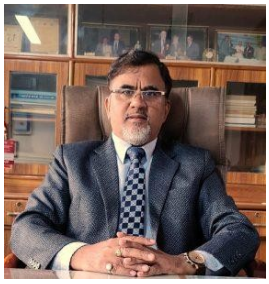

Professor Diwan S Rawat joined the Department as a Reader in July 2003, and was promoted to Professor in March 2010. He obtained his master's degree from Kumaun University, Nainital in 1993 and was honoured with the merit certificate for securing first position in the University. He did his Ph.D. in Medicinal Chemistry from Central Drug Research Institute, Lucknow. He worked two years in a Pharmaceutical Industry and did postdoctoral work at Indiana University and Purdue University, USA. He was an Assistant Professor of Medicinal Chemistry at National Institute of Pharmaceutical Education and Research (NIPER), Mohali, before joining University of Delhi in 2003. Prof. Rawat has published over 158 research papers, authored a book, three book chapters, and nine patents to his credit. His work has been cited over 5678 times with h–index of 42 and i-index of 122. His research interests lies in the areas of development of small organic molecules as anticancer, antimalarial, antimicrobial and anti-Parkinson agents and nano-catalysis. One of his molecule has been licenced to Boston based pharmaceutical industry for the development as a drug for the treatment of Parkinson`s disease.

Prof. Rawat was a Sectional President of Indian Science Congress (2019-2020) and is a recipient of CRSI young scientist award (2007); ISCB young scientist award (2010); Prof. D. P. Chakraborty 60th Birth Anniversary Commemoration Award (2007); VC`s Pratik Chinha Samman, Kumaun University Nainital (2011); Gold Badge and Diploma, International Scientific Partnership Foundation, Russia (2015); Professor RC Shah Memorial LectureAward, Indian Science Congress (2015); Professor SP Hiremath Memorial Award, Indian Council of Chemist (2016); Special Appreciation Award for Exemplary Services, University of Delhi (2021); Platinum Jubilee Lecture, Indian Science Congress (2021). Prof Rawat is a Visiting Professor, Japan Advanced Institute of Science and Technology (JAIST), Japan. He iselected fellow of National Academy of Sciences, Fellow of Royal Society of Chemistry (FRSC) and CChem (London). Prof. Rawat has supervised twenty six PhD students.

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Dr. Vishal Rai obtained his Ph.D. in Chemistry from IIT Bombay (2003-2008). He subsequently held a postdoctoral position and MITACS-Elevate fellow position 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.

Positions, Awards, and Honours:

He is the Founder and Director of *Plabeltech Private Limited*. The state-of-the-art protein and antibody engineering technologies such as LDM®, Gly-Tag®, and Maspecter® empower the company. Recently, his team established the PrecisionAntibody Engineering CEnter (*SERB-PACE*) to meet India's technological demands in biologics. Also, he is the recipient of the Swarnajayanti Fellowship, Ramanujan Fellowship, CRSI Bronze Medal, CDRI Award for excellence in drug research, SERB Technology Translation Award, RSC-WIS Young Scientist Award, and DAE Young Scientist Award. Recently, he joined the *ACS Chemical Biology* team as an Early Career Board member. He hasbeen involved in scientific outreach activities as national co-chair (India) for the InternationalChemical Biology Society (ICBS). Also, he is an invited Fellow of the Royal Society of Chemistry (FRSC), UK.

Research interests:

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

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Education:

1978–1982 B.S., Chemistry, Chonbuk National University
1982–1984 M.S., Organic Chemistry, Seoul National University
(Advisor: Prof. Eun Lee)
1989–1992 Ph.D., Organic Chemistry, Seoul National University
(Advisor: Prof. Eun Lee)

Experience:

1993-1994 Postdoctoral Fellow, Duke University (U.S.A)
(Professor M. C. Pirrung)
1995 Postdoctoral Fellow, Ohio State University (U.S.A)
(Professor L. Paquette)
2000 Visiting Professor, Michigan State University (U. S. A)
(Professor W. Wulff)
1995-2016 Assistant professor, Associate professor, Professor
2016-Present Chunma Distinguished Professor

Awards:

2008 Academic Advanced Award by Korean Chemical Society, Republic of Korea
2012 Outstanding Research Award by Yeungnam University, Republic of Korea
2014 Outstanding Research Award by the Ministry of Education, Republic of Korea
2017 Outstanding Research Award by Organic Division of the Korean Chemical Society, Republic of Korea
2018 Outstanding Research Award by Yeungnam University, Republic of Korea
2020 Taikyue Ree Academic Award, Korean Chemical Society, Republic of Korea
2020 TCI-SEJIN Academic Award, Korean Society of Organic Synthesis, Republic of Korea
2023 Outstanding Research Award by Yeungnam University, Republic of Korea

Research Interests:

1. Organic material synthesis
2. Natural product, medicine synthesis, and biological screening
3. Development of new methodologies for the synthesis of heterocycles
4. Nanomaterial synthesis and application

Construction of Biologically Interesting Aromatics *via* Benzannulation

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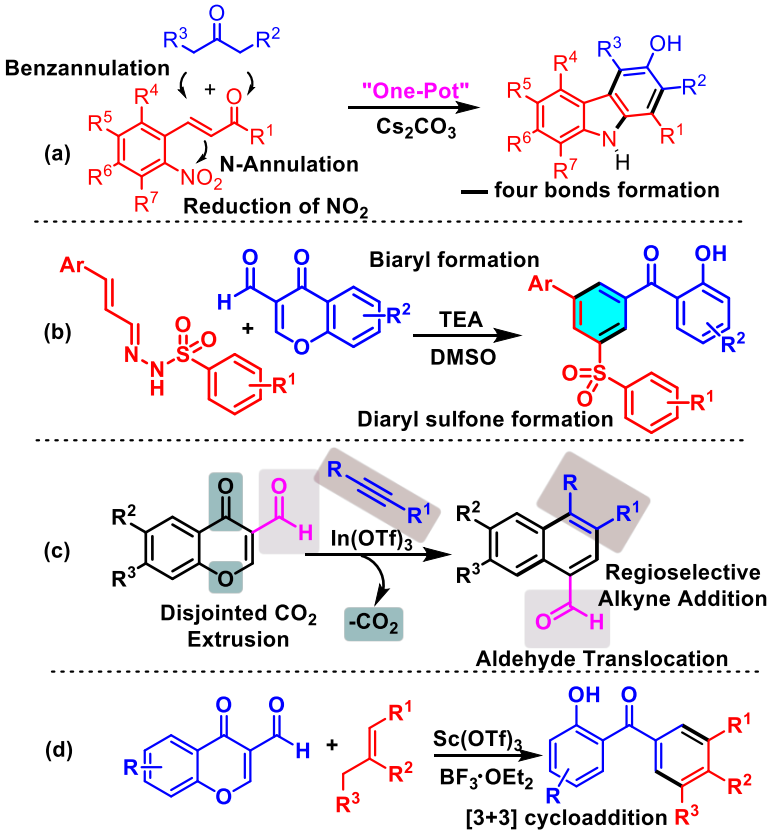
The benzannulation reaction is widely used in the synthesis of diversely functionalized aromatic molecules with myriad properties. The construction of functionalized and diverse aromatic *via* benzannulation plays a vital role in advanced synthetic organic chemistry. Recently, we have interested in the synthesis of aromatics and heteroaromatics *via* benzannulation. In this presentation, we describe facile and efficient synthetic approaches of biologically interesting aromatics such as carbazoles, biaryls, xanthones, biarylsulfones, naphthaldehydes, and 2-hydroxybenzophenones *via* benzannulation (Scheme 1).



Scheme 1. Synthetic strategies for aromatics via benzannulation

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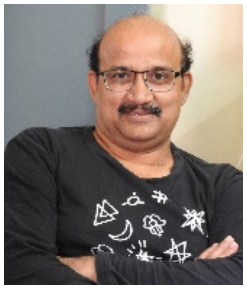

Parthasarathi Das received his Ph D degree from CSIR-National Chemical laboratory, Pune, India in 1999 (Prof. Ganesh Pandey). He did postdoctoral studies (1999-2003) at the RWTH-Aachen, Germany (Prof. H-J. Gais), Tohoku University, Japan (Prof. M. Hirama) and Harvard University, USA (Prof. Y. Kishi). In 2003 he moved to India to join Discovery Research of Dr. Reddy's Laboratories Ltd., Hyderabad and worked in medicinal chemistry group having research focus on various therapeutic areas e.g., oncology, metabolic disorder and antibacterial. After completing ten years in Industry, in 2012 he moved to academia and joined CSIR-Indian Institute of Integrative Medicine, Jammu. In 2017 he moved to Indian Institute of Technology (ISM) Dhanbad and joined as faculty in the Department of Chemistry and Chemical Biology. His current research interests include medicinal chemistry, development of new synthetic tool, synthesis of biologically active natural products and Drug impurities. He has been selected for Chemical Research Society of India (CRSI) Bronze Medal, 2019 for his contribution to research in chemistry. He serves as an International Advisory Board Member of New Journal of Chemistry (NJC) from RSC Publishing Home. He is Fellow of the Royal Society of Chemistry (FRSC) and at present he is the Head of Department of Chemistry and Chemical Biology, IIT (ISM) Dhanbad.

Expanding Discovery Chemistry Toolbox: From Concept to Practice

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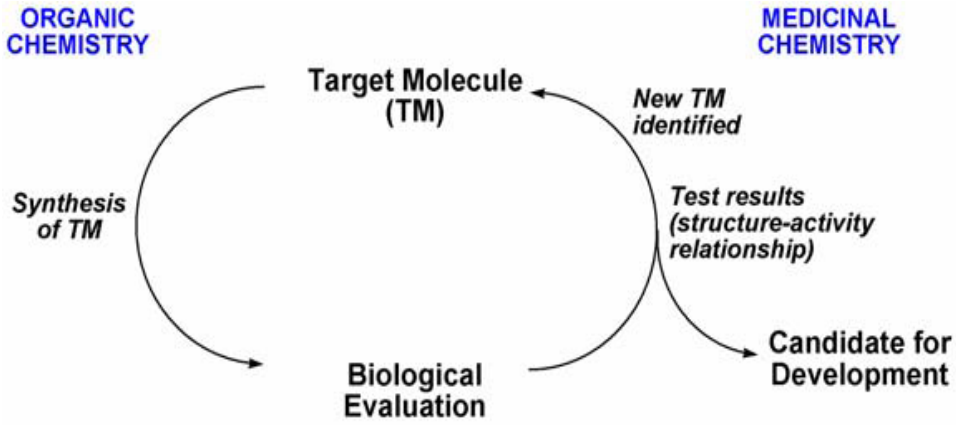
The pharmaceutical industry remains solely reliant on synthetic methodology to prepare drugs or drug like molecules for their discovery/process program. The expansion of synthetic methodology in recent years has greatly facilitated the preparation of molecules that would once have been considered an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



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Dr. Arseniyadis received his PhD from the University of Strasbourg under the guidance of Dr Charles Mioskowski. After various postdoctoral stints in industry (Rhodia Chirex, Boston, USA, in collaboration with Prof. Stephen L. Buchwald, MIT) and in academia with Prof. Alan C. Spivey (Imperial College London, UK) and Prof. K. C. Nicolaou (The Scripps Research Institute, La Jolla, USA), he started his academic career in France as a permanent CNRS Researcher in 2005 and was promoted to the rank of CNRS Director in 2015. The same year, he moved to London and joined Queen Mary University of London as a Reader in Organic Chemistry. His group is interested in the development of new synthetic methods, with a special emphasis given to asymmetric catalysis and photoredox, with applications in natural product synthesis.

Outputs: *>80 publications, 8 Book chapters, 2 books, 2 patents.* ***Distinction & awards:*** *recipient of the 2014 Thieme Chemistry Journal Award and the 2015 CNRS Bronze medal. Fellow of the Royal Chemical Society and elected member of the Organic Chemistry Division Bureau of the French Chemical Society (2015-2021).*

Revisiting Pd-AAA chemistry: Towards the development of active, selective, and stable single component chiral pre-catalysts

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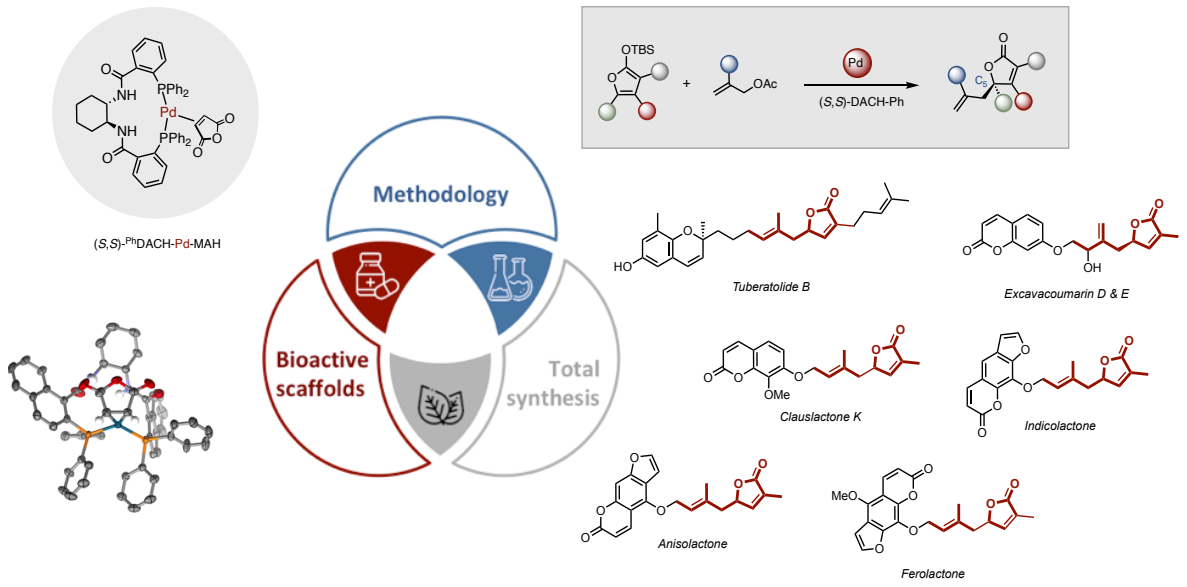
For the past two decades, the group has focused on developing new synthetic tools with a special emphasis given to structural and functional complexity. These methods span within the areas of asymmetric transition metal catalysis, organocatalysis and, more recently, bio-hybrid catalysis. In this context, we've been particularly interested in applying palladium-catalysed asymmetric allylic alkylation chemistry to various heterocyclic scaffolds with direct applications in natural product synthesis.[1] We've also recently developed a series of bench stable, single component chiral pre-catalysts exhibiting improved reactivity and selectivity across the field. I'll present some of these results.



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Prof. Anil Kumar obtained his Ph.D. in Chemistry from University of Delhi in 2004 under the supervision of Prof. SMS Chauhan. He subsequently moved to USA for a post-doctoral position with Prof. Keykavous Parang at University of Rhode Island, Kingston (2004-2006). He joined BITS Pilani, Pilani Campus as Assistant Professor in 2006 and was promoted to Professor in 2018. He has published over 185 articles with >5600 citations. Fifteen candidates have been awarded Ph.D. degree and seven students are working under his guidance. His research interest lies in the development of reaction methodologies with focus on direct C-H functionalization using transition metal catalysts as well as radical mediated reactions, green chemistry and medicinal chemistry.

Awards and Honours:

- Bronze Medal (2020), Chemical Research Society of India (CRSI), Bangalore.
- INSA-DFG Visiting Scientist Fellowship (2019), INSA New Delhi.
- Prof. S. Venkateswaran Faculty Excellence Award (2018), BITSAA, BITS Pilani.
- Dr. Arvind Kumar Memorial Award (2014), Indian Council of Chemists, Agra.
- ISCB Young Scientist Award in Chemical Sciences (2013), Indian Society of Chemists and Biologists (ISCB), Lucknow.
- Harrison McCain Foundation Award (2012), Acadia University, Canada.
- NET and Research Fellowship (JRF/SRF 1999 – 2004), CSIR-UGC, New Delhi
- Science Meritorious Award (1998-99), University of Delhi, Delhi.
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Synthesis of N-Fused Polycyclic Heterocycles via Transition-Metal-Catalyzed Annulation Reactions

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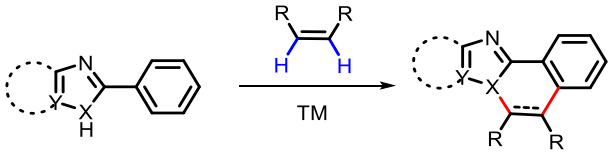
Nitrogen-containing polycyclic heterocycles have received considerable attention because of their presence in numerous biologically active molecules, including natural products and pharmaceuticals. Considering the structural variety and biological activities of N-fused polyheterocyclic molecules, there has been enduring interest to develop new and elegant synthetic approaches for these heterocycles.

In recent years, transition metal-catalyzed C−H activation/C−H functionalization has played a vital role in modern synthetic organic chemistry. The direct conversion of a C−H bond to other functionalities is highly attractive as it removes the need for pre-functionalization steps and, therefore, streamlines synthetic strategies. These reactions have also been used for the intermolecular functionalization of C−H/X−H bonds enabling annulation processes. This approach allows annulation of various pharmacophores and natural products with different coupling partners to generate complex architecture in an easy single step reaction.[1-3] Our research group has been working towards synthesis of heterocyclic compounds through transition-metal-catalyzed C−H functionalization/annulation reactions. Some of our efforts towards synthesis of N-fused heterocyclic frameworks *via* transition-metal catalyzed annulation reactions will be discussed (Scheme 1).[4-7]



Scheme 1*:* Synthesis of N-fused polycyclic heterocycles by transition-metal-catalyzed annulation reaction

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7. N. Meena, D. S. Nipate, P. N. Swami, K. Rangan and A. Kumar, *J. Org. Chem.*, **2024**, DOI: 10.1021/acs.joc.3c02229.

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Brian M. Stoltz was born in Philadelphia, PA in 1970. After spending a year abroad at the Ludwig Maximilians Universität in München, Germany, he obtained his B.S. degree in Chemistry and B.A. degree in German from the Indiana University of Pennsylvania in Indiana, PA. Following graduate studies at Yale University in the lab of John L. Wood and an NIH postdoctoral fellowship at Harvard in the group of Professor E. J. Corey, he took a position at the California Institute of Technology. A member of the Caltech faculty since 2000, he is currently the Victor and Elizabeth Atkins Professor of Chemistry and an Investigator of the Heritage Medical Research Institute. His research interests lie in the development of new methods for general applications in synthetic chemistry and biologically active small molecules. Among his many distinctions, Professor Stoltz has been the recipient of the Arthur C. Cope Scholar and the E. J. Corey Awards from the American Chemical Society, the Presidential Early Career Award in Science and Engineering (PECASE) from the White House, the 2009 Raymond and Beverly Sackler Prize in the Physical Sciences for Chemistry, and was the 2015 recipient of the Mukaiyama Award by the Society of Synthetic Organic Chemistry, Japan. He was named the recipient of the 2018 American Chemical Society Award for Creative Work in Synthetic Organic Chemistry and in 2019 became a Fellow of the American Chemical Society. Professor Stoltz has trained more than 200 students and postdocs, who have gone on to successful independent careers in industry and academia. In 2017, he was awarded the Richard P. Feynman Prize for Excellence in Teaching at Caltech, the highest honor for teaching at the institute.

Complex Natural Products as a Driving Force for Discovery in Organic Chemistry

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Our laboratory is deeply interested in the discovery and development of new reaction methodology *en route* to the chemical synthesis of complex bioactive molecules. Over the course of many years, research in our group at the California Institute of Technology has been pursued in the general area of synthetic chemistry, with a focus on the development of new strategies for the preparation of complex molecules. Concurrent to this program of target driven synthesis is a strong effort directed toward the development of new catalytic reaction methods, which will be useful for a range of applications. Typically, the complex target structure is used as an inspiration for the discovery of new reactions and technologies that may eventually be regarded as general synthetic methodology. Consequently, this approach provides access to a) novel, medicinally relevant structures, b) a general method for their synthesis, and c) new synthetic methods that will be beneficial for a host of applications. These topics will be discussed in the lecture.

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