# A National Conference on Organic Synthesis- 2025



PG Department of Chemistry Berhampur University, Bhanja bihar, Odisha-760007



# **Sponsors**























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### Prof. Geetanjali Dash

Vice- Chancellor
Berhampur University



#### Message

It's my pleasure and privilege that, P.G. Department of Chemistry, Berhampur University, Odisha, India is organizing a National Conference on "National Conference on Organic Synthesis-2025; N-COS-2025" during 15-17<sup>th</sup> December 2025.

It gives me great pleasure to extend my warm greetings to all participants of the *National Conference on Organic Synthesis*-2025 (*N-COS*-2025). This conference provides an exceptional platform for researchers, educators, industrial practitioners, and young scientists to share their latest insights and breakthroughs in the ever-advancing field of organic synthesis.

Organic chemistry continues to play a pivotal role in shaping modern science—driving innovations in pharmaceuticals, materials, agrochemicals, and sustainable technologies. As we stand at the intersection of scientific discovery and societal need, N-COS-2025 serves as a timely opportunity to discuss emerging methodologies, green synthetic approaches, catalytic advancements, and interdisciplinary collaborations that will define the future of molecular design and chemical innovation.

I am confident that the exchange of ideas and knowledge during this conference will inspire new directions in research and foster meaningful scientific partnerships. I extend my best wishes to the organizing committee for their dedicated efforts and to all the delegates for a productive and enriching experience.

Wishing N-COS-2025 great success.

I extend my warm wishes to organizer for their vision and dedication. Greeting to all the delegates, participants, media person and wish for the success of conference. Let us use this occasion not only to expand our knowledge but also to inspire one another toward greater achievements.

Chairperson & Patron N-COS-2025

### Prof. Ashok K. Ganguli

Director

**IISER** Berhampur



#### Message

I am truly pleased to learn that the Post Graduate Department of Chemistry, Berhampur University, Odisha, India, is organizing the National Conference on Organic Synthesis-2025 (N-COS-2025), to be held from 15-17 December 2025. The conference aims to provide an interactive platform for young researchers, senior scientists, internationally recognized experts, and industry professionals to engage in meaningful discussions on recent applications of organic synthesis in biology and medical science for building a disease-free society.

Organic synthesis has become an essential pillar of modern life, enabling the design and creation of molecules that advance human health, strengthen agricultural productivity, and enhance overall societal well-being. In the field of medicine, synthetic organic chemistry has driven the discovery of life-saving drugs, advanced therapeutic molecules, and powerful diagnostic tools.

In agriculture, the development of modern pesticides and agrochemicals relies extensively on synthetic strategies to produce compounds that protect crops, improve yields, and ensure global food security. With growing environmental concerns, organic synthesis is increasingly central to designing safer, more selective, and eco-friendly agrochemicals. Its impact is therefore directly connected to human health—through both the medicines. we depend on and the food systems that sustain us. Continued progress in synthetic methodologies, green chemistry, and interdisciplinary research holds the promise of a healthier and more sustainable future driven by molecular innovation.

Organic synthesis allows precise design of semiconducting molecules and polymers with customized electrical, thermal, and sensing capabilities. These engineered materials are adapted for diverse uses—from flexible electronics to advanced fire-fighting equipment that offers improved heat resistance and real-time hazard detection.

This three-day symposium brings together a diverse range of talks focusing on organic synthesis for human health and agriculture. The field offers immense potential to deliver innovative solutions that harmonize scientific progress with ecological responsibility. By reducing environmental impact, increasing efficiency, and promoting sustainable practices, we can collectively work toward a brighter, more sustainable future.

I believe this conference provides an excellent opportunity for researchers, academicians, and industry professionals to exchange knowledge and ideas. I am confident that the deliberations will highlight how ongoing research is contributing to sustainable organic synthesis and its societal benefits through advanced and environmentally responsible synthetic methodologies.

Prof Ashok K Ganguli Director, IISER Berhampur

### Prof. Sukanta K. Tripathy

Chairman, P.G. Council Berhampur University



#### Message

I am very happy to learn that Post Graduate Department of Chemistry, Berhampur University, Odisha, India is organizing a National Conference on "National Conference on Organic Synthesis-2025; N-COS-2025" during 15-17th December 2025.

Organic synthesis plays a crucial role in shaping modern life by enabling the design and production of molecules that improve human health, enhance agricultural productivity, and ensure overall societal well-being. In the field of medicine, synthetic organic chemistry has led to the discovery of life-saving drugs, advanced therapeutic agents, and innovative diagnostic tools. From antiviral and anticancer drugs to antibiotics and targeted therapies, organic synthesis remains the foundation of pharmaceutical innovation. Similarly, the development of modern pesticides relies heavily on synthetic strategies to create compounds that protect crops, increase yields, and support global food security. With growing concerns about environmental sustainability, organic synthesis also contributes to the design of safer, more selective, and eco-friendly agrochemicals. Ultimately, the impact of organic synthesis extends directly to human health—both through the medicines we depend on and the agricultural systems that sustain us. Continued advancements in synthetic methodologies, green chemistry principles, and interdisciplinary research promise a healthier, safer future driven by molecular innovation.

This three-day symposium features a diverse range of talks on Organic Synthesis for human health and agriculture. The field of organic synthesis holds immense potential to pioneer innovative solutions that seamlessly integrate scientific progress with ecological responsibility. By minimizing environmental impacts, improving efficiency, and championing sustainable practices, we can pave the way for a brighter and more sustainable future. I believe this conference represents a unique opportunity to unite the expertise of researchers, academics, and industry leaders.

I am sure that the conference will cover regarding, how research is contributing towards sustainable organic synthesis for sustainable applications and societal benefits through sustainable synthetic methodology in organic synthesis.

I wish the conference a grand success.

Co-Chairperson & Patron N-COS-2025

### Dr. Satyanarayana Sahoo

Head, P.G. Dept of Chemistry Berhampur University



#### Message

It is my proud privilege to write a few lines on the occasion of the National Conference on Organic Synthesis (N-COS-2025) organized by the P.G. Department of Chemistry, Berhampur University, during December 15-17, 2025.

Nowadays, Chemical Science has emerged as a foundational subject for all types of technical and interdisciplinary research across various leading branches of Science. All the day-to-day materials, such as food, clothing, medicines, fuels, fertilizers, cosmetics, etc., used by modern society are the blessings of Chemistry. It is impossible to imagine an advanced, comfortable and healthy life without the progress in Chemistry. Organic Synthesis is the core branch of Chemistry for drug design and development, interacting with biological targets to treat diseases, from initial discovery and structure-activity relationship studies to large-scale production. It provides the principles for understanding the structure, function, and modification of drugs for better efficacy, safety, and delivery.

P. G. Department of Chemistry, Berhampur University, is organizing this National Conference with the aim of discussing recent advancements in the subject to create interest and enthusiasm among young people for creative research. The Conference also aims to address issues pertaining to various advanced areas of Organic Synthesis, as well as related interdisciplinary areas.

I am glad to know that more than 40 eminent speakers from different parts of the Country are going to deliver their lectures during the Conference on the various emerging areas of Organic Synthesis. The Conference will provide a great opportunity for participants to interact with distinguished Academicians from different parts of India. Finally, suggestions may emerge from the deliberations regarding the implementation of recent research findings in the subject, ultimately benefiting humanity.

I am highly grateful to our Honourable Vice-Chancellor and Chairperson of the Conference, who has been a constant source of inspiration to make the Conference a grand success. I am also grateful to the Chairman of the P.G. Council and the Patron of the Conference, as well as to the members of the Advisory and Organizing Committees, for their continuous support throughout the organization of the Conference.

I would like to express my sincere thanks and appreciation to everyone.

Dr. Satyanarayana Sahoo P.G. Dept of Chemistry

#### Dr. Laxmidhar Rout

P.G. Dept of Chemistry Berhampur University



#### Message

It is my pleasure to welcome all distinguished researchers, academicians, industry professionals, and students to the "National Conference on Organic Synthesis (N-COS)-2025", during December 15-17, 2025 at Berhampur University. This conference will serve as a vibrant platform for exchanging ideas, discussing recent advances, and exploring emerging trends in the dynamic field of organic synthesis.

Organic synthesis remains a cornerstone of chemical sciences, driving innovation in pharmaceuticals, materials science, agrochemicals, natural product chemistry, and sustainable technologies. In recent years, this field has witnessed remarkable progress in areas such as green synthetic methodologies and catalytic transformations. NCOS-2025 aims to bring together experts from across the country to share their insights and inspire new collaborations that will shape the future of synthetic chemistry.

We are honored to host a series of plenary lectures, invited lectures, flash posters, and poster presentations that showcase cutting-edge research and practical solutions to contemporary scientific challenges. I am confident that these discussions will spark curiosity, encourage interdisciplinary perspectives, and foster a meaningful environment of scientific engagement.

I extend my sincere gratitude to all participants, sponsors, advisory committee members, and organizing team members for their continuous support in making this conference possible. Your enthusiasm and contributions are what enrich this academic gathering. I am also grateful to the Vice-Chancellor, PGC-Chairman, and Head of Department of Chemistry for their invaluable support.

Wishing everyone an intellectually stimulating and memorable experience at NCOS-2025.

> Convener N-COS-2025

### Convener



**Dr. Laxmidhar Rout**UGC-Assistant Professor
P.G. Department of Chemistry
Berhampur University

### **Organizing Committee**



Dr. Satyanarayana Sahoo Head P.G. Dept. of Chemistry Berhampur University



**Dr. Bibhuti Bhusan Parida**Assistant Professor
P.G. Dept. of Chemistry
Berhampur University



Dr. Rabinarayana Sahu Microanalyst P.G. Dept. of Chemistry Berhampur University



**Dr. Bedabyas Behera**Assistant Professor
P.G. Dept. of Chemistry
Berhampur University



**Dr. Sunanda Panda**Assistant Professor
P.G. Dept. of Chemistry
Berhampur University

#### **Research Scholar Committee**



Pradyota K. Behera Berhampur University



Papita Behera Berhampur University



Amlan Swain Berhampur University



Ajeena Sahoo Berhampur University



Eitishree Behera Berhampur Universit



Amit K. Behera Berhampur University

# **National Advisory Committee**



Prof. Ashok K. Ganguli IISER Berhampur



Prof. J. S. Yadav CSIR-IICT Hyderabad



Prof. Abu T. Khan IIT Guwahati



Prof. Anandi C. Dash Utkal University



Prof. Ganesh P. Pandey BHU Varanasi



Prof. Satyaban Jena Utkal University



Prof. S. Chandrasekharan IISc Bangalore



Prof. Diwan S. Rawat University of Delhi



Prof. Deevi Basavaiah University of Hyderabad



Prof. Akhilesh K. Verma University of Delhi



Prof. Akhila K. Sahoo University of Hyderabad



Prof. T. Punniyamurthy IIT Guwahati



Prof. Partha Sarathi Das IIT-ISM Dhanbad

# **Chairpersons**



Prof. Satyaban Jena Utkal University, BBSR



Prof. T. Punniyamurthy IIT Guwahati



Prof. D. Basavaiah University of Hyderabad



Prof. J. S. Yadav CSIR-IICT Hyderabad



Prof. Abu T. Khan IIT Guwahati



Prof. Bhisma K. Patel IIT Guwahati



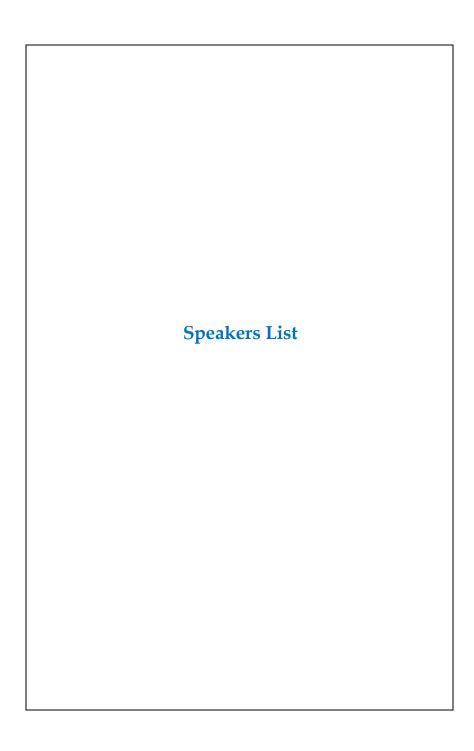
Prof. Debendra K. Mohapatra CSIR-ICT Hyderabad



Prof. Akhila K. Sahoo University of Hyderabad



Prof. Ponneri C Ravikumar IISER Tirupati



### **Plenary Lectures**



Prof. Abu T. Khan IIT Guwahati



Prof. Chepuri V. Ramana CSIR-NCL Pune



Prof. D. Basavaiah University of Hyderabad



Prof. T. Punniyamurthy IIT Guwahati



Prof. Akhila K. Sahoo University of Hyderabad



Prof. Bhisma K. Patel IIT Guwahati

### **Invited Lectures**



Prof. Alakesh Bisai IISER Kolkata



Prof. Debendra K. Mohapatra CSIR-ICT Hyderabad



Prof. S. S.V. Ramasastry IISER Mohali



Dr. Satpal S. Badsara BHU Varanasi



Prof. Chandrakumar Appayee IIT Gandhinagar



Prof. Ponneri C Ravikumar IISER Tirupati



Dr. Jaya Prakash Das Ravenshaw University



Prof. Malaya K. Rana IISER Berhampur



Prof. Harekrushna Sahoo NIT Rourkela



Dr. Priyabrata Dash NIT Rourkela



Dr. Thirupathi Barla IISER Berhampur



Dr. Adinarayana Doddi IISER Berhampur



Dr. Rajendra Goreti IISER Thiruvananthapuram



Dr. Gokarneswar Sahoo NIT Rourkela



Dr. Parikshit Moitra IISER Berhampur



**Dr. Tabrez Khan** IIT Bhubaneswar



Prof. G. B. Ramani IIT Jammu



Dr. Prosenjit Daw IISER Berhampur



Prof. Niranjan Panda NIT Rourkela



Prof. Shantanu Pal IIT Bhubaneswar



Dr. Nagendra Sharma NISER Bhubaneswar



Prof. Prasenjit Mal NISER Bhubaneswar



Dr. Janakiram Vaitla IIT Delhi



Dr. Thangavelu Saravanan University of Hyderabad



Dr. Vignesh Palani IISc Bangalore



Dr. Amit K. Simlandy IISER Berhampur



**Dr. Rambabu Dandela**ICT Bhubaneswar



**Dr. Durga Prasad Hari** IISc Bangalore



Dr. Kiran K. Pulukuri IISER Tirupati



Dr. Chandrakanta Dash Central University of Rajasthan



## National Conference on Organic Synthesis (N-COS 2025)

15th December 08:15 AM to 17th December 02:00 PM Venue: New Conference Hall, Berhampur University

Day 1: 15th December 2025, Monday				
08:15 - 09:00 AM	REGISTRATION			
	(Coffee/Breakfast)			
09:00 - 09:40 AM	INAUGURATION			
	Opening Remarks: <b>Dr. Laxmidhar Rout</b> (Convener, N-COS 2025)			
	,			
	Welcome Address: Prof. Sukanta K. Tripathy (PGC Chairman, Berhampur University)			
	Inaugural Address: <b>Prof. Geetanjali Dash</b> (Vice-Chancellor, Berhampur University)			
	Guest of Honor: Prof. A. K. Ganguli, (Director, IISER Berhampur)			
Technical Session-1				
09:45 - 11:05 AM	Chairperson: Prof. SATYABAN JENA (Honorary Professor, Utkal University) OSHEC SESSION			
09:45 - 10:15 AM	PL-01: Prof. D. Basavaiah (University of Hyderabad) The Baylis-Hillman concept of C-H (sp2) functionalization: Four decades of our contributions and experience. IL-01: Prof. J. R. Vaitla			
10:40 - 11:05 AM	(IIT Delhi) Unifying Carbene Precursors: Synthetic Opportunities with Vinyl Sulfoxonium Ylides and Diazo Compounds.  IL-02: Prof. G. B. Ramani			
	(IIT Jammu) Photochemical Alkynyl Carbene Transfer Reactions.			
	11:05 - 11:20 AM: Tea / Coffee			
Technical Session-2				
11:20 AM - 01:30 PM	Chairperson: Prof. J. S. YADAV (Former Director, CSIR-IICT Hyderabad)			
11:20 - 11:50 AM	PL-02: Prof. A. K. Sahoo (University of Hyderabad) Harnessing Conjugation via Difunctionalization of Ynamide.			
11:50 AM - 12:15 PM	IL-03: Prof. J. P. Dash (Ravenshaw University)			

	Stereoselective Claisen Rearrangement towards construction			
	of Quaternary Stereocenters, Lactones, and precursors of			
	natural products.			
12:15 - 12:40 PM	IL-04: Prof. S. S. V. Ramasastry			
	(IISER Mohali) Metal-Free Chemistry Facilitated by Phosphines.			
12:40 - 01:05 PM	IL-05: Prof. N. K. Sharma			
12.40 - 01.03 1 101	(NISER Bhabaneswar)			
	Tropolone Beyond Natural Products: A Unique Scaffold for			
	Biomolecular Design.			
01:05 - 01:30 PM	IL-06: Prof. N. Panda			
	(NIT Rourkela)			
	Thermally Generated "Cation Pools" and Their Synthetic Applications.			
	01:30 - 02:30 PM: Lunch			
	02:00 - 02:30 PM (Poster Session)			
Chairperso	n: Prof. K. R. Prasad & Prof. Akhila K. Sahoo			
	Technical Session-3			
02:30 - 04:15 PM	Chairperson: Prof. B. K. Patel			
	(IIT Guwahati)			
	DUTTCO SESSION			
02:30 - 03:00 PM	PL-03: Prof. A. T. Khan			
0.000	(IIT Guwahati)			
	Reactivity Study of 4-Hydroxydithiocoumarin Towards the			
	Synthesis of Novel Organosulfur Compounds.			
03:00 - 03:25 PM	IL-07: Prof. C. Appayee			
	(IIT Gandhinagar)			
03:25 - 03:50 PM	Chiral Organocatalysts: Synthesis and Applications.  IL-08: Prof. G. Sahoo			
03:23 - 03:30 FM	(NIT Rourkela)			
	Vicinal Diols as Potentially Greener H-Bond Donors:			
	Application to an Accelerated MBH Protocol.			
03:50 - 04:15 PM	IL-09: Prof. S. Thangavelu			
	(University of Hyderabad)			
	Expanding the Catalytic Horizons of DERA:			
	Photobiocatalytic Enantioselective β-Alkylation of Enals			
	04:15 - 04:30 PM: Tea / Coffee			
	Technical Session-4			
04:30 - 06:10 PM	Chairperson: Prof. A. K. Sahoo			
	(University of Hyderabad)			
04:30 - 04:55 PM	IL-10: Prof. P. Daw			
	(IISER Berhampur)			
04 55 05 00 70 5	Bifunctional Catalysts for Renewable Hydrogen Production.			
04:55 - 05:20 PM	IL-11: Prof. H. K. Sahoo			
	(NIT Rourkela)			

	Impact of Micro- and Macro-Environment on Protein				
	Conformation and Dynamics				
05:20 - 05:45 PM	IL-12: Prof. P. Dash				
	(NIT Rourkela)				
	Heterogeneous Photocatalysis towards Sustainable Synthesis				
05:45 - 06:10 PM	IL-13: Prof. P. Moitra				
	(IISER Berhampur)				
	Development of Novel Nanomaterials for Molecular				
Diagnosis of Certain Rare Genetic Disorders					
06:20 - 07:00 PM: Cultural Programme					
07:00 PM ONWARDS: DINNER					

Day 2: 16 <sup>th</sup> December 2025, Tuesday				
09:00 - 09:30 AM: BREAKFAST New Conference Hall				
	Technical Session-5			
09:30 - 11:15 AM	Chairperson: Prof. D. Basavaiah			
	(University of Hyderabad)			
	S&T, ODISHA SESSION			
09:30 - 10:00 AM	PL-04: Prof. T. Punniyamurthy			
	(IIT Guwahati) Strategic C-H Functionalization and Cascade Synthesis			
	toward Bioactive Heterocyclic Frameworks.			
10:00 – 10:25 AM IL-14: Prof. A. Doddi				
	(IISER Berhampur)			
Novel Ancillary Ligands: Bridging Metal-Free and Metal- Based Approaches in Homogeneous Catalysis				
10:25 - 10:50 AM				
(NISER Bhubaneswar)				
CsPbBr3 Perovskites in Visible-Light-Driven Organic Synthesis.				
10:50 - 11:15 AM	IL-16: Prof. S. Pal			
	(IIT Bhubaneswar)			
	Novel Strategies for the Construction of Bioactive Benzimidazole Fused N-Heterocycles			
	· ·			
11:15 - 11:30 AM: Tea / Coffee				
	Technical Session-6			
11:30 AM - 1:40 PM	Chairperson: Prof. A. T. Khan			
	(IIT Guwahati)			
11:30 AM - 12.00 PM	PL-05: Prof. B. K. Patel			
	(IIT Guwahati)			
	Taming Radicals: Strategies for Bond Activation and Functionalization.			
	1 unchonanzadon.			

12.00 PM - 12:25 PM	IL-17: Prof. V. Palani				
	(IISc Bangalore)				
	A three-phase, one-pot protocol to enable 1,3-translocation of				
	aryl ketones.				
12:25 - 12:50 PM	IL-18: Prof. R. Goretti				
	(IISER TVM)				
	Enantioselective Approaches for the Structure Assignment of				
	Abietane Diterpenoids.				
12:50 - 1:15 PM	IL-19: Prof. T. Barla				
	(IISER Berhampur)				
	Total Synthesis: A Critical Tool for the Structural				
	Reassignment of Natural Products.				
1:15- 1:40 PM	IL-20: Prof. T. Khan				
	(IIT Bhubaneswar)				
	Aiming Sustainability via Visible-Light Photoredox Catalysis				
	and Anthropogenic Gas Capture for Functionalized				
	Molecules				

### 1:40 - 2:30 PM: Lunch

### 02:00 - 02:30 PM (Poster Session)

Chairperson: Prof. K. R. Prasad & Prof. Akhila K. Sahoo

### **Technical Session-7**

2.30- 4.10 PM	Chairperson: Prof. D. K. Mohapatra				
	(CSIR-IICT Hyderabad)				
2:30 PM - 12.00 PM	IL-21: Prof. P. C. Ravikumar				
	(IISER Tirupati)				
	Weak Chelation Assisted C-H Functionalization using Cobalt				
	Catalyst: A Sustainable Approach.				
2.55 PM - 3:20 PM	IL-22: Prof. D. P. Hari				
	(IISc Bangalore)				
	Radical-Polar Crossover for Molecular Remodelling.				
3:20 PM - 3:45 PM	IL-23: Prof. K. K. Pulukuri				
	(IISER Tirupati)				
	Synthesis of Sesquiterpenoids through Siteselective				
	Functionalization				
3:45 PM - 4.10 PM	IL-24: Prof. M. K. Rana				
	(IISER Berhampur)				
	Integrated Artificial Intelligence (AI)-Molecular Dynamics				
	(MD) Approach for Drug Discovery to Overcome				
Chemoresistance in Triple Negative Breast Cancer.					
	4:10 PM - 5:25 PM: Tea / Coffee				
4.10 1 W = 5.25 1 W. Tea/ Coffee					
4:25 PM-5:25 PM: FLASH POSTER SESSION I					
(CHAIR BY PROF. S. S. V. RAMASASTRY & PROF. D. P. HARI)					
16:25 PM-16:35 PM	FP-01: Abhaykumar Vishwakarma				
	(IIT Bhubaneswar)				

16:35 PM-16:45 PM	FP-02: Akshaya S (IISER Berhampur)		
16:45 PM-16:55 PM	FP-03: Ankita Mandal (IISER Berhampur)		
16:55 PM-17:05 PM	FP-04: Harsh Hirpara (ICT-IOC Bhubaneswar)		
17:05 PM-17:15 PM	FP-05: Madhab Chandra Maity (IIT Bhubaneswar)		
17:15 PM-17:25 PM	FP-06: Manas Kumar Sahu (NISER Bhubaneswar)		
07:00 PM ONWARDS: DINNER			

Day 3: 17 <sup>th</sup> December 2025, Wednesday			
	09:00 - 09:30 AM: BREAKFAST New Conference Hall		
09:30 A	M-10:20 AM: FLASH POSTER SESSION II		
(CHAIR BY	PROF. P. C. RAVIKUMAR & PROF. A. DODDI)		
09:30 AM-09:40 AM	FP-07: Manas Ranjan Swain (KIIT Bhubaneswar)		
09:40 AM-09:50 AM	FP-08: Rageshree Dash (IISER Berhampur)		
09:50 AM-10:00 AM	FP-09: Ranjan Kumar Panigrahi (KIIT Bhubaneswar)		
10:00 AM-10:10 AM	FP-10: Subhra Kanti Mahato (IISER Berhampur)		
10:10 AM-10:20 AM	FP-11: Shubham Kumar Dhal (IISER Tirupati)		
	10.20 AM - 10:35 AM: Tea / Coffee		
	Technical Session-8		
10.35-12.45 PM	Chairperson: Prof. J. S. Yadav		
10:35 AM-11:00 AM	(Former Director, CSIR-IICT Hyderabad)  IL-25: Prof. R. Dandela		
10.55 AW-11.00 AW	(ICT Bhubaneswar)		
	The Efficient Construction of Functionalized Heterocyclic Compounds		
11:00 AM-11:25 AM	IL-26: Prof. A. K. Simlandy		
	((IISER Berhampur) Conformational Rigidity Controlled Copper Catalyzed Chemodivergent Annulation		

11:25 AM-11:50 AM	IL-27: Prof. S. S. Badsara				
	(BHU, Varanasi)				
	Site-Selective Electrochemical Functionalization of Indolizine				
	Frameworks Enabled by N-Centered Radical Translocation.				
11:50 AM-12:15 PM	IL-28: Prof. C. Dash				
	(Central University of Rajasthan)				
	Transition-Metal-Catalyzed Carbazole Synthesis via				
	Intramolecular C-H Amination				
12:15 PM-12:45 PM	PL-06: Prof. C. V. Ramana				
	(CSIR-NCL Pune)				
	Catalysis for Sustainable Total Synthesis.				
12:45 AM-1:30 PM: VALEDICTORY SESSION, POSTER PRIZE					
DISTRIBUTION					
	1:30 PM ONWARDS: LUNCH				

THE END

Delegates Profile

#### S. Chandrasekharan

Distinguished Professor, IISc Bangalore

#### **Contact**

**Phone:** +91-9886088344 **Email ID:** scn@iisc.ac.in

Website: fellows.ias.ac.in/profile/v/FL1989004

#### **Education**

Ph.D.: University of Madras.

M.Sc.: Vivekananda College, University of Madras.

#### Career

Professor (1985-1989): Dept. of Chemistry, IIT Kanpur.

Assistant Professor (1981-1985): Dept. of Chemistry, IIT Kanpur.

Lecturer (1978-1980): Dept. of Chemistry, IIT Kanpur.

Postdoctoral (1976-1977): with Prof. E. J. Corey, Harvard University, USA.

(1975-1976): Syntex Research, California, USA.

(1973-1975): with Prof. E. J. Corey, Harvard University, USA.

#### Area of Research

a) New Synthetic Methodology.

b) Total Synthesis of Natural Products.

c) Organic Materials / Catalysis/ Green Chemistry.

#### Awards & Honours

1988: Basudeb Banerjee Memorial Medal & Prize, ICS, India.

1989: Shanti Swarup Bhatnagar Prize, CRI, India.

1992: Elected Fellow, IASc (FNNA); FTWAS

1999: Elected Fellow, INSA.

2000: Elected Fellow, World Academy of Sciences.

2000: Honorary Professor, JNCASR, Bangalore.

2002: CRSI Silver Medal.

2004: IISc Alumni Award.

2005: Medal of the Material Research Society of India.

2006: JC Bose National Fellow, DST.

2007: INSA Golden Jubilee Commemoration Medal.

2009-2011: Chairman, IUPAC, INSA.

2014: SERB Distinguished Fellow, IISc Bangalore.



N-COS 2025 Profile

### Jhillu Singh Yadav

Former Director, CSIR-IICT Hyderabad

#### Contact

Email ID: yadav@iict.res.in, yadavpub@iict.res.in

Website: http://www.iictindia.org/staff/jsy/20150626-JSY-cv.pd

**Education** 

Ph.D.: M.S University, Baroda

M.Sc.: BHU Career

Current Position: CSIR Bhatnagar Fellow, CSIR-IICT, Hyderabad

Director (2003-2012): CSIR-IICT Hyderabad Scientist G (1999-2003): CSIR-IICT Hyderabad Scientist F (1994-1999): CSIR-IICT Hyderabad Scientist EII (1990-1994): CSIR-IICT Hyderabad

Scientist EI (1986-1990): Regional Research Laboratory, Hyderabad

Scientist C (1980-1986): NCL Pune

#### Area of Research

- To develop methodologies for preparation of insect pheromones and Popularize ecofriendly pheromone application technology (PAT) for pest control strategies
- To sharpen and advocate the acquired expertise in synthesizing enantiomerically pure compounds from Natural Products via asymmetric Synthesis.
- To contribute and develop modern Synthetic methods and reagents for the ease of synthesis of complex organic molecules
- To develop unique and viable affordable routes for the synthesis of common drugs/agrochemicals

#### **Awards & Honors**

1987: FAPCCI Award by Federation of Andhra Pradesh Chamber of Commerce and Industry

1991: Shanti Swarup Bhatnagar Award in Chemical Sciences

22nd Khwarizmi International Award, IROST-UNESCO, Iran

1999: Vasvik Award for Chemical Sciences & Technology

2000: Ranbaxy Research Award in Pharmaceutical Sciences

2002: Prof.S.Swaminathan Commemorative Lecture Award

2003: Vigyan Ratna Award, Uttar Pradesh

2003: Goyal Award for Chemical Sciences

2003: CRSI Silver Medal

2003: Andhra Pradesh Scientist Award

2004: Vigyan Gaurav Samman Award, Uttar Pradesh

2008: Jagadish Chandra Bose Fellowship Award

2009: Pandit Jawaharlal Nehru National Award from Madhya Pradesh Department of

Science & Technology, Madhya Pradesh

2010: Banaras Hindu University Alumnus Award

### Satyaban Jena

Former Professor, Utkal University

#### Contact

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#### Education

Ph.D.: Utkal University.

M.Sc.: Utkal University (Gold Medalist).

#### Career

President (2016): President, Orissa Chemical Society (OCS).

Director (2015-2020): KIIT University, Bhubaneswar.

Professor (1999-2014): Dept. of Chemistry, Utkal University.

Reader (1991-1999): Dept. of Chemistry, Utkal University.

Senior Lecturer (1986-1991): Dept. of Chemistry, Utkal University.

Lecturer (1985-1986): Dept. of Chemistry, Utkal University.

Lecturer (1981-1985): Dept. of Chemistry, Ravenshaw University.

Lecturer (1979-1981): Dept. of Chemistry, Gangadhar Meher College, Sambalpur.

**Postdoctoral** (1990-1991): Maxwell's Institute, UK. **Postdoctoral** (1989-1990): University of Leeds, UK.

#### Area of Research & Teaching

a) Synthetic Organic Chemistry

#### Awards & Honours

2002: Mahatab Samman.

#### **Books**

#### (with Dr. L. Rout, Indu Book Service Pvt. Ltd., New Delhi-110002)

- 1. Name reaction, Rearrangements and Mechanism; Problem Solving Approach, 2024; ISBN No.: 978-81-19907-53-3.
- 2. Pericyclic and Photochemistry; Problem Solving Approach, 2024; ISBN No.: 978-81-19907-91-5.
- **3.** Advanced Organic Spectroscopy; Problem Solving Approach, 2024; ISBN No.: 978-81-19907-76-2.
- **4.** Reagent and Mechanism in Organic Synthesis; Problem Solving Approach, 2024; ISBN No.: 978-81-19907-48-9.
- **5.** Retrosynthesis and application; Problem Solving Approach, 2024; ISBN No.: 978-93-91-377-78-6.
- **6.** Stereochemistry, Conformations and Asymmetric Synthesis; Problem Solving Approach, 2024; ISBN No.: 978-81-19907-67-0.
- 7. General Organic Chemistry; Problem Solving Approach, 2024; ISBN No.: 978-81-19907-72-4.
- 8. Advanced Heterocyclic Chemistry; Problem Solving Approach, 2024; ISBN No.: 978-81-19907-98-4.



N-COS 2025 Profile

### Ashok K. Ganguli

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#### **Education**

Ph.D.: IISc Bangalore.

#### Career

Director (2023 - till date): IISER Berhampur India.

Prof N K Jha Chair (2022 - 2023): Dept. of Chemistry, IIT Delhi.

**Deputy Director** : Strategy & Planning, IIT Delhi. **Institute Chair Professor** (2019 – 2021) : IIT Delhi. **Visiting Professor** (2016) : EPFL, Lausanne.

Founding Director (2013 - 2018): INST Mohali.

**Visiting Scientist** (2004 – 2005): Ames Laboratory, Iowa State University, USA.

**Postdoctoral** (1991 – 1993): Ames Laboratory, Iowa State University, USA. **Visiting Scientist** (1990 – 1991): Dupont Company, USA.

### **Area of Research**

- a) design of nanostructured materials for applications in water purification.
- b) solar energy conversion and microfluidic devices.
- c) high-temperature superconductivity.

#### **Awards & Honors**

- 1990 : Sud borough Medal.
- 2006: MRSI Medal.
- FRSC, FNASc, FIAS, Fellow of Asia-Pacific Association of Materials.
- Bangalore India Nano award given by Karnataka Govt.
- Chemical Excellence Award by Indian Society of Chemists and Biologists.
- CRSI-Silver Medal, MRSI-Medal, the C.N.R. Rao-CRSI National Award.
- National Award of Nano Science and Nanotechnology, DST, India.



### Kavirayani R. Prasad

Professor, IISc Bangalore



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#### Education

**Ph.D.:** National Chemical Laboratory, Pune **M.Sc.:** Sri Krishnadevraya Univesrity, Anantapur

#### Career

Professor (2014- Present): Department of Organic Chemistry, IISc Bangalore Professor (2015- 2015): SPS, JNU

Associate Professor (2008-2014): Department of Organic Chemistry, IISc Bangalore Assistant Professor (2003-2008): Department of Organic Chemistry, IISc Bangalore Research Scientist (2003-2003): Praecis Pharmaceuticals Inc (presently Glaxo Smith

Kline), Waltham, MA.USA

Postdoctoral (2000-2003): Department of Chemistry, Temple University, Philadelphia, USA

(1998-2000): Alexander von Humboldt Foundation, Postdoctoral Fellow, Organisch-Chemisches Institut, Universität Münster, Germany.

#### Area of Research

- Total Synthesis of natural products.
- Synthetic Methods
- Medicinal Chemistry

#### **Awards & Honours**

2006: Swarnajayanthi fellowship of the Department of Science and Technology, New Delhi

2012: Rajib Goyal Prize.

2012: NASI (National Academy of Sciences)-SCOPUS Young Scientist award

2013: Prof. N. S. Narasimhan Endowment Lecture Award, University of Pune.

2014: Shanti Swarup Bhatnagar prize for chemical Sciences.

2015: Fellow, Indian Academy of Sciences

2022: Fellow, National Academy of Sciences

**2024:** JC Bose Fellowship

N-COS 2025 Profile

#### Akhilesh K. Verma

Professor, University of Delhi



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#### **Education**

Ph.D.: University of Delhi.

M.Sc.: Bipin Bihari PG College, Jhansi, UP

#### Career

Professor (2013- Present): Dept. of Chemistry, University of Delhi.

Professor (2015- 2015): SPS, JNU

Associate Professor (2009-2013): Dept. of Chemistry, University of Delhi.

**Assistant Professor** (1998-2009): ACBR University of Delhi **Postdoctoral** (2001-2002): University of Florida, USA

#### **Area of Research**

Hydroamination of alkynes; Metal/Iodine-catalyzed reactions of alkynes.

Design of benzotriazole-based ligands for the coupling reaction.

• Tandem/cascade reaction and C-H activation/functionalization.

#### Awards & Honours

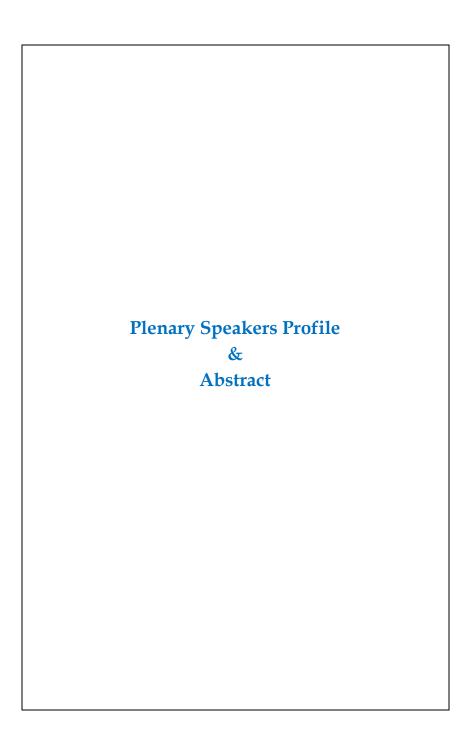
2007: BOYSCAST Fellow (2007-2008)

2021: Elected Fellow (FNA), Indian National Science Academy (INSA)

2021: Bronze Medal: CRSI

2021: Elected Fellow: Royal Society of Chemistry (FRSC)

2021: Senior Fellow, Institution of Eminence (IoE); University of Delhi



#### Deevi Basavaiah

Professor, University of Hyderabad



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#### **Education**

**Ph.D.**: Chemistry Department, BHU. **M.Sc.**: Chemistry Department, BHU.

#### Career

**Professor** (1996-till date): SoC, University of Hyderabad. **Reader** (1987-1996): SoC, University of Hyderabad. **Lecturer** (1984-1987): SoC, University of Hyderabad.

**Scientist** C (1984-1984) : NCL, Pune **Postdoctoral :** Purdue University, U.S.A.

#### Area of Research

Organic Chemistry

a) Baylis-Hillman Reaction

b) Chiral Catalysis

#### **Awards & Honors**

**2014**: Honorary Professor, BHU, Varanasi. **2012**: BHU Distinguished Alumnus Award.

**2009 :** INSA Commemoration Medal. **2008 :** JC Bose National Fellow, DST.

2008 : CRSI Silver Medal.2006 : Elected Fellow, FNA.2000 : CRSI Bronze Medal.

1997: Elected Fellow, FASc, Bangalore.

### The Baylis-Hillman concept of C-H (sp2) functionalization: Four decades of our contributions and experience Prof. D. Basavaiah

School of Chemistry, University of Hyderabad, Hyderabad-500046, India

**Abstract:** C-H functionalization is one of the important and fundamental reactions in organic chemistry. The Baylis-Hillman reaction (also known as the Morita-Baylis-Hillman reaction) is a well-known (sp2) C-H functionalization process involving an atom-economy carbon-carbon bond forming reaction via the coupling of α-position of activated alkenes with electrophiles under the influence of a catalyst (mostly organic catalyst) providing diverse classes of densely functionalized molecules containing proximal functional groups.1,2 Now this reaction represents a new continent in organic chemistry offering unending challenges and opportunities for continuous development both in fundamental level as well as in application point of view. We have been working for the past four decades with the main objective of developing it as a useful and powerful tool in synthetic chemistry and in fact, have made significant contributions to this effect.1,3,4 This talk will present our vision, four decades of our experience in this area of Baylis-Hillman reaction and contributions towards the continuous growth of this reaction.

#### References:

- (a)D. Basavaiah, R. T. Naganaboina New J. Chem. 2018, 42, 14036-14066. (b) D. Basavaiah, G. Veeraraghavaiah Chem. Soc. Rev. 2012, 41, 68-78. (c) D. Basavaiah, B. S. Reddy, S. S. Badsara Chem. Rev. 2010, 110, 5447-5674. (d) D. Basavaiah, K. V. Rao, R. J. Reddy Chem. Soc. Rev. 2007, 36, 1581-1588.; (e) D. Basavaiah, A. J. Rao, T. Satyanarayana Chem. Rev. 2003, 103, 811-891.
- (a)Y. Wei, M. Shi Chem. Rev. 2013, 113, 6659-6690. (b) T. Y. Liu, M. Xie, Y. C. Chen Chem. Soc. Rev. 2012, 41, 4101-4112. (c) V. Declerck, J. Martinez, F. Lamaty Chem. Rev. 2009, 109, 1-48. (d) V. Singh, S. Batra Tetrahedron 2008, 64, 4511-4574.
- (a)D. Basavaiah, K. R. Reddy, N. Kumaragurubaran Nature Protocols 2007, 2, 2665-2676.
   (b) D. Basavaiah, T. Satyanarayana Chem. Commun. 2004, 32-33.
   (c) D. Basavaiah, A. J. Rao, Chem. Commun. 2003, 604-605.
   (d) D. Basavaiah, T. Satyanarayana Org. Lett. 2001, 3, 3619-3622.
   e) D. Basavaiah, S. Roy Org. Lett. 2008, 10, 1819-1822.
- (a)D. Basavaiah, V. V. L. Gowriswari Tetrahedron Lett. 1986, 27, 2031-2032. (b) D. Basavaiah, V. V. L. Gowriswari, T. K. Bharathi Tetrahedron Lett. 1987, 28, 4591-4592.
   (c) D. Basavaiah, T. K. Bharathi and V. V. L. Gowriswari, Tetrahedron Lett., 1987, 28, 4351-4352. (d) D. Basavaiah, V. V. L. Gowriswari, P. K. S. Sarma and P. D. Rao, Tetrahedron Lett., 1990, 31, 1621-1624. (e) D. Basavaiah, S. Pandiaraju and P. K. S. Sarma, Tetrahedron Lett., 1994, 35, 4227-4230.

### Chepuri V. Ramana

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#### **Education**

**Ph.D.:** University of Hyderabad. **M.Sc.:** Andhra University, Waltair

Career

Scientist (2001 - Present): NCL, Pune.

Research Associate (1997-2001): ETH Zürich, Switzerland

### **Area of Research**

a) Total Synthesis.

### **Awards & Honors**

2017: CNR Rao National Prize in Chemical Sciences

2016: Dr. A.V. Rama Rao Foundation Prize Lecture in Chemistry.

2013: CRSI Bronze Medal in chemical sciences (2013)

2011: Professor D. K. Banerjee Memorial Lecture Award - IISc Bangalore

2009: NCL's Scientist of the Year award.

2003: CSIR Young Scientist award in Chemical Sciences.



### Catalysis for Sustainable Total Synthesis

#### Prof. C. V. Ramana

Organic Chemistry Division, CSIR-National Chemical Laboratory Dr. Homi Bhabha Road, Pune-411008 (MH), India

**Abstract:** The design and deployment of novel catalytic transformations is central to modern synthetic chemistry. Our work focuses on developing strategies for the total synthesis of complex natural products and bioactive molecules that strictly adhere to green chemistry principles, aiming to minimize environmental impact and maximize resource efficiency. This mandates the use of intelligent bond disconnections and pioneering retrosynthetic strategies to forge molecular complexity in the fewest possible steps. In this presentation, we will detail several successful total syntheses from our group, all funded and executed around this core concept of sustainable catalytic efficiency.

#### References:

- 1. Khobragade, V. R.; Ramana, C. V. Org. Lett. 2025, 27, 5931.
- 2. Shet, M. N.; Ramana, C. V. J. Org. Chem. 2024, 89, 16923.
- 3. Halnor, S. V.; Ramana, C. V. Tetrahedron 2024, 167, 134301.
- 4. Srinivas, K.; Ramana, C. V. Org. Lett. 2017, 19, 6466.
- 5. Reddy, B. N. Ramana, C. V. Chem. Commun. 2013, 49, 9767.
- 6. Narute, S. B.; Ramana, C. V. Tetrahedron, 2013, 69, 1830.

#### Abu Taleb Khan

Distinguished Professor, IIT Guwahati



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#### **Education**

**Ph.D.:** Kalyani University **M.Sc.:** Kalyani University.

#### Career

Professor (2004 - Present): IIT Guwahati

**Associate Professor** (2001 - 2004): IIT Guwahati **Assistant Professor** (1996 – 2001): IIT Guwahati

Scientist C (1996 – 1996): RRL Jorhat, Assam (CSIR Lab) Postdoctoral (1992 – 1994): University of Konstanz, Germany.

#### **Area of Research**

- Total Synthesis of Natural Products
- Newer Methodologies in Carbohydrate Chemistry
- Synthesis of Heterocycles through MCRs
- New Reagents & Peroxovanadium Chemistry

# Reactivity Study of 4-Hydroxydithiocoumarin Towards the Synthesis of Novel Organosulfur Compounds

#### Prof. Abu Taleb Khan

Department of Chemistry, IIT Guwahati, Guwahati-781039, Assam

**Abstract:** 4-Hydroxydithiocoumarin and 4-hydroxythiocoumarin are well-known thio-analogues of 4-hydroxycoumarin. The reactivity of 4-hydroxycoumarin is well established, and numerous heterocycles have been synthesised using it as a key precursor, with the hydroxy group and the C3-position being primarily involved in these transformations. The non-natural compound warfarin is a derivative of 4-hydroxycoumarin **II**, used as a medication. Similarly, both thio-analogues 4-hydroxydithiocoumarin **III** and 4-hydroxythiocoumarin **IIII** are widely employed as precursors for the construction of diverse organosulfur heterocyclic frameworks. Notably, each of these compounds contains three prominent reactive sites, making their reactivity studies both more complex and more fascinating. They also share structural resemblance except the O, which is placed in the 4-hydroxythiocoumarin **III** ring, whereas S is in the case of 4-hydroxydithiocoumarin **III**, as presented in **Scheme 1**.

The presentation will focus on the reactivity study of 4-hydroxydithiocoumarin (III) towards the synthesis of novel organosulfur compounds.<sup>2-5</sup>

4-Hydroxycoumarin 4-Hydroxydithiocoumarin

4-Hydroxythiocoumarin

**Scheme 1**. 4-hydroxythiocoumarin **I** and its thio-analogues 4-hydroxydithiocoumarin **II** and 4-hydroxythiocoumarin **III**.

**Keywords:** 4-hydroxydithiocoumarin, 4-hydroxythiocoumarin, Organosulfur compounds.

#### References:

- M. Belal, S. Mondal, S. Yashmin, and A. T. Khan, Org. Biomol. Chem., 2022, 20, 715-726.
- 2. Ali, S. Faraz, and A. T. Khan, Org. Biomol. Chem., 2024, 22,1426–1433.
- Ali, S. Begam, K. Mehta, P. V. Bharatam, A. T. Khan, J. Org. Chem., 2025, 90, 8857– 8868.
- Ali, S. Mondal, M. Sood, P. V. Bharatam and A. T. Khan, Org. Chem. Front., 2025, 12, 6288-6300.
- 5. Ali, N. Amin, P. K. Khanra, S. S. Ghosh, A. T. Khan, submitted to Nat. Synth.

# Bhisma K. Patel

Professor, IIT Guwahati

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# **Education**

**Ph.D.:** IIT Kanpur.

**M.Sc.**: Sambalpur University.

# Career

Professor (2005- Present): Dept. of Chemistry, IIT Guwahati.

**Associate Professor** (2001 – 2005): Dept. of Chemistry, IIT Guwahati. **Assistant Professor** (1999 – 2001): Dept. of Chemistry, IIT Guwahati.

Visiting Associate Professor (1997 – 1999): Dept. of Chemistry, IIT Guwahati.

Postdoctoral (1994 - 1997): Max-Planck Institute, Goettingen, Germany

# **Area of Research**

- a) Bio-Organic Chemistry
- b) Newer Methodologies.

# Awards & Honors

2016: Costal Chemical Research Society Award (CCRS-2016)

2014: Bronze Medal by Chemical Research Society (CRSI) of India.

1998: R. C. Tripathy young scientist award by Orissa Chemical Society (OCS)



# Taming Radicals: Strategies for Bond Activation and Functionalization

#### Prof. Bhisma K Patel

Indian Institute of Technology Guwahati

**Abstract:** Radical-mediated reactions play a pivotal role in organic synthesis as they enable unique bond-forming pathways that are often inaccessible through traditional ionic or concerted mechanisms. Our research group has been generating nitrogen-, sulfur-, and carbon-centred radicals via thermal, photochemical, and electrochemical methods, leading to a variety of useful organic transformations. tert-Butyl nitrite (TBN) has proven to be a versatile precursor, functioning as both N and N-O synthon, enabling efficient C-N and N-O bond formations in the synthesis of various nitrogenous heterocycles.<sup>[1]</sup> An intermolecular radical-based distal selectivity in appended alkyl chains has been developed. The selectivity is maximum when the distal carbon is y to the appended group and decreases by moving from  $y \to \delta \to \epsilon$ positions.[2] The EDA (Electron Donor-Acceptor) complex-based photochemical synthesis is important in modern organic chemistry as it absorbs visible light directly, often without any photocatalysts, leading to useful C-C, C-N, C-S, and C-O bond-forming transformations.[3] Further demonstrated is an external photo-sensitizer-free singlet oxygen-enabled solvent-dependent tertiary hydroxylation and aryl-alkyl spirocyclic etherification of C3-maleimidated quinoxalines.<sup>[4]</sup> An operationally simple EnT-mediated C3-*N*-heteroarylation of 2-aryl quinoxalines decarboxylative radical-radical cross-coupling (Csp<sup>2</sup>-Csp<sup>2</sup>) with oxime esters is accomplished.[5]

**Keywords:** Heterocycles, Energy transfer, Reagentless synthesis, Radical reaction, Remote Functionalization

#### References and Notes:

- Patel, B. K. et.al. J. Org. Chem. 2017, 82, 6358; J. Org. Chem. 2018, 83, 1056; Org. Lett. 2019, 21, 4966; Org. Lett. 2020, 22, 3728; J. Org. Chem. 2020, 85, 2118.
- Rajamanickam, S.; Saraswat, M.; Venkataramani, S.; Patel, B. K. Chem. Sci. 2021, 12, 15318.
- Barik, D.; Chakraborty, N.; Sahoo, A. K.; Dhara, H. N. Patel, B. K. Chem. Commun., 2024, 60, 12577. (b) Dhara, H. N.; Rakshit, A.; Barik. D.; Ghosh, K. Patel, B. K. Chem. Commun., 2023, 59, 7990.
- Ghosh, S.; Khandelia, T.; Mahadevan, A.; Panigrahi, P.; Kumar, P.; Mandal, R.; Boruah, D.; Venkataramani, Patel, B. K. Chem Eur. J., 2024, e202400219.
- Mandal, R.; Ghosh, S.; Laha, S.; Panigrahi, P.; Bhattacharyya, K.; Patel, B. K. Org. Lett. 2025, 27, 4257.

# Tharmalingam Punniyamurthy

Professor, IIT Guwahati

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# **Education**

**Ph.D.**: Indian Institute of Technology Kanpur. **M.Phil.**: Bharathidasan University, Tiruchirappalli. **M.Sc.**: Bharathidasan University, Tiruchirappalli.

# Career

Dean (2020 - 2023): Dean, Faculty Affairs, IIT Guwahati.

Visiting Professor (2020): NIPER Guwahati.

Head (2017 - 2020): Dept. of Chemistry, IIT Guwahati.

HAG Professor (2015): IIT Guwahati.

**Visiting Professor** (2013): The Scripps Research Institute.

Visiting Professor (2011): Kyushu University.

Professor (2008): IIT Guwahati.

Visiting Professor (2007): Oxford University.

Associate Professor (2005 - 2008): IIT Guwahati.

Assistant Professor (2001 - 2005): IIT Guwahati.

Postdoctoral (2000 - 2001): CNRS, Ecole de Chime Montpellier.

(1997 - 1999): JSPS, Kyushu University.

(1995 - 1996): North Dakota State University.

#### Area of Research

Synthetic Organic Chemistry

# **Awards & Honors**

2019: Margadarshak, Assam Engineering College.

2018: Elected Fellow, The National Academy of Sciences.

2016: Elected Fellow, Indian Academy of Sciences.

2015: CRSI Bronze Medal.

**2014**: Fellow, Royal Society of Chemistry.

**2013**: OLF Award.

2012: Fulbright-Nehru Senior Research Fellowship.

2011: JSPS Invitation Fellowship (Short Term).

2010: JSPS Bridge Fellowship.

2007: UKIERI Research Fellowship.

2006: IUPAC Travel Award.



# Strategic C-H Functionalization and Cascade Synthesis toward Bioactive Heterocyclic Frameworks

# Prof. T. Punniyamurthy

Department of Chemistry, IIT Guwahati, Guwahati-781039

**Abstract:** 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 reaction of strained rings with suitable coupling partners can further lead to formation of diverse heterocycles of medicinal interests, which are important in the development of sustainable organic synthesis. Our research work focusses primarily on showcasing miscellaneous methodologies and their subsequent incorporation towards achieving hetero-atom embedded cyclic structural motifs. Lower catalyst loading and the use of readily available synthetic precursors for achieving site-selective functionalization has been our primary aim. Currently, our efforts rely on C-H functionalization using strained ring systems as viable coupling partners to introduce molecular complexity to a simple substrate as well as functionalization of more inert sp³ C-H bonds under milder reaction conditions using abundant 3d-transition metals. Our group has made a significant contribution for the past decade in these active topics and some of the recent results would be presented.

#### Reference:

- 1. Roy, S.; Saha, S.; Bhattacharyya, H.; Punniyamurthy, T. Org. Lett. 2025, 27, 7898.
- Nanjegowda, M. V.; Basak, S.; Paul, T.; Barman, M.; Punniyamurthy, T. Org. Lett. 2025, 27, 5379.
- 3. Debnath, B.; Mandal, S.; Saha, S.; Karjee, P.; Punniyamurthy, T. Chem. Commun. 2025, 61, 7875.
- 4. Sahoo, A.; Paul, T.; Basak, S.; Punniyamurthy, T. Chem. Commun. 2024, 60, 14818.
- 5. Barman, M.; Mishra, M.; Mandal, S.; Punniyamurthy, T. Org. Lett. 2024, 26, 3722.

# Akhila K. Sahoo

Professor, University of Hyderabad

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# **Education**

**Ph.D.**: National Chemical Laboratory, Pune, India. **M.Sc.**: Utkal University, Bhubaneswar, Odisha.

# Career

Professor (2016 - till date): SoC, University of Hyderabad.

**Associate Professor** (2013 - 2016): SoC, University of Hyderabad. **Assistant Professor** (2007 - 2012): SoC, University of Hyderabad.

**Scientist** (2006 - 2007): Sai Advantium Pharma Limited, Hyderabad, India. **Postdoctoral** (2004 - 2006): Kyoto University, Japan (with Prof. A. Osuka).

(2002 - 2004): JSPS, Kyoto University, Japan (with Prof. T. Hiyama). (2002 - 2002): RWTH Aachen, Germany (with Prof. H-J. Gais).

#### Area of Research

- a) Development of novel synthetic methods for organic synthesis.
- **b)** Functionalizations of sp<sup>2</sup> and sp<sup>3</sup> C-H bonds.
- c) Stereoselective C-H functionalizations.
- d) Gold and silver-catalyzed organic transformations.
- e) Synthesis of fused- $\pi$ -conjugated heterocycles.
- f) Synthesis of nitro and nitrogen-rich insensitive high energetic materials

# **Awards & Honours**

2025: Fellow of Indian National Science Academy (FNA)

2021: Fellow of Indian Academy of Sciences (FASc).

**2020:** Fellow of Royal Society of Chemistry (FRSC).

2020: UGC-BSR-Mid Career Award.

**2019:** Fellow of National Academy of Sciences (FNASc).

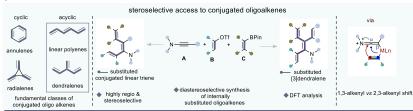
2012: Prof. D. K. Banerjee Memorial Lecture Award, IISc, Bangalore.

# Harnessing Conjugation via Difunctionalization of Ynamide

#### Akhila K. Sahoo

School of Chemistry, University of Hyderabad

Abstract: Acyclic conjugated polyenes represent a privileged scaffold with substantial potential for synthesizing complex molecular architectures.1-3 Traditional de novo synthesis of these molecules often encounters regio- and stereoselectivity challenges, resulting in multistep processes that compromise reaction efficiency.1-3 In this study, we introduce a modular approach for the direct synthesis of nitrogen-substituted polarized conjugated trienes and [3]dendralene derivatives from readily available feedstock reagents.4,5 This transformation is particularly notable for its unprecedented 1,3-alkenyl migration, showcasing an umpolung reactivity. Moreover, it enables the rapid diversification of synthetically challenging triene motifs and [3]dendralenes, demonstrating broad functional group compatibility and facilitating the synthesis of conjugated and cross-conjugated hybrid molecules. Mechanistic insights are supported by control experiments and DFT calculations, highlighting the robustness and versatility of our methodology in advancing the field of conjugated polyene synthesis.



**Keywords:** conjugated triene, [3] dendralene, cationic pallidum catalysis, umpolung reactivity, stereoselective synthesis.

#### References:

- 1. M. Sethi, S. Dutta, A. K. Sahoo Org. Lett. 2024, 26, 15, 3224–3229.
- 2. S. Dutta, S. Shandilya, S. Yang, V. Gandon, A. K. Sahoo. Nat Commun. 2022, 13, 1360.
- S. Dutta, S. Yang, R. Vanjari, R. K. Mallick, V. Gandon, A. K. Sahoo. Angew. Chem., Int. Ed. 2020, 59, 10785–10790.
- M. Sethi, S. Verma, V. Gandon, A. K. Sahoo ACS Catal. 2025, 15, 15606–15616
- 5. S. Verma, M. Sethi, A. K. Sahoo Chem Science 2025, ASAP.

Invited Lecturers
Profile
&
Abstract

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# Education

Ph.D.: Indian Institute of Science, Bangalore ,2008

M Sc.: Alagappan University, 2002

#### Career

Associate Professor (2020-2024): IIT Gandhinagar Assistant professor (2013-2020): IIT Gandhinagar Research (2008-2009): University of Miami, USA

Postdoctoral (2012-2013): Columbia University, New York, USA

(2009-2012): Brooklyn College and the City University of New York

(2008-2009): University of Miami, Florida

# Area of Research

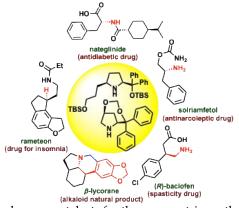
- Organic Chemistry
- Area of asymmetric organocatalysis
- Asymmetric Synthesis of bioactive natural products and drugs

# **Chiral Organocatalysts: Synthesis and Applications**

# Chandrakumar Appayee

Department of Chemistry, IIT- Gandhinagar, Palaj, Gandhinagar-382055 India

**ABSTRACT:** Asymmetric catalysis is one of the most powerful ways to produce single-enantiomer drugs. Asymmetric organocatalysis has become a key tool for making bioactive chiral molecules because it uses non-toxic, airand moisture-stable, cheap, and eco-friendly catalysts. L-Proline and their derivatives such as silyl protected diarylprolinols (Hayashi-Jørgensen catalysts), and Macmillan catalysts have been studied in a wide range of organic transformations. However, the catalyst decomposition, higher catalytic loading (usually 20 mol %), and poor regioselectivity are the major challenges associated with the secondary amine organocatalysis. To address these limitations, novel chiral secondary amine organocatalysts were developed in our laboratory.<sup>1,2</sup> In this talk, I would like to discuss the challenges associated with the development of chiral secondary amine organocatalysts and their applications to the asymmetric synthesis of natural products and drugs.



**Figure:** Chiral organocatalysts for the asymmetric synthesis of drugs.

#### References:

- 1. Kumar, R.; Maurya, V.; Avinash, A.; Appayee, C. J. Org. Chem. 2024, 89, 8586–8600.
- 2. Singh, S.; Kumar, R.; Dubey, N.; Appayee, C. Chem. Commun. 2024, 60, 8768–8771.

#### Gokarneswar Sahoo

Associate Professor, NIT Rourkela



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#### **Education**

Ph.D.: National Chemical Laboratory, Pune

M Sc.: Utkal University

# Career

Associate Professor (2023-Present): NIT Rourkela Assistant Professor (2016-2023): NIT Rourkela

Post-Doctoral (2014-2016): Tekniikan edistämiskeskus (TEKES), Finland

(2011-2013): Academy of Finland

Research Associate (2008-2010): Sai Advantium Pharma Ltd

# Area of Research

- Organocatalysis
- Carbohydrate Chemistry
- Natural Product synthesis
- Mechanistic Interpretation

# **Awards & Honors**

2023- Life Member- Chemical Research Society of India (CRSI)

2023- Patron Member- Orissa Chemical Society (OCS)

2018 & 2019- Executive Member- Orissa Chemical Society (OCS)

**2017-** Prof. R. C. Tripathy young scientist award (Orissa Chemical Society)

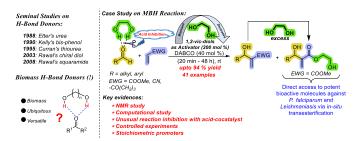
2016- Life Member- Orissa Chemical Society (OCS)

# Vicinal Diols as Potentially Greener H-Bond Donors: Application to an Accelerated MBH Protocol

#### Gokarneswar Sahoo

Department of Chemistry, NIT Rourkela, Rourkela-769008, Odisha

**Abstract:** Herein, the concept of bio-based vicinal diols as an alternative H-bond donor, is presented. Spectroscopic study revealed superior electrophilic enhancement by ethylene glycol in comparison to other H-bond donors, duly supported by computational studies. As a case study, controlled experiments confirmed the superior activation by 1,2-diols over mono-ols, diol regiomers and other H-bond donors in Morita-Baylis-Hillman reaction. Acid co-catalysts, functioning as competing promoters, significantly modulate the H-bonding capacity of the diol promoter through the protonation of electrophilic precursors, thereby effectively diminishing the intricate H-bond interactions involved in the catalytic process. As a practical application of this concept, a thorough investigation and optimisation were carried out as an integrated strategy to mitigate the sluggishness of sp2-C electrophiles, particularly aliphatic aldehydes, in MBH reactions with various pro-nucleophiles. The sluggishness of the aliphatic aldehydes w. r. to aromatic aldehydes has been assigned to the easy formation of amine-trapping side reactions. An extended work built upon the concept dealt with the facile synthesis of molecular-hybridised MBH adducts using known bioactive phenesins as promoters derived from the biomass waste glycerol. Since, both the reacting coupling partners in this case have been proven to be biologically potent, the hybridised MBH adduct are anticipated to exhibit a culminated effect of the active sites/functional groups derived from the reactants. The study also provides a valuable route for the effective valorization of glycerol, a surplus biowaste towards pharmacologically important adducts.



**Keywords:** Vicinal Diol, Dual H-Bond Donor, MBH Reaction, Acid-inhibition, Sustainable Catalysis.

#### References and Notes:

- Preprint at S. Mandal, J. Panda, V. K. Mishra, G. Sahoo, ChemRxiv, 2025 [DOI: 10.26434/chemrxiv-2025-pck4k].
- 2. V. Korpelin, G. Sahoo, R. Ikonen, K, Honkala, J. Catal. 2023, 422, 12-23.
- 3. J. Sahoo, J. Panda, S. Giri, G. Sahoo, J. Org. Chem. 2023, 88 (14), 10147-10155.
- 4. J. Panda, J. Sahoo, J. Dutta, H. S. Biswal, G. Sahoo, Chem.-A Eur. J. 2023, 29 (45), e202300675.

# Harekrushna Sahoo

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# **Education**

Ph.D.: Jacobs University Bremen, Bremen (Germany).

M.Sc.: Utkal University.

#### Career

Associate Professor (2020 - Present): NIT Rourkela.

Assistant Professor (2012-2020): NIT Rourkela.

Postdoctoral (2012-2012): Max-Bergmann Center, Dresden (Germany).

(2010-2011): Technical University Dresden, Dresden (Germany) (2007-2009): UMASS-Amherst, Massachusetts (USA).

# **Area of Research**

- Biophysical chemistry (Peptide and protein folding & extracellular matrix), Ionic Liquids, and Environmental Chemistry
- Nanobiophysical Chemistry

# Awards & Honors

2025: International Resource Person (Qingdao, China)

2023: Ulam fellowship (NAWA, Poland), Fellow: IUPAC, FASc, FNA.

**2022:** ICMR-DHR international fellowship (ICMR, India)

2021: Research Stay Program (DAAD, Germany)

**2018:** Material Resources Program (DAAD, Germany)

# Impact of Micro- and Macro-Environment on Protein Conformation and Dynamics

#### Harekrushna Sahoo

Biophysical and Protein Chemistry Lab, Department of Chemistry, NIT Rourkela, Rourkela-769008, Odisha

**Abstract:** *In vivo* protein folding occurs within the highly crowded and chemically complex cytoplasmic environment, unlike the dilute buffer conditions typically employed in vitro. This dense milieu significantly influences folding pathways, conformational fluctuations, and the stability of folding intermediates. It comprises micro-environmental components, such as inorganic salts, macro-environmental factors like carbohydrates and synthetic polymers, and small-molecule co-solvents including ionic liquids (ILs). Each of these constituents can modulate protein conformations through direct molecular interactions and indirect solvent-mediated effects, thereby altering secondary and tertiary structures, folding intermediates, and kinetic pathways. Understanding these influences is essential for bridging the gap between in vitro and in vivo folding behaviour.

Cellular Retinoic Acid-Binding Protein I (CRABP I) was selected as a model system to probe these effects. To examine the influence of micro-environmental salts, anions (Cl<sup>-</sup>, SO<sub>4</sub><sup>2-</sup>, and HPO<sub>4</sub><sup>2-</sup>) were employed along with macromolecules such as polyethylene glycol and cyclodextrin using optical spectroscopic techniques like fluorescence and circular dichroism (CD) spectroscopy.



#### References:

- 1. PR Hota, DP Behera, and **H Sahoo**, J. Mol. Liq., 2024, 405, 125017
- S. Subadini. K. Bera, J. Hritz, & H. Sahoo, Colloids Surf. B: Interfaces, 2021, 202, 111696
- S. Millan, BC Swain, U Tripathy, PP Mishra, & H. Sahoo, J. Mol. Liq., 2020, 320, 114489
- 4. PR Hota, DP Behera, and **H Sahoo**, J. Ion. Liq., 2025, 5, 100150

# Rajendar Goreti

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# **Education**

**Ph.D.:** IICT Hyderabad **M.Sc.:** Kakatiya University

#### Career

Associate Professor (2024 – Present): IISER-Trivandrum Assistant Professor (2016-2024): IISER-Trivandrum Postdoctoral (2012-2016): Harvard University

# **Area of Research**

- Asymmetric Total Synthesis of Natural Products and Natural Product Analogues.
- Development of New Synthetic Methodologies and Their Application in Organic Synthesis.
- Design and Synthesis of New Ligands and Their Application in Asymmetric Catalysis.

# **Awards & Honors**

2016: Early Career Research Award SERB-Govt of India

2015: Ramanujan Fellowship in Chemical sciences, SERB, Govt of India.

# **Enantioselective Approaches for the Structure Assignment of Abietane Diterpenoids**

# Rajendar Goreti

Indian Institute of Science Education and Research (IISER) Thiruvananthapuram

Abstract: Aromatic abietanes and podocarpanes are important diterpenoids found in various terrestrial plants and are of significant interest in pharmacology due to their diverse biological activities. These compounds typically possess a common [6-6-6] tricyclic 20-carbon framework with an aromatic C-ring, exhibiting distinct oxidation states across the A, B, and C ring systems. Euolutchuols, isolophonthins, nagiol, and ferruginols have been isolated from different plant species, including the roots of Euonymus lutchuensis, the leaves of Isodon lophanthoides var. gerardianus, and Podocarpus nagi. These diterpenoids were synthesized directly through biomimetic cationic polyene cyclization of an epoxy polyene. Various enantio- and diastereoselective oxidation reactions have been employed to generate structurally diverse natural diterpenoids. Different synthetic isomers were prepared and their structures were assigned and revised using NMR spectroscopy and single-crystal X-ray analysis of, providing valuable insights into the structural features of these bioactive compounds.

#### Reference:

- (a) González, M. A. Eur. J. Med. Chem. 2014, 87, 834–842; (b) Kang, J.; Quynh Le, T.; Oh, C. H. Tetrahedron Lett. 2022, 108, 154133; (c) Wang, Y.-D.; Zhang, G.-J.; Qu, J.; Li, Y.-H.; Jiang, J.-D.; Liu, Y.-B.; Ma, S.-G.; Li, Y.; Lv, H.-N.; Yu, S.-S. J. Nat. Prod. 2013, 76 (10), 1976–1983; (d) Okasaka, M.; Takaishi, Y.; Kashiwada, Y.; Kodzhimatov, O. K.; Ashurmetov, O.; Lin, A. J.; Consentino, L. M.; Lee, K.-H. Phytochemistry 2006, 67 (24), 2635–2640.
- (a) Reyno, R. S.; Surendran, S.; James, G.; Rajendar, G. Eur J Org Chem 2023, 26 (43), e202300748; (b) Rajendar, G.; Corey, E. J. J. Am. Chem. Soc. 2015, 137 (17), 5837–5844; (c) Sravya Surendran, Chandrendu K. C., Goreti Rajendar J. Nat. Prod. 2025, 88, 2, 502–512. (d) Surendran, S., Ramachandran, A., and Rajendar, G., Org. Biomol. Chem., 2025, 23, 6924-6930 (e) Surendran, S., Chandrendu K.C., Reyno, R. S., Rajendar, G., "A Concise Approach to Enantioselective Synthesis of Euolutchuols A, B, and D and Their Structure Assignment (Revisions).

# Priyabrata Dash

Professor, NIT Rourkela



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# **Education**

Ph.D.: University of Saskatchewan, Canada

M.Sc.: Utkal University

#### Career

Professor (2020 - Present): NIT Rourkela

**Associate Professor** (2018 – 2023): NIT Rourkela. **Assistant Professor** (2011-2018): NIT Rourkela.

Postdoctoral (2010-2011): University of Ottawa, Canada

# **Area of Research**

- Nanocatalysis
- Photocatalysis
- Gas sensing
- Toxic ion removal

# **Awards & Honors**

**2018:** Prof. R. C. Tripathy Young Scientist Award in Chemical Science by Odisha Chemical Society

**2018:** Applied Surface Science Certificate of Outstanding Contributions in Reviewing

# Heterogeneous Photocatalysis towards Sustainable Synthesis

# Priyabrata Dash

Nanochemistry Laboratory, Dept. of Chemistry, NIT Rourkela, Odisha-769008

**Abstract:** Heterogeneous photocatalysis based on modified g-C<sub>3</sub>N<sub>4</sub> coupled with non-noble bimetallic alloy nanoparticles presents a promising route for visible-light-driven catalytic processes. In this talk, three tailored photocatalyst systems are going to be discussed and presented for various catalytic reactions.<sup>1-3</sup> For example, h-BN doped g-C<sub>3</sub>N<sub>4</sub> (h-BN/ g-C<sub>3</sub>N<sub>4</sub>) decorated with CuNi nanoparticles for enhanced H<sub>2</sub> evolution, citric-acidfunctionalized g-C<sub>3</sub>N<sub>4</sub> (CGCN) supported with CuCo nanoparticles for efficient H<sub>2</sub> production and CO<sub>2</sub> reduction to methanol and ethanol and Zndoped g-C<sub>3</sub>N<sub>4</sub> (ZCN) loaded with CoNi nanoparticles for H<sub>2</sub> generation and photocatalytic transfer hydrogenation of styrene. The rational modification of g-C<sub>3</sub>N<sub>4</sub> through h- BN doping, citric-acid functionalization and Zn incorporation significantly improved charge separation, metal dispersion, and interfacial electronic coupling, leading to superior photocatalytic performance across all systems. To establish the structure-activity relationships, advanced X-ray absorption spectroscopy (XAS) techniques (EXAFS and XANES) were utilized. Overall, the combined catalytic and spectroscopic insights demonstrated that support engineering, together with bimetallic synergy, plays a critical role in tuning adsorption energetics and directing reaction pathways. This study offers a comprehensive design framework for developing next- generation CuCo, CuNi, and CoNi alloybased nanocatalysts for sustainable H<sub>2</sub> production, CO<sub>2</sub> reduction and selective organic transformations.

**Keywords:** Heterogeneous photocatalysis, g-C<sub>3</sub>N<sub>4</sub>, non-noble, bimetallic alloy nanoparticle, XAS.

#### References

- 5. P. Dash *et al*, **2025**. (submitted)
- 6. P. Dash et al, ACS Appl. Mater. Interfaces, **2024**, 16 (50), 69333.
- 7. P. Dash et al, Ind. Engg. Chem. Res., 2024, 63(18), 8054.

# Satpal Singh Badsara

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# **Education**

**Ph.D.:** University of Hyderabad **M.Sc.:** Banaras Hindu University

#### Career

Associate Professor (2024 - Present): Banaras Hindu University

Assistant Professor (2014-2024): University of Rajasthan.

Postdoctoral (2013-2014): National Chung Hsing University, Taichung,

Taiwan

# Area of Research

• Electro-Organic Synthesis

Green and Sustainable Approaches for Organic Synthesis

# **Awards & Honors**

2025: Bronze Medal Award by 'Chemical Research Society of India (CRSI)

2025: MNASc Award by 'The National Academy of Sciences, India (NASI)

**2019:** ISCB Young Scientist in Chemical Sciences Award by Indian Society of Chemists and Biologists, India

**2019:** Member (MRSc) Award by 'Royal Society of Chemistry

2015: DST INSPIRE Faculty Award by Department of Science &

Technology, Government of India

# Site-Selective Electrochemical Functionalization of Indolizine Frameworks Enabled by N-Centered Radical Translocation

# Satpal Singh Badsara

MFOS Laboratory, Department of Chemistry, Institute of Science, Banaras Hindu University (BHU), Varanasi, Uttar Pradesh, India.

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

#### References

- (a) Wang, Y.; Dana, S.; Long, H.; Xu, Y.; Li, Y; Kaplaneris, N.; Ackermann, L. Chem. Rev. 2023, 123, 11269-11335. (b) Kingston, C.; Palkowitz, M. D.; Takahira, Y.; Vantourout, J. C.; Peters, B. K.; Kawamata, Y.; Baran, P. S. Acc. Chem. Res. 2020, 53, 72-83. (c) Badsara, S. S.; Ucheniya, K.; Chouhan, A.; Gurjar, A. Chem. Rec. 2025, 00, e202500092. (d) Jat, B; Yadav, D. K.; Badsara, S. S.; Sharma, S. Org. Biomol. Chem. 2025, 23, 4846-4854.
- (a) Jat, P. K.; Badsara, S. S. J. Org. Chem. 2024, 89, 12263-12276. (b) Ucheniya, K.; Jat, P. K.; Chouhan, A.; Yadav, L.; Badsara, S. S. Org. Biomol. Chem., 2024, 22, 3220-3224. (c) Jat, P. K.; Yadav, L.; Chouhan, A.; Ucheniya, K.; S. S. Badsara, Chem. Commun., 2023, 59, 5415-5418. (d) Chouhan, A.; Ucheniya, K.; Yadav, L.; Jat, P. K.; Gurjar, A.; Badsara, S. S. Org. Biomol. Chem., 2023, 21, 7643-7653. (e) Jat, P. K.; Dabaria, K.; Bai, R.; Yadav, L.; Badsara, S. S. J. Org. Chem., 2022, 87, 12975-12985.

# Malay Kumar Rana

Associate Professor, IISER Berhampur



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Education

Ph.D.: IIT Kanpur

M.Sc.: University of Delhi.

#### Career

**Associate Professor** (2024 – Present): IISER Berhampur **Assistant Professor** (2017-2024): IISER Berhampur

Visiting Assistant Professor (2016-2017): IISER Berhampur

Senior Scientific Officer (2015-2016): IIT Kanpur Postdoctoral (2011-2014): University of Michigan, USA (2010-2011): University of Sassari, Italy

# Area of Research

• Development of effective therapeutics for COVID-19, cancer, and bacterial infections, including studies on porous, crystalline nanomaterials and 2D materials for applications in optoelectronics, sensing, gas separation, and energy storage. State-of-the-art computational methods and complementary experiments are used.

#### **Awards & Honors**

2015: DST Inspire Faculty Award

# Integrated Artificial Intelligence (AI)-Molecular Dynamics (MD) Approach for Drug Discovery to Overcome Chemoresistance in Triple Negative Breast Cancer

# Malay Kumar Rana

Department of Chemical Sciences, IISER Berhampur

Abstract: Triple-negative breast cancer (TNBC) is one of the aggressive subtypes of breast cancer and depends largely on chemotherapy for treatment. However, high recurrence and chemoresistance prevail in TNBC patients, highlighting an urgent need for novel molecular targets and effective discovery pipelines [1]. Emerging evidence suggests that TNBC cells develop chemoresistance through metabolic reprogramming, primarily by de novo nucleotide biosynthesis. Inosine-5'-monophosphate dehydrogenase 2 (IMPDH2), the rate-limiting enzyme of GTP synthesis, is overexpressed in TNBC and controls the enhanced cell proliferation and chemoresistance [2]. Although IMPDH2 has emerged as a promising metabolic vulnerability in recent times, it still lacks a potent inhibitor. Static models, used in conventional drug discovery approaches, fail to capture ligand stability or prolonged stay in the catalytic pocket, underscoring the need for more advanced computational strategies.

To address this, we developed an artificial intelligence (AI)-driven and molecular dynamics (MD)–guided framework [3] to identify potent natural-product-based IMPDH2 inhibitors. Machine learning (ML) models, trained on IC50-annotated ChEMBL datasets, were utilized for activity prediction. High-confidence hits were subjected to ADMET filtering, structure-based docking, extensive MD simulations, and  $\tau$ -RAMD analysis. Among all candidates, MOL3 outperformed the reference inhibitor, Ribavirin Monophosphate, by exhibiting stronger catalytic-site engagement, better stability, and a longer residence time within the protein's catalytic pocket. The novelty of the work lies in the integration of AI-driven QSAR with multiscale MD and  $\tau$ -RAMD simulations to discover natural IMPDH2 inhibitors capable of overcoming chemoresistance by disrupting guanine nucleotide synthesis in TNBC. This framework provides a robust and scalable strategy for accelerating target-focused drug discovery. **References:** 

- Bianchini, G., Balko, J. M., Mayer, I. A., Sanders, M. E., & Gianni, L. (2016). Triplenegative breast cancer: challenges and opportunities of a heterogeneous disease. *Nature Reviews Clinical Oncology*, 13(11), 674–690. https://doi.org/10.1038/nrclinonc.2016.66
- Da Silva Fernandes, T., Gillard, B. M., Dai, T., Martin, J. C., Chaudhry, K. A., Dugas, S. M., Fisher, A. A., Sharma, P., Wu, R., Attwood, K. M., Dasgupta, S., Takabe, K., Rosario, S. R., & Bianchi-Smiraglia, A. (2025). Inosine monophosphate dehydrogenase 2 (IMPDH2) modulates response to therapy and chemo-resistance in triple negative breast cancer. *Scientific Reports*, 15(1), 1061. https://doi.org/10.1038/s41598-024-85094-5
- Shree, A., Pani, P., & Rana, M. K. (2025). A robust ensemble machine learning approach for inhibitor discovery: Case study of HIV-1 NNRTI and validation using MD simulation. *Chemistry – An Asian Journal*, e70340. https://doi.org/10.1002/asia.70340

# Nagendra Sharma

Associate Professor, NISER Bhubaneswar



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# **Education**

Ph.D.: CSIR-NCL Pune & University Of Pune

M.Sc.: Delhi University.

# Career

Associate Professor (2012 - Present): NISER Bhubaneswar

Visiting Faculty (2009-2012): NISER Bhubaneswar

Postdoctoral (2006-2009): University of Utah, Salt Lake City, Utah (USA)

# Area of Research

 Chemical synthesis of biomolecules (Amino acid and Nucleic Acid DNA/RNA)

# Tropolone Beyond Natural Products: A Unique Scaffold for Biomolecular Design

# Nagendra Sharma

School of Chemical Sciences, NISER Bhubaneswar, Odisha, India

Abstract: Tropolone, a non-benzenoid aromatic molecule, is a key constituent of troponoid natural products.[1] It displays unique photophysical properties and a strong affinity for transition metals such as Cu(II), Ni(II), and Zn(II).[2] Several of its derivatives, including colchicine and aminotropones, exhibit remarkable biological activities such as antimicrobial and anticancer effects.[3] By contrast, the aromatic scaffolds of native biomacromolecules (DNA, RNA, and proteins) are exclusively benzenoid in origin, where they play a fundamental role in stabilizing secondary structures through hydrogen bonding and  $\pi$ - $\pi$  stacking interactions.4 Incorporating tropolone into biomolecular frameworks offers an exciting opportunity to explore new structural and functional dimensions. Recently, we have synthesized and studied *troponyl*-modified DNA and peptides, which display distinctive structural, physicochemical, and biochemical behaviors.[4] These findings highlight the potential of tropolone-based biomacromolecules as structural analogues capable of fine-tuning native architectures and biological functions through minimal modifications.



#### Reference:

- a) R. Bentley, Nat. Prod. Rep. 2008, 25, 118-138; b) H. Guo, D. Roman and C. Beemelmanns, Nat. Prod. Rep. 2019, 36, 1137-1155.
- 2. B. E. Bryant, W. C. Fernelius and B. E. Douglas, *Nature* **1952**, 170, 247-248.
- a) M. Dewar, Nature 1945, 155, 141-142; b) T. Nozoe, Nature 1951, 167, 1055-1057;
   c) A. Kumar, P. R. Sharma and D. M. Mondhe, Anti-can. drugs 2017, 28, 250-262.
- a) C. Balachandra and N. K. Sharma, Org. Lett. 2015, 17, 3948-3951; b) A. Bollu and N. K. Sharma, ChemBioChem 2019, 20, 1467-1475; c) C. K. Jena and N. K. Sharma, Chem. Commun. 2022, 58, 8077-8080; d) M. K. Gupta and N. K. Sharma, Org. Biomol. Chem. 2022, 20, 9397-9407; e) S. S. Nayak, A. Patnaik, C. K. Jena and N. K. Sharma, Org. Lett. 2025 (ASAP).

# Thirupathi Barla

Associate Professor, IISER Berhampur



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#### Education

Ph.D.: CSIR-Indian Institute of Chemical Technology, Hyderabad

M.Sc.: Osmania University.

# Career

Associate Professor (2024 - Present): IISER Berhampur.

Assistant Professor (2018-2024): IISER Berhampur.

Associate Research Scientist (2014-2015): Sai Life Sciences, Hyderabad,

India

Postdoctoral (2015-2018): Harvard University, USA

#### Area of Research

- Organic Synthesis
- Total Synthesis of Natural Products
- Aryne Chemistry
- Asymmetric Synthesis

# **Awards & Honors**

2025: Life Member of Chemical Research Society of India

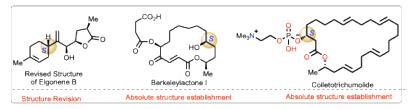
2024: Associated Fellow of Telangana Academy of Sciences

2023: Thieme Chemistry Journal Award

# Total Synthesis: A Critical Tool for the Structural Reassignment of Natural Products

# Thirupathi Barla

Department of Chemical Sciences, IISER Berhampur, Odisha-760010, India



Natural products continue to be the most promising possibilities for drug discovery and development for a variety of human diseases. A majority of FDA-approved drugs between 1981 to 2019 were inspired by natural products or synthetic molecules based on natural product pharmacophores. Determining the absolute configuration is essential, and one of the critical challenges in the field of medicinal chemistry, as it plays a crucial role in drug discovery and development. As part of an ongoing research programme in the total synthesis of natural products in our laboratory, we have revised the absolute configuration of elgonenes, berkeleylactone, and colletotrichumolide via total synthesis.

#### References

- Atanasov, A.G., Zotchev, S.B., Dirsch, V.M. et al. Natural products in drug discovery: advances and opportunities. Nat. Rev. Drug Discov. 20, 200-216.
- 2. D. J. Newman and G. M. Cragg, J. Nat. Pro., 2020, 83, 770-803.
- 3. (a) Mandal, S.; Mahananda, D.; Dey, S.; Bharathavikru, R. S.; Thirupathi, B. *Journal of Natural Products* **2024**, *87*, 152-159.; (b) Mandal, S.; Thirupathi, B. *Org. Biomol. Chem.*, **2022**, *20*, 3922-3929.
- Mandal, S.; Mahananda, D.; Paladugu, D.; Thirupathi, B. J. Org. Chem. 2024, 89, 4165-4175.
- Mandal, S.; Kundu, S.; Ginopragathish, B.; Neelam, Chakrabarty, A.;
   Moitra, P.; Thirupathi, B. J. Org. Chem., 2025, 90, 7902–7909.

**Keywords:** (Total synthesis, macrolide, absolute configuration, natural products).

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# **Education**

Ph.D.: IISc Bangalore

M.Sc.: University Of Madras.

#### Career

Professor (2024 - Present): IISER Tirupati.

Associate Professor (2019-2024): NISER Bhubaneswar.

Reader (2015-2019): NISER Bhubaneswar. Assistant Professor (2010-2015): IIT Mandi

Postdoctoral (2009-2009): Yale University, New Haven, USA

(2007-2008): Duquesne University, Pittsburgh, USA

# **Area of Research**

- oxidatively cleaving carbon-carbon bonds in strained organic molecules.
- C-H bond activation using transition metal catalysts.
- Application of bioactive heterocyclic core structures and valuable organic scaffolds.
- Novel strategies for functionalizing arenes and heteroarenes.

#### **Awards & Honors**

**2024:** Member, Editorial Advisory Board, The Journal of Organic Chemistry.

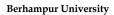
2024: Member, Editorial Advisory Board, ACS Catalysis.

**2023:** Recognized as Pioneering Investigator by the RSC journal Chem Comm.

**2023:** Chemical Research Society of India (CRSI) Bronze medal for significant contribution to Research in Chemistry

2020: Ranked as the top 3% highly cited ACS author from India

**2013:** Received teaching excellence award as well as foundation day awards for institute service while serving at IIT Mandi.



# Weak Chelation Assisted C-H Functionalization using Cobalt Catalyst:

#### A Sustainable Approach

#### Ponneri C. Ravikumar

Indian Institute of Science Education and Research (IISER) Tirupati Sreenivasapuram, Yerpedu, Andhra Pradesh 517619

**Abstract:** During the last century, direct functionalization of inert bonds such as C-C and C-H has been ignored due to their high bond strength and inertness. Since the beginning of the 21st century, there has been renewed interest in functionalizing these inert bonds through metal catalysts to synthesize many useful organic molecules. In this talk, I will briefly introduce sustainable C-H activation reaction and our work using cobalt catalysts, through weak chelation. Over the years we have developed, transformations such as C-H alkylation, alkenylation, and annulation reactions. In this talk, I will specifically talk about the synthesis of C-4 substituted indole acyloins through weak chelation, wherein the in-situ generation of water from trifluoroethanol is the key process that helps in the synthesis of acyloins. Several mechanistic and control studies support the proposed catalytic cycle. If time permits, I will also briefly cover the work we have done with regard to C-C bond functionalization using three-membered strained molecules. **Keywords:** Heterocycles, Metal salts, Hypervalent iodine reagents, Dearommatization.

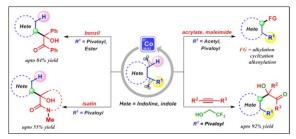


Figure: Cobalt catalyzed C-H bond functionalization of organic motifs.

#### References:

- 1. S. K. Banjare, T. Nanda, B. Vedvyas Pati, G. K. Das Adhikari, J. Dutta, and P. C. Ravikumar ACS Catal. 2021, 18, 11579.
- 2. S. K. Banjare, Rajesh Chebolu, and P. C. Ravikumar. Org. Lett. 2019, 21, 4049.
- 3. T. Nanda, S. K. Banjare, W-Y. Kong, W. Guo, P. Biswal, L. Gupta, A. Linda, B. V. Pati, S. R. Mohanty, D.J. Tantillo and P. C. Ravikumar *ACS Catal.* 2022, **12**, 11651.
- 4. T. Nanda, M. Fastheem, A. Linda, B. V. Pati, S. K. Banjare, P. Biswal and P. C. Ravikumar, ACS Catal. 2022, 12, 13247.
- B. V. Pati, A. Ghosh, K. Yadav, S. K. Banjare, S. Pandey, U. Lourderaj, and P. C. Ravikumar, Chem. Sci. 2022, 13, 2692.

# Alakesh Bisai

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#### Education

**Ph.D.:** IIT Kanpur. **M.Sc.:** BHU, Varanasi.

#### Career

Professor (2020 - till date): Dept. of Chemical Science, IISER Kolkata.

Professor (2018 - 2020): Dept. of Chemistry, IISER Bhopal.

**Associate Professor** (2013 - 2018): Dept. of Chemistry, IISER Bhopal. **Assistant Professor** (2009 - 2013): Dept. of Chemistry, IISER Bhopal. **Postdoctoral** (2006 - 2009): University of California Berkeley, USA.

# **Area of Research**

**a)** Strategy & Tactics for the Total Synthesis of Natural Products of Biological Relevance.

b) Nature-Inspired Strategies.

#### **Awards & Honors**

2026: C. N. R. Rao National Prize in Chemical Science (CRSI)

**2025:** DST Advanced Materials Research Grant (*erstwhile* DST Nano-Mission)

2024: Fellow, The National Academy of Sciences (NASI), (FNASc, 2024)

2023: Elected Fellow, RSC.

**2023:** Prof. A. Srikrishna Memorial Lecture, UoH. **2022:** CDRI Award for Excellence in Drug Research.

2021: Prof. D. Nasipuri Memorial Award.

**2021:** CRS Silver Medal.

2021: SERB Star Award.

2020: CRSI Bronze Medal.

2018: Young Scientist Award by CRSI, India.

**2016:** Lead Lecture at Pfizer Symposium from IISc Bangalore.

2013: Young Scientist Award by SERB, DST, India.

2011: Young Scientist Award by BRNS-DAE.



# **Total Synthesis of Natural Products of Biological Relevance**

#### Alakesh Bisai

Department of Chemical Sciences, IISER Kolkata, Mohanpur, WB, INDIA

**Abstract:** The natural product chemical diversity is more closely aligned with drugs than synthetic libraries, thus making them ideal candidates for drug discovery projects. 1a-b Marine organisms can be considered the most recent source of bioactive natural products in relation to terrestrial plants and nonmarine microorganisms. 2a-c The beauty of Nature is that she produces a variety of complex natural products in entioenriched form (Figure). 3-4 In the above context, naturally occurring alkaloids with impressive diversity of biological activities drew our interest for the development of bio-inspired strategies. 5-6 Towards this, we explored Nature-Inspired strategies that will be discussed in this talk.

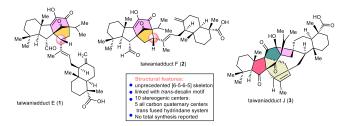


Figure. Architecturally intriguing secondary metabolites of biological relevance.

#### References and Notes:

- 1. (a) C. Jiménez ACS Med. Chem. Lett. 2018, 9, 959 (Marine Products in Medicinal Chemistry). (b) M. Munda, R. Nandi, S. Kundu, V. R. Gavit, S. Niyogi, A. Bisai Chem. Sci. 2022, 13, 11666.
- 2. (a) R. Nandi, S. Niyogi, S. Kundu, V. R. Gavit, M. Munda, A. Bisai *Chem. Sci.* **2023**, *14*, 8047. (b) S. Niyogi, A. Mondal, M. Nandy, A. Bisai, *Org. Lett.* **2024**, *26*, 8643. (c) M. Munda, A. Mondal, N. K. Roy, R. Murmu, S. Niyogi, A. Bisai *Chem. Sci.* **2024**, *15*, 9164.
- 3. (a) R. Murmu, S. Kundu, M. Majhi, S. Pal, A. Mondal, A. Bisai, *Chem. Commun.* **2024**, *60*, 9737. (b) M. Nandy, A. Das, S. Niyogi, A. Khatua, D. Jana, A. Bisai, *Org. Lett.* **2024**, *26*, 1531.
- 4. (a) S. Kundu, D. Jana, N. Mandal, A, Mondal, A. Dutta, A. Bisai *Chem. Sci.* **2024**, *15*, 14946. (b) S. Pal, S. Majumder, P. Shyamal, D. Mondal, B. Das, A. Bisai *Chem. Sci.* **2024**, *15*, 19851. (c) D. Jana, A. Khatua, S. Noskar, M. Nandy, A. Bisai *JACS Au* **2025**, *5*, 1376-1381.
- 5. (a) N. K. Roy, R. Murmu, M. Munda, S. Niyogi, A. Bisai, *Chem. Commun.* **2025**, *61*, 11053. (b) A. Mondal, A. Mondal, T. Roy, A. Bisai, *Org. Lett.* **2025**, *27*, 6878.
- (a) R. Nandi, R. Murmu, S. Sadhukhan, D. Pal, S. Biswas, B. Das, A. Bisai, Org. Lett. 2025, 27, 1531.
   (b) K. Shaw, A. Roy, D. Mondal, P. Shyamal, A. Khatua, A. Bisai, Chem. Commun. 2025, 61, 12944.
   (c) N. K. Roy, R. Murmu, M. Majhi, S. Biswas, A. Bisai, Org. Lett. 2025, 27, 9281.

#### Related Publications:

Chem. Sci. 2022, 13, 11666; Chem. Commun. 2022, 58, 3929; Chem. Sci. 2023, 14, 8047; ACS Catal. 2023, 13, 2118; Chem. Commun. 2024, 60, 9737; Chem. Sci. 2024, 15, 9164; Org. Lett. 2024, 26, 8643; Chem. Sci. 2024, 15, 14946; Org. Lett. 2024, 26, 10803; Chem. Sci. 2024, 15, 19851; Chem. Commun. 2025, 61, 11053; Org. Lett. 2025, 27, 1531; JACS Au, 2025, 5, 1376; Chem. Commun. 2025, 61, 12944.

# Adinarayana Doddi

Associate Professor, IISER Berhampur



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#### **Education**

Ph.D.: Ruhr-University Bochum, Germany

M.Sc.: IIT Madras.

#### Career

Associate Professor (2025 - Present): IISER Berhampur.

Assistant Professor (2019-2025): IISER Berhampur.

Sub-Group Leader (2017-19): TU Braunschweig, Germany

Postdoctoral (2013-2017): Technical University Braunschweig, Germany

# Area of Research

- Main Group and Organometallic Synthesis
- Sustainable Homogeneous Catalysis
- Frustrated Lewis Acid Base Pairs/Applications in Expensive Metal Free Catalysis
- Designing of new Ligand Scaffolds/Cooperative Catalytic Applications of Bimetallic Complexes
- Structure & Bonding Aspects of Metal-Metal Bonded Species of MGs and TMs

# **Awards & Honors**

2025: Life Member of Chemical Research Society of India

**2019:** Ramanujan Fellowship by SERB, Department of Science and Technology, Government of India.

# Novel Ancillary Ligands: Bridging Metal-Free and Metal-Based Approaches in Homogeneous Catalysis

# Adinarayana Doddi

Department of Chemical Sciences, IISER Berhampur, Odisha, India

**Abstract:** In recent times, widespread attention has been devoted towards the isolation of main group element consisting species such as silyl phosphines and NHO supported P(III) compounds, these are in fact stereo-electronically tuned phosphorus compounds.[1-3]Stereo- electronically tuned ligands play crucial role not only for the isolation of various novel, and unusual main-group, organometallic fragments, but also find widespread utility as ancillary ligands in homogeneous catalytic transformations. Phosphine ligands featuring group 13/14 elements supported pincer type ligands have been explored [1-3] but their mono- dentate counterparts have not been studied in organometallic synthesis and in homogeneous catalysis. Among this class of species, the silyl (SiR3) groups functionalized phosphines would offer new reactivity aspects as these are sterically, and electronically tuned reactive species. We have recently introduced N-heterocyclic olefin phosphines namely "NHOPs" as potential systems for stabilization of interesting organometallic species and found to be useful in the small molecule (CE2; E = O,S) activation reactions. Carbon dioxide was continently converted to various N-formylated, and cyclic products under metal free conditions. The silylphosphines with Si-H bonds were treated with various Ru and Pd metal precursors and isolated the corresponding Ru(II) and Pd(II) complexes. In the latter case, Pd(II) insertions into the Si-H bonds were observed to give palladium-silicon bonded species, however, the corresponding reactions with R2PSiMe3 afforded P-coordinated complexes, indicating the superior use of Si-H species over Si-R (R = aryl, phenyl) species in organometallic synthesis. <sup>5,6]</sup> Furthermore, we have isolated a series of electronic rich neutral, and cationic phosphorus (III) species featuring N-heterocyclic olefins, and subsequently used for the isolation of a series of half-sandwich ruthenium-complexes.[4] The details of isolation, structural and catalytic studies will be discussed in this presentation.

#### Reference

- 1. P. Gualco, S. Ladeira, K. Miqueu, A. Amgoune and D. Bourissou, Angew. Chem., Int. Ed., 2011, 50, 8320-8324.
- 2. Doddi, M. Peters, M. Tamm, Chem. Rev. 2019, 119, 6994.
- 3. A. K. Sahoo, A. K. Sahoo, B. Das, S. J. Panda, C. S. Purohit, and A. Doddi, Dalton Trans., 2023, 52, 15549-15561.
- 4. K. Sahoo, B. Das, S. J. Panda, C. S. Purohit, and A. Doddi, Adv. Synth. Catal. 2024, 366, 2468–2476.
- 5. B. Das, A. K. Sahoo, S. K. Banjare, S. J. Panda, C. S. Purohit, and A. Doddi., ChemPlusChem. 2024, e202400623.
- 6. K. Sahoo, R. Dash, S. K. Agrawalla, C. S. Purohit, A. Doddi, Dalton Trans., 2025, accepted.

# Parikshit Moitra

Assistant Professor, IISER Berhampur



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# **Education**

**Ph.D.:** IISc Bangalore **M.Sc.:** IISc Bangalore

#### Career

Assistant Professor (2024 - Present): IISER Berhampur.

**Assistant Research Professor** (2022-2024): Pennsylvania State University, University Park, Pennsylvania, USA

**Research Associate** (2020-2022): University of Maryland Baltimore School of Medicine, Maryland, USA

**Postdoctoral** (2019-2020): University of Maryland Baltimore School of Medicine, Maryland, USA

**Scientist D** (2017-2019): Indian Association for the Cultivation of Science, Kolkata, West Bengal

**Research Associate** (2016-2017): Indian Association for the Cultivation of Science, Kolkata, West Bengal

#### Area of Research

- Programmable Nanoparticles for Selective Sensing of Genetic Diseases
- Advanced Non-Viral Systems for Image Guided Therapeutics

#### Awards & Honors

2025: Member of the Royal Society of Chemistry (MRSC)

2025: Life Member, Materials Research Society of India (MRSI)

2023: Received Young Researcher Award

2017: Received Gandhian Young Technological Innovation (GYTI) Award

# Development of Novel Nanomaterials for Molecular Diagnosis of Certain Rare Genetic Disorders

#### Parikshit Moitra

IISER Berhampur, Odisha, India

Abstract: We are developing new nanomaterials and conjugating them with suitably tuned complementary oligonucleotides targeting certain rare genetic diseases. These oligonucleotides are chosen based on their target binding energy and binding site disruption energy. The oligonucleotide-conjugated nanomaterials were characterized by various analytical techniques including UV-visible spectroscopy, fluorescence spectroscopy, X-ray diffraction, Raman spectroscopy, scanning electron and transmission electron microscopy. These nanomaterials are then used for molecular diagnosis of certain rare genetic disorders, namely Turner syndrome and rare blood genotypes. Changes in spectroscopic and/or electrochemical data were recorded to selectively detect the presence of targeted genetic material. In this talk, I shall be presenting the efforts being undertaken in my laboratory over the last year.

**Keywords:** Covalent Organic Framework; Gold Nanoparticles; Complementary Oligonucleotides; Clinical Diagnosis, Rare Genetic Disorders.

#### References:

- Rijo Rajeev, Paresh Mohanty, Suvro Sankha Datta, Parikshit Moitra\*. Recent Advances in Point-of-Care Testing Devices for Transfusion Medicine. TrAC Trends in Analytical Chemistry 2026, 194, 118490. DOI: https://doi.org/10.1016/j.trac.2025.118490.
- Rijo Rajeev, Paresh Mohanty, Suvro Sankha Datta, Parikshit Moitra\*. Improving transfusion medicine in resource-limited settings by point-of-care diagnostics.
   Nature Reviews Bioengineering 2025, 3, 718–720. DOI: https://doi.org/10.1038/s44222-025-00331-4.
- Neethu KM, Shyamal Karmakar, Baishakhi Sahoo, Navniet Mishrra, Parikshit Moitra\*. Use of Quantum Dots as Nanotheranostic Agents: Emerging Applications in Rare Genetic Diseases. Small 2025, 21, 2407353. DOI: https://doi.org/10.1002/smll.202407353

# **Prosenjit Daw**

Assistant Professor, IISER Berhampur



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# **Education**

**Ph.D.:** IIT Kanpur **M.Sc.:** IIT Kanpur

#### Career

**Associate Professor** (2025 – Present): IISER Berhampur **Assistant Professor** (2019-2025): IISER Berhampur

Senior Postdoctoral Researcher (2018-2019): Weizmann Institute of Science, Israel.

Postdoctoral (2015-2018): Weizmann Institute of Science, Israel.

# **Area of Research**

- Organometallic Chemistry and Homogeneous Catalysis
- Renewable Green Hydrogen Generation

# **Awards & Honors**

2009: Shyama Prasad Mukherjee Fellowship (SPMF), in chemical science

### Bifunctional Catalysts for Renewable Hydrogen Production

#### Prosenjit Daw

IISER Berhampur, Odisha, India

**Abstract:** The development of a new generation of catalysts is always a demanding goal that mainly operates under energy-efficient, cost-effective, and environment-friendly conditions towards a sustainable system.<sup>1</sup> The conversion of biomass and chemical wastes into useful chemical resources is part of the circular economy, where hydrogen can be produced as a by-product.<sup>2</sup> A robust bifunctional NNN-Ru complex shows an excellent catalytic efficiency for the selective hydrogen production from biomass-derived substrates and plastic wastes under mild reaction conditions.<sup>3-6</sup> A series of stoichiometric control experiments and NMR studies revealed the active participation of functionalized ligands during catalysis and supported a metal-ligand cooperativity pathway as well as a secondary-coordination-sphere hydrogen-bonding interaction for the appropriate substrate orientation at the active center. In line with the circular economy, PET plastic waste derivatives are also utilised as a substrate for producing hydrogen gas with a high turnover number.

**Keywords:** Metal-ligand Cooperativity; Hydrogen Economy; Biomass-derived alcohols; Circular Economy.



#### References

- 1. J. Rana, S. T. Sahoo, P. Daw, Tetrahedron 2021, 132473.
- 2. A. Kumar, P. Daw, D. Milstein, Chem. Rev. 2022, 122, 385-441.
- S. T. Sahoo, A. Mohanty, R. Sharma, P. Daw, Dalton Trans., 2023, 52, 15343.
- 4. S. T. Sahoo, A. Mohanty, R. Sharma, S. R. Rout, R. Dandela, P. Daw, Organometallics 2023, 42, 745–751.
- 5. S. T. Sahoo, A. Sinkua,; P. Daw, RSC Adv., 2024, 14, 37082-37086.
- S. T. Sahoo, G. Kenguva, R. Dandela, P. Daw, ChemCatChem., 2025, e202500508.

## Niranjan Panda

Professor, NIT Rourkela



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#### **Education**

**Ph.D.:** IIT Kharagpur **M.Sc.:** IIT Madras.

#### Career

Professor (2020 - Present): NIT Rourkela

**Associate Professor** (2008 – 2020): NIT Rourkela. **Assistant Professor** (2006-2008): NIT Rourkela.

Postdoctoral (2005-2006): Israel Institute of Technology, Israel

#### **Area of Research**

- Natural product synthesis
- Heterocyclic chemistry
- Heterogeneous catalysis

## Thermally Generated "Cation Pools" and Their Synthetic Applications

#### Niranjan Panda

Professor of Chemistry, Dean-SW, NIT Rourkela, Odisha, India

**Abstract:** Conventionally, carbenium and onium ions are prepared in the presence of nucleophiles due to their instability and transient nature. The nucleophiles that are unstable or inert to the reaction media cannot be used for reaction with the cationic species to access the desired compounds. To overcome these limitations, developing methods for generating organic cations irreversibly in the absence of nucleophiles is essential. The "Cation Pool" method stands out as a reliable strategy to generate and accumulate the reactive cations in solution in the absence of nucleophiles. The cation pool method conventionally involves electrochemical redox process to access cations in the absence of nucleophile. Usually such electrochemical redox process was carried out at low temperature to stabilize the transient cations. Moreover, the generation of halogen and chalcogen cations through electrolysis needs extra care because of their low stability. Our effort in generating and accumulating halogen cations as "cation pools," most importantly by simple heating a mixture of dimethyl sulfoxide (DMSO) and 1,2-dihaloethane (DXE, X = Cl, Br, I), and their use in halogenation reaction. Further, condition-dependent Pummerer-type fragmentation of DMSO-stabilized halogen cations to methyl(methylene)sulfonium ions and chlorodimethylsulfonium ions for synthetic applications was explored.1-5

Keywords: Cation Pools, C-C bond formation, C-heteroatom bond formation

- 1. P. G. Dalai, K. Palit and N. Panda, Adv. Synth. Catal. 2022, 364, 1031-1038.
- 2. K. Palit, N. Sepay, and N. Panda, J. Org. Chem. 2023, 88, 2931.
- 3. P. G. Dalai, and N. Panda, Adv. Synth. Catal. 2022, 364, 3736.
- 4. P. G. Dalai, S. Swain, and N. Panda, J. Org. Chem. 2024, 89, 2599.
- 5. S. Mohapatra, N. Panda, J. Org. Chem. 2025, 90, 13496.

#### Chandrakanta Dash

Assistant Professor, Central University of Rajasthan



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#### **Education**

Ph.D.: IIT Bombay

M.Sc.: Fakir Mohan University

#### Career

Assistant Professor (2014 - Present): Central University of Rajasthan

Research Fellow (2013-2014): Nanyang Technological University (NTU),

Singapore

Postdoctoral (2010-2013): University of Texas at Arlington, Texas, USA

#### **Area of Research**

- Organometallic Chemistry
- Green Synthesis and Catalysis
- Metal-catalyzed Organic synthesis
- C-H bond Functionalization

#### **Awards & Honors**

**2015:** Young scientist award from DST

2013: Selected as an UGC-Assistant Professor under the UGC-Faculty

Recharge Programme

**2009:** CSIR partial travel grants to attend the 238th ACS National meeting and Exposition at Washington DC, USA.

## Transition-Metal-Catalyzed Carbazole Synthesis *via*Intramolecular C-H Amination

#### Chandrakanta Dash

Department of Chemistry, Central University of Rajasthan

**Abstract:** Carbazoles are a crucial class of nitrogen-containing heterocycles that are widely found in natural products, pharmaceuticals, and advanced functional materials.<sup>1</sup> Their broader applications have driven extensive research into their synthesis and functionalization. Among these, transition metal-catalyzed C-H activation has emerged as a powerful method for direct functionalization, providing regioselectivity, efficiency, and sustainability. Complementarily, nitrene chemistry, with its longstanding legacy, offers a unique advantage in C-N bond formation. Nitrenes can insert into C-H bonds to form disubstituted amines through C-N bond formation. The transition metal-catalyzed intramolecular amination of biaryl azides through C-H bond activation represents a greener approach to carbazole synthesis, due to its exceptional atom and step economy.2 In this regard, a series of welldefined nickel, cobalt, and zinc complexes bearing bis(imino)pyridine ligands have been employed as catalysts to achieve the regioselective synthesis of diversely substituted carbazoles. These earth-abundant metal systems offer practical benefits in terms of cost, sustainability, and electronic tunability. The synthesis, characterization, and catalytic application for the synthesis of carbazoles will be discussed.

**Keywords:** Carbazoles, Heterocycles, Catalysis, transition metal, C-H amination.

- P. S. Waghmare, A. R. Chabukswar, K. G. Raut, P. T. Giri, *Chirality*, 2025, 37, e70021. (b) H. Zhang, W. Zhang, M. Zhu, A. Awadasseid, 2024, 31, 4826-4849.
- B. J. Stokes, B. Jovanović, H. Dong, K. J. Richert, R. D. Riell, T. G. Driver, J. Org. Chem., 2009, 74, 3225-3228. (b) J. Grover, A. T. Sebastian, S. Maiti, A. C. Bissember, D. Maiti, Chem. Soc. Rev. 2025, 54, 2006-2053.

## Kiran Kumar Pulukuri

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**Education** 

**Ph.D.:** CSIR-CDRI Lucknow **M.Sc.:** Pondicherry University.

Career

**Assistant Professor** (2019-Present): IISER Tirupati **Postdoctoral** (2013-2019): Rice University, USA

### Area of Research

- Total synthesis of natural products
- Synthetic methodology development
- Electro-organic synthesis
- Natural product-based drug discovery.

## Synthesis of Sesquiterpenoids through Siteselective Functionalization

#### Kiran Kumar Pulukuri, 1 Ashutosh Panigrahy\*2

Indian Institute of Science Education and Research (IISER) Tirupati

**Abstract:** Natural products remain a rich source of inspiration for synthetic chemists, combining intricate architectures with remarkable biological activities. Among them, sesquiterpenoids represent one of the most structurally diverse and synthetically demanding classes. In this talk, I will describe our recent efforts to streamline the synthesis of Eudesmane sesquiterpenoids and the guaiane terpenoid nonalabotalide through selective olefin functionalization-based strategies that emphasize efficiency and elegance. By integrating domino reactions, stereocontrolled olefin transformations, and biomimetic approaches, we have developed concise synthetic routes that enable the rapid assembly of these complex targets. These methods not only minimize the number of steps but also broaden opportunities to access structurally diverse and bioactive natural product scaffolds.

#### Figure/Scheme (if any):

**Keywords:** Natural Products, Site-Selective functionalization, Sesquiterpenoids, Hydrogenation and Epoxidation.

- 1. Panigrahy, K. K. Pulukuri, Organic Letters, 2025, 27, 12758–12762.
- 2. Panigrahy, K. K. Pulukuri, Organic Letters, 2025, 27, 11526–11530.

## Prasenjit Mal

Professor, NISER Bhubaneswar



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## **Education**

**Ph.D.:** IIT Kanpur **M.Sc.:** IIT Kharagpur

#### Career

Professor (2024 - Present): NISER Bhubaneswar

Associate Professor (2017 – 2024): NISER Bhubaneswar Assistant Professor (2009-2017): NISER Bhubaneswar Postdoctoral (2008-2009): University of Cambridge, UK (2006-2007): University of Siegen, Germany

#### **Awards & Honors**

2021: CRS Bronze Medal

2008: Marie Curie Fellowship

2006: Alexander von Humboldt Fellowship

## CsPbBr<sub>3</sub> Perovskites in Visible-Light-Driven Organic Synthesis Prasenjit Mal

School of Chemical Sciences, National Institute of Science Education and Research (NISER) Bhubaneswar, An OCC of Homi Bhabha National Institute; PO Bhimpur-Padanpur, District Khurda, Odisha 752050, India

**Abstract:** Cesium lead bromide perovskite (CsPbBr<sub>3</sub>) nanocrystals have rapidly emerged as powerful visible-light photocatalysts for organic synthesis owing to their tunable bandgaps, long-lived excited states, and superior charge-transport properties.<sup>1</sup> This presentation provides an overview of recent advances in perovskite-mediated photocatalysis, with particular emphasis on our own contributions to synthetic applications and mechanistic elucidation.<sup>2</sup> Key photocatalytic transformations will be discussed alongside insights into catalyst stability, and structure-activity relationships.<sup>3, 4</sup> Finally, we will highlight emerging strategies to address current limitations and offer a perspective on future opportunities for translating these highly luminescent nanomaterials from laboratory curiosities to practical photocatalytic platforms.<sup>5</sup>



**Keywords:** CsPbBr<sub>3</sub> Perovskite; Heterogeneous Photocatalysis; Photocatalysis; Visible-light

- 1. P. Nayek, B. Pal and P. Mal, ACS Catal., 2025, 15, 15519-15558.
- 2. Manna, P. Nayek and P. Mal, ACS Energy Lett., 2025, 10, 1499-1507.
- Mathuri, B. Pal, M. Pramanik, A. Manna and P. Mal, Catal. Sci. Technol., 2024, 14, 183-189.
- 4. Pal, A. Mathuri, A. Manna and P. Mal, *Org. Lett.*, 2023, 25, 4075-4079.
- 5. T. K. Dinda, A. Manna, P. Nayek, B. Mandal and P. Mal, *ACS Appl. Mater. Interfaces*, 2024, 16, 49411-49427.

#### Shantanu Pal

Professor, IIT Bhubaneswar



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**Education** 

Ph.D.: IIT Bombay

Career

Professor (2010-Present): IIT Bhubaneswar.

Postdoctoral: Ewha Womans University, Seoul, South Korea & Karmanos

Cancer Research Institute, Detroit, USA

#### Area of Research

Development of novel methodologies using transition metal catalysed C-C, C-X bond formation and total synthesis of natural products or bioactive molecules.

#### Awards & Honors

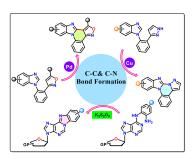
- G.N. Mohapatra Endowment Award from Utkal University
- Life Member: Chemical Research Society of Odisha

## Novel Strategies for the Construction of Bioactive Benzimidazole Fused N-Heterocycles

#### Shantanu Pal

IIT Bhubaneswar, Jatni, Odisha

**Abstract:** The direct construction of C-C and C-N bonds continues to hold a central position in modern organic synthesis. Among nitrogen-containing heterocycles, benzimidazole and its fused analogues represent a privileged structural framework due to their prevalence in bioactive molecules and their versatility as synthetic building blocks. In this presentation, we highlight our recent efforts toward the development of transition-metal-catalyzed dehydrogenative coupling strategies for the annulation of benzimidazole with isoxazoles and pyrazoles, enabling efficient access to biologically relevant benzimidazole-fused N-heterocycles. Furthermore, we introduce a novel  $K_2S_2O_8$ -mediated oxidative deamination protocol that facilitates the construction of benzimidazole-fused purine nucleosides. A detailed mechanistic rationale supporting these transformations will be discussed, along with their broader applicability toward the synthesis of diverse heterocyclic architectures.



**Keywords:** Organic synthesis, Metal catalysed reactions, Benzimidazole fused N-heterocycles

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### Guru Brahamam Ramani

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#### **Education**

**Ph.D.:** University of Hyderabad, Hyderabad **M.Sc.:** University of Hyderabad, Hyderabad

#### Career

Assistant Professor (2019-Present): IIT Jammu

Postdoctoral (2017-2019): Stockholm University, Stockholm, Sweden.

(2013-2017): National Taiwan Normal University, Taipei, Taiwan

#### **Area of Research**

Asymmetric Synthesis, Alkyne & Allene Chemistry, Carbene Transfer Reactions, Hypervalent Iodine Chemistry, Organocatalysis, Photoredox Catalysis, C-H Functionalization, and Organoboranes.

#### **Awards & Honors**

**2017:** Wenner-Gren Foundation Postdoctoral Fellowship (2017-2019), Stockholm, Sweden.

2004: Dr. Reddy's Spirit of Excellence Award for the year

### Photochemical Alkynyl Carbene Transfer Reactions

#### Guru Brahamam Ramani

Indian Institute of Technology Jammu, Jammu

Abstract: Carbenes are versatile reactive intermediates, enabling a wide range of novel transformations in modern organic synthesis. Typically, they have been accessed through the decomposition of different kinds of diazo compounds. In this context, alkynyl diazo compounds offer a unique synthetic platform, as the presence of the alkyne group provides an additional functional handle that can facilitate increased molecular complexity. Recently, our research group synthesized alkynyl diazo acetates through oxidation of unprotected alkynyl hydrazones and utilized them for metalcatalysed carbene transfer reactions. 1-3 Inspired by the growing potential of visible-light driven methodologies, we explored the photochemical reactivity of alkynyl diazoacetates and developed the first visible-light induced alkynyl carbene insertion into furans, affording stereoselective π-enriched conjugated dienynals and dienynones with excellent selectivity. 4 Building on this reactivity, we established a novel metal-free photochemical strategy for synthesizing 2-alkynyl substituted pyrans via a carbene mediated ring expansion of tetrahydrofuran (THF). Additionally, we achieved highly regioselective (>20:1) y-insertion of alkynyl carbenes into O-H bonds under visible light irradiation to obtain diversified propynyl ethers of 2,2,2-trifluoroethanol (TFE).5 On the other hand, we observed exclusive a-insertion with non-fluorinated alcohols under similar reaction conditions. In summary, the study highlights the synthetic versatility of alkynyl diazoacetates in metal-free photochemical carbene transfer reactions, thereby expanding the range of visible light-mediated alkynyl carbene transformation

**Keywords:** Diazo Compounds, Photochemical reactions, Homologation, Carbenes Insertions.

- Sharma, A.; Jamwal, P.; Vaid, H.; Gurubrahamam, R. Org. Lett. 2023, 25, 1889-1894.
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- Sharma, A.; Vaid, H.; Kotwal, R.; Mughal, Z.-N.; Gurubrahamam, R. Org. Lett. 2024, 26, 4887-4892
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- 5. Vaid, H.; Nganthoinganbi, Y.; Tsai, M.-K.; Gurubrahamam, R. Manuscript under revision.

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#### **Education**

**Ph.D.:** CSIR-IICT Hyderabad **M.Sc.:** Kakatiya University.

#### Career

**Associate Professor** (2020 – Present): IIT Delhi. **Postdoctoral** (2019-2020): Emory University, U.S.A

(2018-2019): University of Tromsø - The Arctic University of

Norway, Norway

(2016-2018): University of Tromsø - The Arctic University of

Norway, Norway

### **Area of Research**

Ylide and carbene-mediated transformations

• Synthesis of natural product

#### **Awards & Honors**

2025: Merck Young Scientist Award (Scientific Excellence) - Merck Group

**2022:** Teaching Excellence Award – IIT Delhi

2020: Thieme Chemistry Journals Award - Thieme Chemistry.

2018: FRIPRO mobility grant (Research Council of Norway and (COFUND)

- Marie Curie Actions)

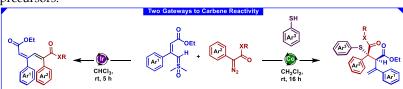
**2017:** Certificate of Outstanding reviewing from Tetrahedron Journal (Elsevier)

## Unifying Carbene Precursors: Synthetic Opportunities with Vinyl Sulfoxonium Ylides and Diazo Compounds

#### Srashti Bhardwaj, Dinesh Kumar Gopalakrishnan, and Janakiram Vaitla

Indian Institute of Technology Delhi, Delhi

**Abstract:** Carbene transfer reactions play a pivotal role in modern organic synthesis. Among carbene precursors, vinyl sulfoxonium ylides<sup>1</sup> and diazo compounds have recently emerged as versatile and complementary platforms for developing stereoselective transformations. This study explores the unique reactivity and selectivity arising from the interaction of these two carbene sources through distinct mechanistic paradigms. A carbene-mediated stereoselective cross-olefination strategy established,<sup>2</sup> coupling vinyl sulfoxonium ylides with diazo compounds. This transformation proceeds under mild conditions to deliver substituted alkenes with excellent stereochemical control and broad substrate compatibility.<sup>3</sup> Complementarily, a metalloradical catalytic approach was developed to achieve gem-difunctionalization of diazo compounds with vinyl sulfoxonium vlides and thiols. Utilizing cobalt(II)-based metalloradical catalysis, this method orchestrates concurrent C-C and C-S bond formation via controlled radical intermediates, affording densely functionalized products with high stereoselectivity.4 Together, these complementary methodologies demonstrate the untapped potential of combining vinyl sulfoxonium ylides and diazo esters as dual carbene precursors.



**Keywords:** Sulfoxonium ylides, Diazo esters, Metal carbenes, Carbene radicals, Olefines.

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- 2. D. S. Davas, S. Bhardwaj, R. Sen, D. K. Gopalakrishnan, and Janakiram Vaitla, *Adv. Synth. Catal.*, 2022, 364, 3122.
- 3. D. K. Gopalakrishnan, S. Bhardwaj, S. Kumar, T. Karmakar, and J. Vaitla, *Chem. Commun.*, 2024, 60, 3846 3849.
- 4. S. Bhardwaj, D. K. Gopalakrishnan, S. Deshwal, R. Sen, V. Tiwari, T.

## Debendra K. Mohapatra

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## **Education**

**Ph.D.:** CSIR-IICT Hyderabad **M.Sc.:** Ravenshaw University

#### Career

Professor (2025 - Present): IISER Berhampur

Chief Scientist (2008 - Present): CSIR-IICT Hyderabad

Scientist (2002-2008): CSIR-NCL Pune

Postdoctoral (2000-2002): U.S.A

#### Area of Research

Development of new methodologies

• Asymmetric reactions and applications towards the stereoselective total synthesis of complex natural products.

#### **Awards & Honors**

2023: CRSI Bronze Medal

2017: NASI-Reliance Industries Platinum Jubilee Award

2014: CSIR-Technology Award

2008: AVRA Young Scientist Award

2007: CDRI Award for Excellence in Drug Research

2005: D & O Pharmachem Inc., U.S.A. Young Scientist Award

2004: ICT Foundation Day Young Scientist Award

2002: INSA Young Scientist Award

## Molecular Mysteries - The Art of Structure Elucidation in Drug Research

#### Debendra Kumar Mohapatra

Organic Synthesis and Process Chemistry Department

CSIR-Indian Institute of Chemical Technology, Hyderabad-500007, Telangana, INDIA

Abstract: Despite significant advances in NMR spectroscopy and other analytical techniques, structure elucidation of natural products with limited availability, is still a challenging task for chemists. From the year 2000 to 2020, more than 300 natural products have been incorrectly assigned (stereochemical and/or structural). Surprisingly, the examples cover almost all class of compounds, including steroids, terpenes, indole alkaloids, peptides and encompass molecules of all sizes and stereochemical complexity. The first asymmetric convergent total synthesis of four isomers of proposed structures of cryptorigidifoliol K² (1a, 1b, 1c, and 1d) and discrepancies between the spectroscopic data of synthetic isomers of cryptorigidifoliol K and the data reported for the natural product, suggested that the structure proposed for the natural products needs revision.<sup>3</sup>

In this talk, the first asymmetric total synthesis of proposed structures, correct structure and absolute configuration of cryptorigidifoliol K, Monocillin VII, and Diplopyrone will be discussed.<sup>3-6</sup>

#### References

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#### **Education**

**Ph.D.:** University of Mumbai **M.Sc.:** University of Mumbai

#### Career

Assistant Professor (2018- Present): IIT Bhubaneswar

Postdoctoral (2012-2013): The Scripps Research Institute, California

(2011-2012): Hyderabad Central University

(2010-2011): IISc Bangalore

#### Area of Research

- Heat-/Light-/Electricity-mediated Catalytic/Non-catalytic Synthetic Method Development for Functionalized Heterocycles/Carbocycles synthesis.
- Greener Synthetic Strategies employing Cycloadditions Strategy, metalfree late-stage C-H functionalization approaches, and other modern methods.
- Repurposing the existing chemical space for developing new methodologies.
- Symmetric Total Synthesis of Bioactive Marine Alkaloids, Terpenoids, and Natural products of mixed biosynthetic origin

#### **Awards & Honors**

**2013:** Fulbright-Nehru Postdoctoral fellowship from the United States-India Education Foundation (USIEF), New Delhi, India

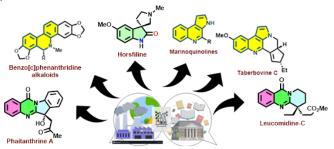
**2008:** Best Poster Award at Trombay Symposium for Radiation and Photochemistry from the Department of Atomic Energy, Govt. of India **2007:** Best Talk Award at Ph.D Student Symposium from the Royal Society of Chemistry- West India Section

## Aiming Sustainability via Visible-Light Photoredox Catalysis and Anthropogenic Gas Capture for Functionalized Molecules

#### Tabrez Khan

Organic Synthesis Laboratory, School of Basic Sciences, Indian Institute of Technology Bhubaneswar

**Abstract:** The Greenpeace report indicates that India is the leading emitter of SO<sub>2</sub> in the world, contributing more than 15% of global anthropogenic emissions. Due to the enormous SO<sub>2</sub> production every year, utilizing SO<sub>2</sub> gas to access value-added products is becoming a lucrative strategy in organic synthesis. To address the pressing need to transform waste to wealth (W2W), our laboratory is engaged in the development of visible-light-assisted methodologies utilizing anthropogenic gas capture<sup>1.5</sup> for the synthesis of value-added products inspired by natural products, driven by our interest in natural product synthesis.<sup>6-11</sup> Some of these recent endeavors will be presented in the talk.



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- 2. Vishwakarma, T. K. Sahu, S. G. Patra, C. Paul, S. Behera, S. Sahoo, and T. Khan, Eur. J. Org. Chem. 2025 (Just Accepted)
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## Thangavelu Saravanan

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#### Education

Ph.D.: IIT Madras

M.Sc.: Madurai Kamaraj University.

#### Career

Assistant Professor (2019-Present): University of Hyderabad

Postdoctoral (2016-2019): University of Groningen, Netherlands

(2014-2016): Technical University of Darmstadt, Germany

#### Area of Research

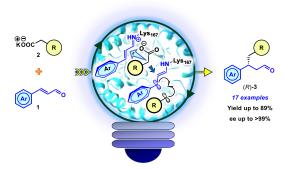
- Use of enzyme catalysis in the asymmetric synthesis of active pharmaceutical ingredients (APIs)
- Development of (chemo-)enzymatic cascade process for valuable pharmaceuticals
- Photo-Biocatalysis: Enzyme catalysis in combination with light for sustainable synthesis
- Discovery of novel enzymes & exploring it towards new chemical reactions
- Enhancing the enzyme properties by directed evolution and protein engineering techniques

## Expanding the Catalytic Horizons of DERA: Photobiocatalytic Enantioselective β-Alkylation of Enals

#### Thangavelu Saravanan

School of Chemistry, University of Hyderabad

ABSTRACT: Aldolases, particularly 2-deoxyribose-5-phosphate aldolase (DERA), are versatile biocatalysts for constructing chiral building blocks of pharmaceutical relevance. Extending their catalytic repertoire beyond natural substrates and mechanisms opens new avenues in asymmetric synthesis.1 While protein engineering has broadened substrate scope, the catalytic potential of aldolases beyond the thermal domain remains largely unexplored. We recently introduced a photobiocatalytic strategy that exploits the promiscuous iminium-ion pathway of DERA to achieve enantioselective β-alkylation of enals.<sup>2</sup> Direct photoexcitation of iminium intermediates enables electron donor-acceptor (EDA) complexation with potassium salts of aryl(alkyl)acetic acids, serving as alkyl radical precursors. This methodology was validated across diverse donor and acceptor substrates, affording  $\beta$ -alkylated products in good yields (up to 89%) and excellent enantiopurity (>99% ee). By merging iminium-ion catalysis with photochemical activation, this approach pioneers radical-based C-C bond formation with high enantiocontrol, significantly broadening the synthetic repertoire of aldolases. Detailed insights into reaction development and the challenge



Keywords: Asymmetric Synthesis, Biocatalysis, Aldolases, Protein Engineering

#### References:

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- S. Dheeraj, S. Pulikkathodi, S. O. Valappil, K. Samanta and T. Saravanan, ACS Catal, 2025, 15, 2531 – 2539.

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#### **Education**

**Ph.D.:** University of California, Berkeley, USA **M.Sc.:** University of Minnesota-Twin Cities, USA

#### Career

Assistant Professor (2023- Present): IISc Bangalore

Postdoctoral (2021-2023): Massachusetts Institute of Technology, USA

#### **Area of Research**

- Methodology-driven total synthesis of bioactive molecules
- New skeletal editing tools

#### **Awards & Honors**

**2024:** INSPIRE faculty fellowship **2023:** Infinite Expansion Award

2016: Tobacco-Related Disease Research Program (TRDRP) Predoctoral

Fellowship Stauffer award

2016: ACS Division of organic chemistry most outstanding senior,

undergraduate student award

## A three-phase, one-pot protocol to enable 1,3-translocation of aryl ketones

#### Vignesh Palani

Indian Institute of Science, Bangalore

**ABSTRACT:** Molecular skeletal editing refers to scaffold remodeling that alters the core framework of the molecule without affecting the appended functionalities. The editing could include either a single atom or a group of atoms within the core skeleton or at the periphery of the molecular framework. This emerging direction would involve an organic transformation to rapidly arrive at a completely elusive molecular skeleton and, thus, serve as a valuable step towards late-stage diversification of druglike molecules. This, in turn, would open doors to a library of retrosynthetic tools that were previously inaccessible. The function of an organic molecule is generally attributed to its associated functional groups (FGs). Hence, transformations pertaining to the introduction, removal, or interconversion of FGs are highly significant in drug discovery. Despite these advances, methodologies to selectively translocate functionalities to unactivated remote C-H positions have remained largely unexplored. This peripheral editing strategy offers an ideal 100% atom economy for translocating FGs to inaccessible C-H sites without introducing any other alterations to the molecule.

This work will disclose peripheral skeletal editing involving selective movement of the aryl ketone functional group along the periphery of the molecular framework. In particular, our work is aimed toward selective 1,3-translocation of aryl ketone functionality in a saturated carbocycle, thereby venturing into a challenging three-dimensional space. An aryl appendage bearing a carbonyl functionality would be a significant choice considering its widespread presence in several naturally occurring molecules and therapeutic drugs. In addition, the versatility in translating this FG to various other functionalities would add to the synthetic utility of the proposed transposition. In summary, this translocation strategy will be of high importance both in the late-stage diversification of drug molecules and in unorthodox retrosynthetic disconnections.

Keywords: Functional group translocation, skeletal editing, late-stage diversification

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#### Rambabu Dandela

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#### **Education**

**Ph.D.:** Dr. Reddy's Institute of life sciences, University of Hyderabad campus,

Hyderabad

M.Sc.: Kakatiya University

#### Career

**Assistant Professor** (2018-Present): Institute of Chemical Technology, India Oil Odisha Campus (IOC), Bhubaneswar.

Postdoctoral (2013-2017): Ben-Gurion University of the Negev, Israel Research scientist (2004-2008): Matrix Labs Ltd (Now Mylan Lab Ltd), Hyderabad

#### Area of Research

- Organo Catalysis
- Flow Chemistry
- Synthetic Methodology
- Drug application

#### **Awards & Honors**

2022: Ramanujan Faculty Fellow by DST, Govt. of India

2019: Associate fellow of the Telangana Academy of Sciences

**2017:** Associate fellow of the Andhra Pradesh Academy of Sciences

**2011:** Young Scientist award (2011) in Oral presentation at the "National Seminar on Indian Council Chemists" seminar conducted by the Department of Chemistry, Osmania University, Hyderabad.

## The Efficient Construction of Functionalized Heterocyclic Compounds

#### Rambabu Dandela

Department of Industrial and Engineering Chemistry, Institute of Chemical Technology, Indian Oil Odisha Campus, Samantpuri, Bhubaneswar-751013, India.

ABSTRACT: Heterocyclic compounds are intriguing structures that include one or more heteroatoms—like nitrogen, oxygen, or sulfur—within a ring. This inclusion of heteroatoms affects the compound's properties compared to all-carbon rings. The most common heterocycles feature five- or six-membered rings that include heteroatoms such as nitrogen (N), oxygen (O), or sulfur (S). Some of the best-known simple heterocyclic compounds are pyridine, pyrrole, furan, and thiophene. A key aspect of many heterocyclic compounds is their structural versatility, allowing for the incorporation of functional groups either as substituent or as part of the ring itself. This flexibility enables these compounds to effectively provide or mimic various functional groups, enhancing their utility in a wide range of chemical applications. Considering all aspect of having significant properties and applications, here in, we have effectively engaged to develop a list heterocyclic valuable scaffold like 1,5disubstituted pyrazoles, 3,3-diindolyl derivatives, 1,3,4-oxadiazoles, 2,5-disubstituted oxazoles, 2,4,6-triarylpyridines, 2-(dimethylamino) pyrimidine, 2-substituted benzimidazoles, substituted imidazoles, 2-arylquinolines, etc, which is shown in Schem<sup>1</sup>

**Scheme 1.** Development of various important heterocyclic moieties.

**Keywords:** Pyrazoles, Oxazoles, Triarylpyridines, Benzimidazoles, Arylquinolines.

#### References:

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- 5. S. Bhukta, R. Chatterjee, D. Rambabu. Green Chemistry., 2023, 25, 3034-3039.

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**Education** 

Ph.D.: IISc Bangalore

M.Sc.: Visva-Bharati Central University, Santiniketan, India

#### **Career**

Assistant Professor (2024-Present): IISER Berhampur

Postdoctoral (2021-2023): The Scripps Research Institute, La Jolla, USA.

(2018-2021): Indiana University, Bloomington, USA.

Research Associate (2018-2018): IISc Bangalore

#### Area of Research

- Asymmetric Catalysis
- Synergistic Catalysis
- Organometallics
- Olefin Functionalization

#### **Awards & Honors**

**2018:** GRC Carl Storm International Diversity (CSID) Award to attend the **2018:** GRC in Stereochemistry, USA

## Conformational Rigidity Controlled Copper Catalyzed Chemodivergent Annulation

#### **Amit Kumar Simlandy**

IISER Berhampur

**ABSTRACT:** Conformational rigidity of the substrate plays a pivotal role in controlling the reaction outcome which is measured in terms of either the reactivity of the substrate or the selectivity in the product<sup>1</sup>. Despite this importance, conformational rigidity controlled mechanistic divergence remain underexplored. Herein we report a Cucatalyzed [3+2] annulation reaction where, the rigidity of the  $\alpha$ -aminoketones controls the switch in mechanism under identical set of reaction conditions. This copper catalyzed strategy utilizes allenylidene<sup>2</sup> derived allenal<sup>3</sup> which is generated from the ethynylethylene carbonate. This protocol provides valuable nitrogenous heterocycles which were either difficult to synthesize or unattainable previously, opening new avenues for drug discovery<sup>4</sup>.

**Keywords:** Conformational Rigidity, Mechanistic Divergence, Annulation, Allenal, Copper.

#### References:

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## Durga Prasad Hari

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#### **Education**

Ph.D.: University of Regensburg, Germany

M.Sc.: IIT Madras.

#### Career

Assistant Professor (2021-Present): IISc Bangalore

Postdoctoral (2018-2021): Marie Curie Research Fellow, University of Bristol,

UK

(2014-2018): EPFL, Switzerland

#### Area of Research

- Ring-Strain-Driven Reaction Discovery
- Synthesis and Applications of New Carbenes
- Deconstructive Functionalization

#### **Awards & Honors**

2025: INSA Young Associate for the year 20252024: Thieme Chemistry Journals Award2023: Infosys Young Investigator Award2019: Marie-Curie Individual Fellowship

2010: GRK 1626 Chemical Photocatalysis Fellowship, Germany.

### Radical-Polar Crossover for Molecular Remodelling

#### Durga Prasad Hari

Department of Organic Chemistry, Indian Institute of Science, Bangalore

**Abstract:** Radical-Polar Crossover (RPC) is an effective method in organic synthesis that integrates both radical and ionic species. Since the reactivities of radical and ionic intermediates are orthogonal, using these two mechanisms in sequence offers significant advantages in molecular remodelling. In this lecture, I will first discuss a photoredox-catalyzed Dowd-Beckwith ring-expansion/RPC strategy for synthesizing functionalized medium-sized carbocyclic compounds.<sup>1</sup> Recently, deconstructive strategies have garnered attention as efficient methods for molecular remodelling. However, the selective cleavage and functionalization of inert C-C bonds, particularly within unstrained cycles, remains a considerable challenge. In the second part of the lecture, I will present an RPC Interrupted Dowd-Beckwith reaction, which provides a robust approach for C-C bond cleavage and functionalization.<sup>2</sup> This deconstructive strategy is applicable to medium-sized (hetero)carbocycles and macrocycles, thereby expanding its utility for challenging synthetic transformations. Finally, I will discuss a strain-enabled RPC strategy for the unified synthesis of spiro-, fused-, and enantioenriched aza/oxa-bicyclo[3.1.1]heptanes.3

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## S. S.V. Ramasastry

Professor, IISER Mohali



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#### **Education**

Ph.D.: IISc Bangalore

M.Sc.: Andhra University, Visakhapatnam.

#### Career

Professor (2023- Present): IISER Mohali

**Associate Professor** (2017-2023): IISER Mohali **Assistant Professor** (2011-2017): IISER Mohali

Senior Research Scientist (2010-2011): Jubilant Biosys Ltd., Bangalore, India Senior Research Investigator (2008-2010): Bristol-Myers Squibb Biocon Research Center (BBRC), Syngene International Ltd., Bangalore, India Postdoctoral (2005-2008): The Scripps Research Institute, La Jolla, CA, USA

#### Area of Research

- Development of novel stereoselective reactions relevant to both medicinal and natural product chemistry.
- Development of green and sustainable synthetic chemistry and atom economic reactions.
- Application of aforementioned strategies in the total synthesis of bioactive natural products and pharmaceutically important compounds.

#### **Awards & Honors**

2025: Silver Star Medal 2025 by Chirantan Rasayan Sanstha (CRS)

2025: Selected as an INSA Associate Fellow (IAF)

2022: Recipient of the CDRI Award for Excellence in Drug Research

2018: A. V. Rama Rao Research Foundation (AVRA) Young Scientist Award

2018: Organisation of Pharmaceutical Producers of India (OPPI) Young

Scientist award

2018: Chemical Research Society of India (CRSI) Bronze Medal

2016: Young Scientist award from the organizing committee of 'Chemical

Frontiers Goa.'

### **Metal-Free Chemistry Facilitated by Phosphines**

#### S. S. V. Ramasastry

IISER Mohali

**Abstract:** Our laboratory has been actively engaged in developing new synthetic strategies to access diverse heterocyclic scaffolds from readily available starting materials. In this pursuit, we have established several new metal-catalyzed methods for constructing privileged structures.<sup>1</sup> In parallel, we have made significant advances in metal-free approaches to various carboand heterocycles by harnessing the Lewis basicity of trivalent organophosphines.

The major focus of my presentation will be on our phosphine-promoted methodologies, including the enantioselective intramolecular Morita-Baylis-Hillman (IMBH) reaction,<sup>2</sup> reductive aldol and vinylogous aldol reactions,<sup>3</sup> the  $\alpha$ -spirannulative IMBH reaction,<sup>4</sup> as well as related developments.

Keywords: Metal-free, Phosphines, Orgnocatalysis

- Some representative articles: (a) Dhiman, S.; Mishra, U. K.; Ramasastry, S. S. V. Angew. Chem. Int. Ed. 2016, 55, 7737. (b) Bankar, S. K.; Singh, B.; Tung, P.; Ramasastry, S. S. V. Angew. Chem. Int. Ed. 2018, 57, 1678. (c) Singh, B.; Bankar, S. K.; Kumar, K.; Ramasastry, S. S. V. Chem. Sci. 2020, 11, 4948. (f) Kumar, P.; Kumar, P; Venkataramani, S.; Ramasastry, S. S. V. ACS Catal. 2022, 12, 963.
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# Stereoselective Claisen Rearrangement towards construction of Quaternary Stereocenters, Lactones, and precursors of natural products

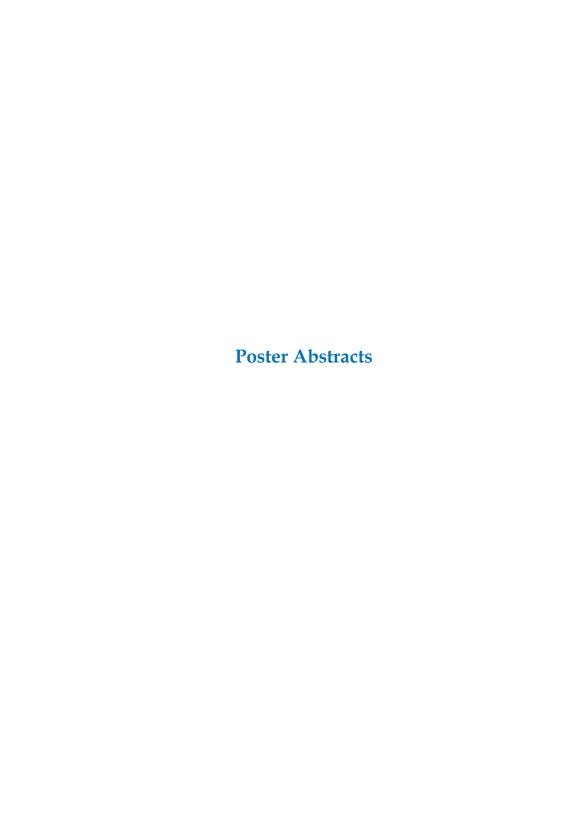
#### Jaya Prakash Das

Organic Synthesis and Catalysis Laboratory, Department of Chemistry, Ravenshaw University, Cuttack-753003, India.

Abstract: The Claisen rearrangement is considered one of the most efficient methods for the construction of a C-C single bond, along with the formation of γ,δ-unsaturated carbonyl compounds. This reaction proceeds through a six-membered (Zimmermann-Traxler) transition state, which itself provides diastereoselectivity. Furthermore, the construction of all carbon quaternary stereogenic centres, along with a contiguous stereo centre in an acyclic system, remains a challenge to achieve. The strategy focuses on the design of a novel domino process that consists of a metal-catalysed C-O bond coupling and a subsequent Claisen Rearrangement with diastereo-, and enantioselectivity, which leads to the construction of two adjacent stereocenters along with the desired all-carbon quaternary stereocenter.1 The envisioned transformation starts with vinyl iodides, which are synthesised from simple ynamides either through regio- and stereocontrolled carbocupration followed by iodination<sup>2a</sup> or by our recently developed hydroiodination of vnamides using DPPO/NIS couple<sup>2b</sup>. Another strategy includes an efficient Lewis-acid catalysed transformation of chiral ynamides to  $\gamma$ ,  $\delta$ -unsaturated amides with contiguous stereocenters, along with an all-carbon quaternary centre in good to excellent yields following Claisen-type stereoselective [3,3]- sigmatropic rearrangement reaction.<sup>3</sup> High diastereoselectivity and excellent enantioselectivity have been achieved along with access to structurally diversified lactones with excellent enantio-induction, which can be used as precursors for various natural product synthesis. The methodology is further extended towards the synthesis of chiral allenes with very good yields and moderate to good diastereoselectivity. A large range of chiral ynamides, allyl alcohols, and propargyl alcohols has been utilised for the synthesis of complex molecular architectures.

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## P-01; 1,2-Sulfonylative-Arylation of Acrylamides via Strain-Release-/Aromaticity-Driven Radical Generation and SO<sub>2</sub>-capture under Photoredox Catalysis

#### Abhaykumar Vishwakarma, and Tabrez Khan\*[a]

**Abstract:** Among N-heterocycles, the prevalence of 2-oxindoles in bioactive natural products and pharmaceutically active molecules underscores their significance as a privileged scaffold.[1-3]. Besides, y-keto sulfones, being a medicinally relevant building block, have never been integrated with the bioactive oxindole scaffolds. On the other hand, strategies involving SO2 capture in organic molecules to access value-added products are gaining momentum. Therefore, with the growing significance of visiblelight-promoted photoredox catalysis and our ongoing interest [4,5], a strategy en route to  $\gamma$ -keto alkylsulfonylated oxindoles bearing a  $\beta$ -all-carbon quarternary center is disclosed. Toward this goal, the bis-functionalization of N-(hetero)arylacrylamides has been realized via the strain-release driven ring-scission of strained 3°-cyclopropanols in the presence of DABSO and the aromaticity-driven bond-scission in pro-aromatics like 4-alkyl-1,4-DHPs in the presence of  $Na_2S_2O_5$  under visible-light photoredox catalysis to access a library of  $\gamma$ -keto/ alkylsulfonylated oxindoles featuring a  $\beta$ -allcarbon quaternary center. The reaction optimization, broad substrate scope along with the mechanistic probing studies that have been complemented with DFT calculations, and bioactivity profiling will be presented through the poster.



Scheme: 1,2-sulfonylative-arylation of N-phenyl acrylamides

Keywords: photoredox catalysis • oxindoles • cyclopropanols • SO<sub>2</sub>-capture • acrylamides

#### References:

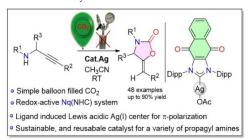
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## P-02; Redox-active NqNHC Bearing Silver(I) Complexes; Synthesis, and Promising Catalysts for Carboxylative Cyclization of Propargylamines from CO2

Aiswarya Moharana, Jyotikiran Sahoo and Adinarayana Doddi\*

Abstract: N-Heterocyclic carbene (NHC)-supported transition metal complexes represent a rapidly emerging area in homogeneous catalysis. In this study, we have synthesized a series of neutral and cationic silver complexes incorporating two different redox-active NHC ligands. NHC complexes of the type Nq(IDipp)AgOCOR (R = CH<sub>3</sub> (2a), Ph (2b), CF<sub>3</sub> (2c)) were obtained by the reaction of free carbenes or the corresponding imidazolium salts with suitable silver precursors. In contrast, cationic complexes of the type  $[(Nq(NHC)_2Ag)]X$  (NHC = IDipp, X = BF<sub>4</sub> $^-$ (3a), SbF<sub>6</sub> $^-$ (3b); NHC = IMes,  $X = BF_4^-$  (3c),  $SbF_6^-$  (3d)) were synthesized using AgX salts. Among these, 2b was explored as a molecular catalyst for the carboxylative cyclization of propargylamines with CO2. This transformation enabled the development of a new and efficient catalytic protocol for the synthesis of a broad range of oxazolidine-2-ones in good to excellent yields. Notably, catalyst 2b exhibited excellent catalytic performance under mild conditions, operating effectively at low CO2 concentrations and without the need for added bases or other additives. In addition, the practical applicability of catalyst 2b was highlighted through its successful use in the synthesis of the antidepressant drug Toloxatone and a Linezolid-inspired antimicrobial precursor. Future studies will focus on "sustainable metal-free approach to amide N-formylation via naphthoquinone-annulated redox-active NHC catalysis" and "Nq(NHC) supported air-stable Copper borohydride complexes and their reactivity towards small moleculeactivations".



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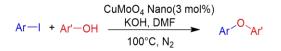
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## P-03; Bimetallic CuMoO4 Nano Catalyst for Csp2-O Cross-Coupling Reaction.

Ajeena Sahoo,1 and Laxmidhar Rout2\*

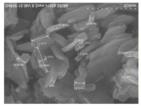
**Abstract:** Now-a-days the use of nano-sized transition metal catalysts in coupling reaction has attracted a lot of attention because of their high surface-to-volume ratio, high surface energy, and reactive morphology allows for rapid *C–O* bond formation under mild and ligand-free conditions. *C–O* bond present in many drug molecules thus synthesis of ether is highly important in medicinal and pharmaceutical industries. Based on that we developed Oxygen bridged Nano catalyst which has large surface area, high TOF and high TON, environmentally friendly, Heterogeneous and recyclable CuMoO<sub>4</sub> catalyst for *C-O* coupling reaction to give unactivated 2,4-dichlorophenol derivatives that could be used as potential herbicides.

**Keywords:** Nano-Catalyst, Bimetallic, Cross-Coupling, Ether, Transition metal.



Nano Catalyst Recyclable Ligand free Heterogeous

34 examples upto 95% yield





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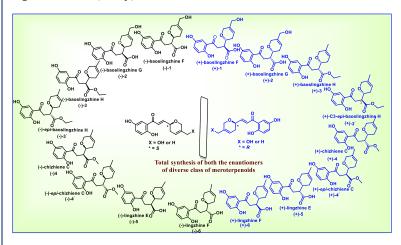
Research Area: Synthetic Organic Chemistry

# P-04; Collective Total Synthesis of (+)- and (-)-Baoslingzhines F-H, (+)- and (-)-Chizhiene C, and (+)- and (-)-Lingzhines E-F

Nityaprakash Patra, Akshaya S, Barla Thirupathi\*

**Abstract:** We report a collective modular approach to the total syntheses of 12 naturally occurring diverse meroterpenoid natural products, (+)- and (-)-baoslingzhines F-H,<sup>1</sup> (+)- and (-)-chizhiene C,<sup>2</sup> and (+)- and (-)-lingzhines E-F,<sup>3</sup> together with their enantiomers and diastereomeric congeners. The strategy centred on the efficient preparation of key intermediates, which enabled divergent synthetic routes by a Michael addition with TBS-MAC, followed by meticulously designed deprotections and functional group manipulations.

## Figure/Scheme (if any):



Keywords: Total synthesis, natural products, baoslingzhines, TBS-MAC.

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**Research Area:** Total synthesis of bioactive natural products.

## P-05; Metal-Free C-S Coupling Enables Access to Sulfur-**Containing Bioactive Noscapinoids**

Amit Kumar Pradhan, and Dr. Laxmidhar Rout2\*

**Abstract:** Sulfur-containing pharmaceuticals—such as sulfonamides, thioethers, sulfones, and penicillin-represent essential scaffolds that have been widely explored for both their synthesis and therapeutic applications. Organosulfur compounds account for roughly 25% of all pharmaceutical drugs, making sulfur the third most common heteroatom in medicines, following nitrogen and oxygen. Several organosulfur-based drugs, including ritonavir, arbidol, and baricitinib, are currently undergoing clinical trials for their efficacy against SARS-CoV-2. Among notable examples, cotarnine, a tetrahydroisoquinoline derivative derived from noscapine, demonstrated promising biological activity. Recently, a metal-free C-S coupling method has been established using sulfur derivatives and cotarnine analogs, providing excellent chemoselectivity, scalability, straightforward product isolation. Ongoing biological evaluations aim to further assess the therapeutic potential of these synthesised compounds.

$$R_1$$
 R-SH  $CH_3OH$   $OMe\ S$   $R$   $R_1$   $R_2$   $R_3$   $R_4$   $R_4$   $R_5$   $R_6$   $R_7$   $R_8$   $R_8$   $R_9$   $R$ 

**Scheme:** metal-free synthesis of sulfur-based tetrahydroisoguinoline derivative.

**Keywords:** metal-free, bioactive, noscapine, C-S coupling.

#### References:

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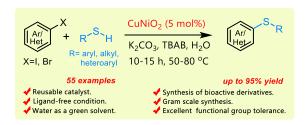
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Research Area: organic synthesis

# P-06; CuNiO<sub>2</sub> Nano Catalyst for Efficient Csp<sup>2</sup>-S Bond Formation in Water: Toward Green Synthesis of Bioactive Molecules

Amlan Swain, 1 Dr. Laxmidhar Rout, \*2 Prof. D. K. Mohapatra\*3

Abstract: Sulfur compounds display tunable biological activity, and in general, approximately 20% of all drugs approved by the FDA contain organosulfur compounds as a core unit [1]. Metal-catalyzed Csp2-S crosscoupling has been an indispensable tool for this purpose. A Green and efficient method for Migita-type Csp2-S cross-coupling of aryl halides with thiols has been developed using a heterogeneous CuNiO2 bimetallic nanocatalyst. This low-cost, easily synthesized catalyst operates under ligandfree conditions in water, enabling the coupling of aliphatic, aromatic, and heterocyclic thiols with challenging electrophiles like 3-bromopyridine, 2bromoquinoline, and 5-bromo-1H-indole. The methodology has been extended for the synthesis few drug molecules, such as Vortioxetine, Potent β-HSD-1 Inhibitor, and some other molecules with anticancer and antibacterial properties. Control experiments confirm a synergistic effect between Cu and Ni, while DFT calculations indicate that the reaction preferentially occurs at the Ni center, with an overall Gibbs free energy change of -102.7 kcal/mol.



**Scheme 1:** CuNiO<sub>2</sub> catalysed C-S cross coupling in aquous medium.

**Keywords:** nano catalyst,  $C_{sp2}$ -S Cross-coupling, ligand free, water solvent, DFT calculation.

### References and Notes:

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**Email ID:** as.rs.chem@buodisha.edu.in<sup>1</sup>, ldr.chem@buodisha.edu.in<sup>2</sup>, mohapatra@iict.res.in<sup>3</sup> **Research Area:** Sustainable Organic Synthesis, Bimetallic Catalysis

## P-07; Efficient Renewable Hydrogen Production from Glycerol Using Water Soluble Bifunctional Ruthenium Catalyst

Ankita Mandal, 1 Satabdee Tanaya Sahoo, Dr. Prosenjit Daw\*2

**Abstract:** Considering the increasing global energy and environmental challenges, the replacement of non-renewable sources, which currently fulfill more than 90% of our energy requirements and serve as feedstocks for the chemical industry is essential. Thus, the synthesis of value-added chemicals from biomass or its derivatives is considered as a key tactic in reducing the global dependency on fossil resources and including renewable resources in a circular economy. In this context for the production of green hydrogen from biomass derived feedstock, we employed a water-soluble, bifunctional NNN-Ru system bearing protic arms in a ligand scaffold. This complex is highly liable for a metal-ligand cooperativity pathway as well as a secondarycoordination-sphere with hydrogen-bond interaction for the appropriate substrate orientation at the active center. Our water-soluble catalyst exhibits superior performance for hydrogen evolution, rather than the catalyst which employs alternative organic solvents like diglyme, demonstrating enhanced efficiency in green hydrogen production. Along with this a high catalytic efficiency for the selective production of hydrogen and lactic acid from glycerol under mild reaction conditions, where a TON of 11,116 was achieved. Keywords: Lewis acids, Claisen rearrangement, ynamide, lactones.

**Keywords:** Water- soluble, Circular Economy, Bifunctional, Metal-ligand Cooperativity, Green Hydrogen.

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Research Area: Organometallic, Homogenous catalyst & Renewable Energy lab.

# P-08; Cu-Catalyzed Acylsilylation of Allenes Using Silylboronates and Acyl Fluorides

<u>Bikash Kumar Sahoo</u><sup>a</sup>, Purabi Kara, Jyotsnarani Panda<sup>a</sup>, Saikat Berab and Debobrata Sheetb and Saroj Kumar Rout\*

**Abstract:** A copper-catalyzed acylsilylation of allenes with silylboronate and acyl fluorides to access  $\beta$ -silyl  $\beta$ ,  $\gamma$ -unsaturated ketones<sup>1-3</sup>. Acyl fluorides were found to be more effective than acyl chlorides, showing higher reactivity under mild reaction conditions. This project is currently in the developmental stage, focusing on a detailed investigation of the reaction scope and mechanism<sup>4,5</sup>

**Keywords:** Copper-catalyzed, silylboronates, allene, acyl fluoride and acylsilylation.

### References

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**Research Area:** Organic Chemistry

# P-09; Asymmetric synthesis of (+)-isoboonein, (-)-boschnialactone, (+)-scholarein (putative structure) and the (+)-dioxa-[5.5.5.6]fenestrane core present in asperaculin A

### Biswajit Panda, Tabrez Khan\*

Abstract: Intramolecular Pauson-Khand reaction (IPKR) has emerged as a compelling strategy for accessing fused cyclopentenones embedded in diverse natural products.¹Given the immense synthetic potential of IPKR, we too exploited the same for accessing diverse iridoid monoterpenoids<sup>2</sup> and the dioxa[5.5.5.6]fenestrane core of sesquiterpenoid asperaculin A, in a racemic fashion.3 However, here we demonstrated A chiral pool strategy for divergent access to (+)-isoboonein, (-)-boschnialactone, (+)-scholarein (putative structure), and the (+)-dioxa-[5.5.5.6] fenestrane core present in asperaculin A. The synthesis features a stereoselective intramolecular Pauson-Khand reaction (IPKR) on a chiral envne ether and other synthetic manipulations stereoselective to access monoterpenoids. Also, easy accessibility to enediyne ether-based precursor enables one-pot access to the tetracyclic fenestrane core of asperaculin through a tandem IPKR.

$$\begin{array}{c} \text{H.} \\ \text{H.} \\$$

**Keywords:** Asymmetric synthesis  $\bullet$  intramolecular Pauson-Khand reaction  $\bullet$  chiral enyne ether  $\bullet$  asperaculin A  $\bullet$  fenestrane core

### Reference:

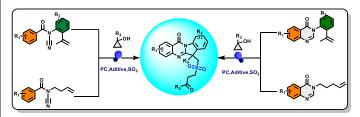
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Research Area: Total Synthesis of Bioactive Natural Products

## P-10; Visible-Light Promoted Photoredox Catalysed Strategies Embracing Activated and Unactivated alkene Bis-Functionalization for Synthesis of S(VI)-Functionalized Polyheterocyclic Quinazolinone

### Chandrakanta Sahoo, 1 Tabrez Khan\*2

Abstract: Polycyclic quinazolinones represent a structurally diverse class of fused heterocycles with significant importance in medicinal and synthetic organic chemistry. Their rigid frameworks and hydrogen-bonding capabilities contribute to a broad spectrum of biological activities, including anticancer, antimicrobial, antiviral, and anti-inflammatory properties<sup>1</sup>. Over the past few decades, researchers have synthesised this core in various approaches like metal-catalysed annulation, intramolecular cyclisation, and multicomponent reaction in classical thermal ways, microwave-assisted, and a few in photochemical conditions. This makes enthusiasm to develop a novel method under visible light photo-redox conditions. A new functionality in polycyclic quinazolinone core, i.e,  $\gamma$ -keto alkylsulfonylation<sup>2</sup>, has been synthesised by using an activated and unactivated alkene-containing quinazolinone core or N-cyanamide functionality with radical precursor cyclopropanol, followed by SO<sub>2</sub>- fixation using DABSO, additive  $K_2S_2O_8$ , solvent DMSO at 456 nm with moderate to excellent yield. This method features mild reaction conditions, readily available starting materials, and valuable synthetic utility with a broad substrate scope.



**Keywords:** (Visible Light Photo-redox reaction, Polycyclic Quinazolinone, Cyclopropanol, γ-keto alkylsulfonylation).

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Research Area: Total Synthesis of bioactive natural products, Synthetic method development in photochemical and electrochemical conditions

# P-11; 1,6-Hydrosulfonylation of p-Quinone Methides Enabled via Strain-Release-/Aromaticity-Driven Alkyl Radical Generation and SO2-Capture: Synthesis and Antiproliferative Studies of Sulfonylated Diarylmethanes

### Dipun Kumar Penthi, 1 Tabrez Khan \*2

Abstract: The integration of γ-keto sulfones, despite being a medicinally relevant building block with the bioactive diarylmethane motif, remains elusive. On the other hand, the fixation of SO2 in organic molecules for accessing value-added products is gaining wide attention in organic synthesis. Herein, we disclose the 1,6hydrosulfonylation of p-quinomethides via the strain-release driven ring-scission of strained 3°-cyclopropanols in the presence of a SO2-surrogate like K2S2O5 and a Bronsted acid under visible-light photoredox catalysis to access a library of y-keto alkylsulfonylated diarylmethanes in moderate to good yields. Also, the 1,6hydrosulfonylation of p-quinone methides is developed via the aromaticity-driven bond-scission in pro-aromatics like 4-alkyl-1,4-DHPs in the presence of K<sub>2</sub>S<sub>2</sub>O<sub>5</sub> and a Bronsted acid under visible-light photoredox catalysis to access a library of alkylsulfonylated diarylmethanes. The efficiency of the developed reactions has been established through broad substrate-scope studies, and the mechanistic probing studies have been complemented with DFT calculations to support the proposed mechanisms. In addition, antiproliferative studies revealed oral cancer activity for some of the synthesized sulfonylated diarylmethane derivatives.

Keywords: Photoredox Reaction, p-QMs, Hantzsch ester, Cyclopropanol,  $SO_2$  surrogates

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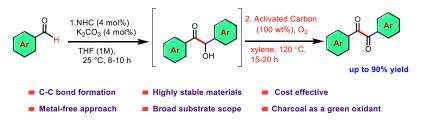
Research Area: Heat-/Light- mediated Catalytic / Non-Catalytic Synthetic Method Development for Functionalized Heterocycles/ Carbocycles Synthesis.

## P-12; A Green One-Pot Strategy for the Direct Synthesis of Benzil

### Jayshree Nandkumar Solanke, Rambabu Dandela\*

**Abstract:** A practical and green methodology has been developed for the direct synthesis of arylated 1,2-diketones from aldehydes utilizing 4 mol% of N-heterocyclic carbenes (NHC) organocatalysts and activated carbon. The design of this method is a one-pot, two-step sequence: NHC-catalysed benzoin condensation followed by aerobic oxidation in the presence of activated carbon (AC) and molecular O<sub>2</sub>, offers good to high yields, tolerating various functional groups. This method demonstrates a sustainable and ecofriendly protocol for efficiently synthesizing benzil scaffolds from a wide range of aldehydes directly through one-pot conversions. Catalyst loading, solvent screening, and mechanistic experiments were also performed to understand the roles of NHC catalysts and activated charcoal.

## Figure:



**Keywords:** • Benzoin • benzil • activated carbon • N-heterocyclic carbene (NHC) • organocatalysis

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Research Area: Organocatalysis

## P-13; Heteroleptic Coinage Metal Complexes Bearing Redox-Active Carbenes and Carbazoles towards Alkyne-Azide Cycloaddition Reaction

### Ivotikiran Sahoo and Adinarayana Doddi\*\*

ABSTRACT: N-Heterocyclic carbenes (NHCs), distinguished by their finely tunable steric and electronic properties, have become indispensable in both main-group and transition-metal organometallic chemistry. Their strong o-donor ability and structural adaptability make them highly effective ancillary ligands in homogeneous catalysis, where they play pivotal roles in diverse small-molecule activation processes.[1] Among the various classes of NHCs, those incorporating redox-active functionalities exhibit intriguing and often unusual chemical and physical properties. In this context, naphthoquinone-annulated NHCs represent a particularly interesting yet relatively unexplored subclass, despite their proven synthetic accessibility.<sup>[2]</sup> These NHCs form strong σ-donor bonds with metal centres, thereby enhancing catalytic activity and selectivity in diverse transformations such as cross-coupling and polymerisation reactions. Furthermore, NHC-based complexes contribute to the development of advanced materials, including conducting, magnetic, and optically active systems. The stabilisation and electronic tuning of metal centres by such ligands open avenues for innovative material design. In this regard, a series of redox-active metal complexes bearing cyclic and acyclic amide substituents has been synthesised and structurally characterised. The photophysical and electrochemical properties of these newly synthesised Carbene-Metal-Amide complexes will be presented along with their catalytic activity towards the 'Click' reaction.

Scheme. Redox-active NHC carbene-based amide complexes and their application

**Keywords:** N-heterocyclic carbenes, Redox active, organometallic chemistry, Photophysical properties, Click

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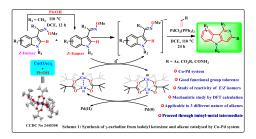
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# P-14; Mechanistic Insights into E/Z-Selective Reactivity of Indolyl Ketoximes in Cu-Pd Catalysed γ-Carboline Synthesis

### Madhab Chandra Maity, Prof. Shantanu Pal\*

ABSTRACT: y-Carbolines are biologically significant nitrogen heterocycles with broad pharmaceutical potential.1 Hence, there is growing interest in developing efficient routes from indolyl ketoximes and alkenes, but isomeric selectivity of the ketoximes remains a major challenge for y-carboline formation. Existing methods lack clear insight into this selectivity and have largely failed to achieve γ-carboline synthesis with copper salts instead of silver.2 Here, we report an efficient Cu-Pd bimetallic strategy for synthesizing y-carbolines in high yield and with wide substrate scope from alkenes and O-methyl indolyl ketoximes. We systematically studied the isomeric selectivity and reactivity of indolyl ketoximes. UV-visible spectroscopy and crystallography revealed that Cu(OAc)2 in presence of pivalic acid exists as a Cu(OPiv)2 dimer in solution. Mechanistic analysis supported by DFT calculation revealed that reaction is initiated by the N-O bond cleavage via single electron transfer (SET) from Cu2(OPiv)4 to indolyl ketoxime form iminyl Cu intermediate. Then it undergoes transmetalation with Pd(II) followed by alkenylation and C-N bond formation to yield γ-carbolines. This study delivers a practical Ag-free route to γcarbolines and uncovers fundamental principles of Cu-Pd cooperation in heterocyclic synthesis.



Keywords: γ-Carboline, Cu-Pd system, Selectivity, Reactivity, Cu<sub>2</sub>(OPiv)<sub>4</sub> dimer, SET

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Research Area: Transition metal catalysed C-H activation and functionalization

# P-15; Cobalt-Catalyzed Deoxygenative Coupling of Ethers to Alkanes

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ABSTRACT: Alkanes have extensive applications in diverse fields and their natural abundance is dwindling. Ethers are prevalently present in biomolecules and synthetic compounds; however, despite recent progress in their transformations they are considered as unreactive functionalities, and widely used as solvents in transition metal catalyzed reactions. Hence, catalytic synthesis of alkanes from bio-ample ethers is highly desirable. A simple cobalt catalyzed double C-O bond activation of ethers is attained now; diverse symmetrical and unsymmetrical arylmethyl ethers (ArCH2OCH2Ar') are selectively transformed to 1,2-diaryl alkanes. This protocol is extended towards unsymmetrical arylmethyl alkyl ethers which furnished linear alkyl arenes. Synthesis of biologically active compounds is also achieved utilizing this catalytic method. Consumption of ethers in catalytic deoxygenative coupling to alkanes follows first-order kinetics. Mechanistic studies indicate that the reactions proceed through molecular intermediates and involve arylmethyl and alkyl radicals. DFT analysis reveals that the in situ generated radical either abstracts a proton from silane, resulting in C-H bond formation or attacks the aryl silyl ether, leading to C-C coupling. The reaction mechanism involves intermediates with different spin multiplicities and spin crossover through minimum energy crossing points (MECPs).



**Keywords:** cobalt pincer complex • C-O activation • deoxygenative coupling • DFT calculations • minimum energy crossing points • homogeneous catalysis

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Research Area: Organometallic Catalysis, Organic Synthesis

# P-16; N-Heterocycle-Functionalized Resorcin[4]arene Cavitands: Design, Synthesis, and Biological Applications

Manas Ranjan Swain, Manini Nayak, Anita Pati\*

**ABSTRACT:** Resorcin[4]arenes constitute a unique class of supramolecular typically synthesized through the acid-catalyzed building blocks condensation of resorcinol with aldehydes. Their well-defined cyclic tetrameric architecture, enriched with a π-electron-dense cavity, provides a versatile platform for structural modification. Functionalization at the upper and lower rims, along with the presence of multiple hydroxyl groups, enables the creation of diverse resorcin[4] arene-based cavitands with broad utility in host-guest chemistry, nanoscience, catalysis, and medicinal chemistry. Nheterocyclic moieties play essential roles in biochemistry, pharmaceutical chemistry, and materials science. The incorporation of tetrazole, pyrrole, pyridine and triazole units into resorcinol frameworks significantly enhances their functional value, enabling a broader range of advanced applications. A survey of the literature indicates that N-heterocycle-based resorcin[4] arene cavitands exhibit significant interactions with bovine serum albumin (BSA), emphasizing their potential in biomedical pharmacological applications. These interactions highlight the promise of Nheterocyclic resorcin[4]arene derivatives as emerging pharmaceutical candidates, paving the way for further exploration of their biomolecular recognition capabilities. Therefore, the present work focuses on the design and synthesis of N-heterocycle-functionalized resorcinarene cavitands and the investigation of their biological applications.

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Research Area: Synthetic Organic Chemistry and Supramolecular Chemistry

## P-17; A Novel Heterogeneous CuMoO<sub>4</sub> Nanocatalyst for Heck Reactions

### Papita Behera, 1 Laxmidhar Rout\*

**Abstract:** The Heck reaction is a cornerstone transformation in modern synthetic chemistry. It is widely employed for the synthesis of internal alkene-based small drug molecules as well as complex multistep drug intermediates. This reaction is especially prominent in forming C(sp)²-C(sp)² bonds in pharmaceutical and material science applications. Here, we report an oxo-bridged CuMoO4 bimetallic nanocatalyst for the Heck reactions of alkenes with iodoarenes. The heterogeneous catalyst is easily synthesized via simple precipitation and features an oxo-bridge between the copper and molybdate centers. This bimetallic system enables ligand-free Heck couplings, affording *trans*-selective products with broad tolerance to various functional groups. Notably, this oxo-bridged catalyst exhibits excellent recyclability by retaining high catalytic activity for up to four cycles in DMSO without significant metal leaching. Furthermore, this protocol effectively synthesizes several biologically active molecules with anticancer, antifungal, and antibacterial properties.

Heterogeneous • Ligand-free • No leaching • Recyclable • Moderate temperature
 • Trans-selectivity • Broad substrate scopes • Gram-scale up

**Keywords:** Oxo-bridged, Nanocatalyst, *Trans*-olefins, Drug Molecules, Recyclable.

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Research Area: Synthetic Organic Chemistry

# P-18; Cu-O-Se Bridged Catalyst for Ligand-Free Sonogashira Coupling

### Pradyota Kumar Behera, Laxmidhar Rout\*1

**Abstract:** Most non-palladium catalysts for Sonogashira cross-coupling require elevated temperatures (120–140 °C) and tailored ligand architectures, while palladium systems typically rely on bulky electron-rich phosphines to achieve high efficiency. In contrast, we present a mild and practical protocol for C\_sp-C\_sp2 Sonogashira cross-coupling using the inexpensive and commercially available CuSeO<sub>3</sub> 2H<sub>2</sub>O catalyst. A broad range of terminal alkynes undergo coupling with aryl iodides and bromides to afford diaryl and aryl-alkyl acetylenes in high yields under ligand-free conditions. The method accommodates alkyl acetylenes, ethynylsilanes, and alkynols, demonstrating wide functional-group tolerance. DFT studies support a mechanism involving an oxygen-bridged Cu-O-Se bimetallic framework. Importantly, the reaction is palladium-free, with residual Pd levels verified to remain below 0.2 ppm.

Figure 1: CuSeO<sub>3</sub> Catalyst for Sonogashira Coupling

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Research Area: Synthetic Organic Chemistry

# P-19; Cascade Annulation Approach to Highly Functionalized Spiro[cyclopenta[c]pyrrole-indene] Triones under mild Metal-Free Conditions

Priteeparna Das, Sahil Mondal, Sayanta Roy, Rambabu Dandela\*, Thirupathi Barla\*

**Absract:** The development of concise synthetic routes to architecturally complex spiroand polycyclic frameworks remains an important challenge in modern organic synthesis. In this study, we describe a transition-metal-free strategy that enables the efficient construction of 3H-spiro[cyclopenta[c]pyrrole-4,2'-indene]-1',3,3'-triones through the intermolecular reaction of (*E*)-1-benzyl-4-benzylidenepyrrolidine-2,3dione with 2-keto-1,3-indandione.<sup>1-3</sup> The transformation proceeds under mild conditions and delivers the spiro-fused products in moderate to excellent yields across a diverse substrates. This method provides rapid access to densely functionalized heterocyclic architectures and demonstrates the utility of diketone-based cascade reactivity for assembling structurally intricate molecular frameworks.

### Scheme:

**Keywords:** Spirotrione frameworks, Spirocyclic compounds, Diketone cascade reaction, Polycyclic heterocycles, Annulation mechanisms

### References:

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**Research area:** Development of methodologies to synthesize heterocyclic compounds with significant biological properties.

## P-20; Ambiphilic Silyl-phosphine Ligands in Transition-Metal Chemistry: Utilisation in C-C Coupling Reactions and Transformation of CO<sub>2</sub> into value-added products.

Rageshree Dasha, Amiya Sahooa, and Adinarayana Doddi\*

**Abstract:** Phosphine ligands functionalized with Lewis acidic moieties — namely elements from groups 13 and 14 in their +3 and +4 oxidation states, respectively — have been extensively explored as ambiphilic ligands in coordination and organometallic chemistry. 

1 Ortho-silyl arylphosphines bearing Si–R substituents (R = H, CH<sub>3</sub>, Ph) display distinctive coordination and reactivity patterns toward transition metals. 

12 In this work, we describe the synthesis and structural characterization of a series of square-planar Pd(II) complexes incorporating silylphosphine ligands. 

3 Treatment of Si–H functionalized phosphines with  $[Pd(\eta^3-allyl)X_2](X = Cl, Br, I)$  affords dimeric  $[\{P,Si\}PdX]_2$  complexes via Si–H bond activation, leading to well-defined Pd–Si bonds. One representative Pd–Si complex was evaluated as a molecular catalyst for hetero carbon–carbon coupling reactions, producing alkynyl products in good to excellent yields while effectively suppressing Glaser-type homocoupling.

In addition, both neutral and cationic Cu complexes supported by silylphosphine ligands featuring Si-H agostic interactions have been investigated. The cationic Cu complex efficiently catalyzes the selective conversion of amines to *N*-formylated amines using CO<sub>2</sub>.

Keywords: Silyl phosphines, Sonogashira coupling, and N-formylation.

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Research Area: Organomettalic chemistry and homogenous catalysis.

# P-21; Exploration of titanocene(III) chloride in de-iodination reaction of active iodide

### Ranjan Kumar Panigrahi and Samaresh Jana\*

**Abstract:** Titanocene (III) chloride mediated deiodination reaction of benzyl iodide has been reported. The reaction proceeds through a benzyl radical. This benzyl radical reacts with another benzyl radical to form a bibenzyl product. Also, the radical has been trapped using one electron deficient double bond. Titanocene(III) chloride is generated by using Cp<sub>2</sub>TiCl<sub>2</sub> and activated Zn dust in deoxygenated THF under argon condition. As Ti(III) is a single electron donor, it can readily reduce the active iodo compound to form the corresponding carbon radical, which further reacts with appropriate functionality to obtain the desired product. The product obtained from the reaction mixture does not require any purification on column chromatography.

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## P-22; REGEOSELECTIVE HYDRO-HETEROARYLATION OF 1,6-DIYNE VIA CARBOXAMIDE ASSISTED INDOLE C(2)-H ACTIVATION USING COBALT CATALYST

Saista Afreen, a,b , Ponneri C. Ravikumar\*a,b

**Abstract:** In this study, the novel reactivity of a cobalt (III) catalyst in the functionalization of 1,6-diynes was presented. The reaction mechanism was analyzed, revealing the in-situ generation of a six-membered cobalta cycle, which subsequently underwent further functionalization with 1,6-diynes. Experimental evidence from radical quenching experiments indicated the involvement of an ionic pathway in this conversion. Furthermore, the hydrogen scrambling experiment lent further support to the proposed mechanism. Significantly, this methodology exhibited extensive versatility, accommodating a diverse array of electronically distinct substrates and reactive partners in a highly atom-efficient manner.

**Keywords:** Hydroindolation; 1,6-diyne; Earth abundant cobalt catalyst; C H activation; Strong-chelation

### References and Notes.

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# P-23; N-Heterocyclic Vinyl Phosphines Enabling Metal-Free CO<sub>2</sub> Insertion and Reductive Formylation

S.K. Maharana, A.K. Sahoo and Adinarayana Doddi\*

**Abstract:** Since the pioneering work by Stephan and co-workers in 2009, the activation of small molecules such as CO2 and CS2 using Lewis basic phosphine donors has garnered significant attention within the domain of main-group chemistry<sup>1</sup>. While frustrated Lewis pair (FLP) systems have demonstrated remarkable efficiency as metalfree platforms for the activation and transformation of these substrates, systems that rely exclusively on Lewis bases-particularly phosphine donors-have remained comparatively underexplored<sup>2</sup>. This limitation stems primarily from the intrinsic instability of the resulting adducts in the absence of a complementary Lewis acid, posing both synthetic and mechanistic challenges. Nevertheless, the exploration of phosphine donors as standalone activators offers an exciting and largely untapped avenue in small molecule activation and sustainable catalysis. Herein, we report for the first time the design, synthesis, and structural characterisation of highly nucleophilic phosphine donors coordinated to n-heterocyclic olefins (NHOs), which serve as robust platforms for the activation of small molecules. The NHO-phosphine systems of the general formula (NHO)PR<sub>2</sub> (R = Ph, tBu) have been successfully prepared and fully characterised by spectroscopic and crystallographic methods<sup>3</sup>. These phosphines exhibit remarkable reactivity toward small molecule substrates such as CO2 and CS2, furnishing insertion products of the type [(NHO)CE<sub>2</sub>PR<sub>2</sub>] (E = O, S), including cyclic carbonates and thiocarbonates, which are highly valued as synthetic intermediates and functional materials. Furthermore, the N-heterocyclic vinyl phosphine derivatives derived from these systems have been employed as efficient transition metal-free catalysts for the reductive formylation of amines and amides, thereby offering a sustainable and environmentally benign approach to carbon-heteroatom bond formation4.

Keywords: Small molecules, main group chemistry, N-heterocyclic olefin phosphine

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Research Area: Organometallic and main group Chemistry

# P-24; Mechanochemical synthesis of phosphoryl amides and esters from diphenylphosphoryl azides under mild conditions

### Savita Gat,1 Rambabu Dandela \*2

**Abstract:** A simple, efficient, and one-step synthetic procedure to construct phosphoryl amides and esters has been developed applying mechanochemistry. A ball-milling technique easily facilitated the amination and esterification of diphenylphosphoryl azides (DPPA) in the presence of molecular iodine and sodium carbonate via cleavage of P-N bond. The metalfree mechanochemical protocol enables the transformations to provide a variety of alkyl phosphoryl amides and esters under solvent-free conditions and at room temperature. Moreover, readily available, and inexpensive starting materials, excellent functional group compatibility, rapid synthesis, high yields of the products, and mild conditions are the notable features of the present method.

**Keywords:** Mechanochemistry, Metal-free methodology, phosphoryl amides, phosphoryl ester.

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Research Area: Organic Synthesis

# P-25; Three-Component Reaction through Rh(III) Catalyzed Strain Release of Bicyclo[1.1.0]butanes

### Shubham Dhal, Ponneri C. Ravikumar\*

**Abstract:** A three-component reaction through Rh(III)-catalyzed strain release of bicyclo[1.1.0]butanes (BCBs) to synthesize substituted acrylamides was realized. This protocol represents the first example of nucleophilic attack on the Rh(V) nitrenoid complex generated by the coupling of phenoxyacetamides and strained BCBs. The reaction proceeds under mild conditions and demonstrates broad compatibility with various functional groups on both phenoxyacetamides and nucleophiles, affording valuable substituted acrylamides. Furthermore, the products can be further transformed into important synthetic building blocks. Preliminary mechanistic studies support the proposed catalytic cycle.

Keywords: (Strain release, Three component, BCB).

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**Research Area:** (Transition metal catalysis)

# P-26; Strategies to Alter the Typical Reactivity of Cu-Allenylidene and Anilines

## Subhra Kanti Mahato, 1 Dr. Amit Kumar Simlandy\*2

**Abstract:** Altering the typical reactivity of a substrate is of prime interest as it has the potential to create new avenues that would expand the chemical space. In this study, we have utilized two crucial parameters: hydrogen bonding and steric to alter the well-established reactivity of propargylic carbonated-derived Cu-allenylidene intermediate and aniline derivatives. These two parameters reduce the nucleophilicity of the aniline, thereby allowing time to convert the initially formed Cu-allenylidene intermediate to allenal. These slow-reacting amines thereby react with the allenal, providing either a sterically congested secondary enaminal or undergo annulation to produce the nitrogenous heterocycles. It was found that the conformational rigidity of the aniline derivatives plays a decisive role in controlling the chemo selectivity.

**Keywords:** Conformational rigidity, Mechanistic divergence, Annulation, Allenal.

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Research Area: Asymmetric Catalysis and organic synthesis

# P-27; Synthesis of Spiro[indane-1,3-dione-2-pyrrolidines] by the Reaction of 2-(2'-Ketoalkyl)-1,3-Indandiones with Triazinanes

### Susmita Sahoo, Biral K Pal, Barla Thirupathi\*

Abstract: As part of an ongoing research interest in the exploration of the various reactions by 2-(2'-Ketoalkyl)-1,3-indandiones.1-4 We became interested in utilizing 1,3,5-triazinanes as one of the reacting partners with 2-(2'-Ketoalkyl)-1,3-indandiones. Because 1,3,5-triazinanes have emerged as an important class of such synthons. Structurally, they can be regarded as cyclictrimers of formaldehyde imine, and functionally, they act as masked equivalents of reactive iminium or aminoalkyl intermediates. Spiropyrrolidines, derivatives are specially privileged motifs that have conquered an inevitable space in the modern therapeutic world. These types of structural frameworks have been found to be the core structure of many alkaloids and natural products with amazing biological properties, which enhance the quality of human life. A straightforward and transition metal-free approach for the synthesis of highly functionalized spiro[indane-1,3-dione-2-pyrrolidines] has been demonstrated. The reaction of 2-(2'-ketoalkyl)-1,3-indandiones with triazinanes proceeds efficiently to afford a wide range of spirocyclic products in good to excellent yields.<sup>5</sup> The versatility of the method was further demonstrated by the successful incorporation of various drug molecules and chiral amines, highlighting its potential for application in medicinal and synthetic organic chemistry.

**Keywords:** 2-(2'-Ketoalkyl)-1,3-indandiones; Spiro[indane-1,3-dione-1-pyrrolidine]; Spirocycles, Heterocycles

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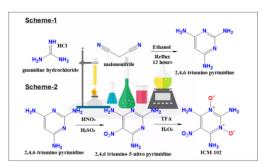
Research Area: Synthetic methodology development

## P-28; Cost-Effective Synthesis and Alternative Oxidation Strategies for N-Oxide Derivatives of 2,4,6-Triaminopyrimidine (TAP)

### Harsh Hirpara<sup>1</sup>, Dr. Rambabu Dandela\*<sup>2</sup>

Abstract: 2,4,6-Triaminopyrimidine (TAP) is a valuable heterocyclic precursor, but its high cost and reliance on column chromatography limit broader applications. In the previously described procedure, the use of base during synthesis often led to increased impurities, complicating purification. In our novel method, the base was eliminated and the reaction time extended to 12 hours (Scheme-1). Our work resulted in fewer impurities while maintaining a good yield, offering advantages of reproducibility, cost-effectiveness, and simplified purification compared to the conventional approach. Beyond methodology, TAP prepared through this route was successfully utilized in the synthesis of an insensitive energetic material (Scheme-2), demonstrating its practical utility in advanced material development. The ability to access TAP more economically and cleanly enhances its potential for scalable heterocyclic chemistry and specialized applications. This work highlights methodological innovation and application, balancing cost-effectiveness, sustainability, and reproducibility in organic synthesis.

### Scheme/diagram:



**Keywords:** Base-free synthesis, Insensitive Energetic Molecule, N-oxide formation, Cost-effective methodology

### References and Notes:

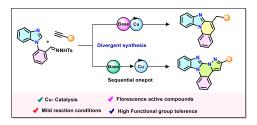
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## P-29; Cu-Catalyzed Divergent Synthesis of Benzimidazole-Fused N-Heterocycles via C-C and C-N Bond-Forming Reactions Manthri Atchuta Rao, 1 Prof. Shantanu Pal\*2

Abstract: Polycyclic nitrogen-containing frameworks are widely recognized for their prevalence in natural products, pharmaceuticals, and functional materials. Among these, benzimidazole and pyrazole scaffolds stand out due to their characteristic reactivity profiles and broad applications. The fusion of diverse heterocyclic motifs with the benzimidazole core has enabled the development of structurally rich polyheterocycles exhibiting notable photoelectronic and biological properties [1]. Recent advances in copper-catalyzed transformations have further accelerated progress in this area, offering efficient and versatile tools for heterocycle construction [2]. In this context, we report a straightforward and divergent synthetic strategy for accessing benzimidazole-fused polyheterocycles through intramolecular C-C and C-N bond-forming processes, modulated by the controlled introduction of a copper catalyst. Mechanistic studies indicate that the reaction proceeds via intra molecular C-C coupling and other another one is benzimidazole-assisted dehydrogenative C-N coupling that liberates H2 gas, ultimately affording the desired fused heterocycles in good yields. The generality of this method is highlighted by its compatibility with various substrates, enabling the efficient synthesis of structurally diverse benzimidazole-fused systems. Moreover, the resulting compounds exhibit strong fluorescence emission with high quantum yields, underscoring their potential utility in optoelectronic and photophysical applications [3].

### Scheme/diagram:



Keywords: Cu-Catalysis, Fused N-hetrocycles, Organic synthesis

### References and Notes:

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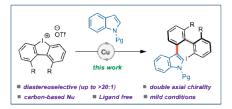
Research Area: Organic synthesis

# P-30; Diastereoselective Synthesis of Double Axially Chiral Indole Derivatives via Friedel-Crafts Biarylation

Arijit Banerjee, 1 Akanksha Yadav, Prasoon Raj Singh, Dr. Amit Kumar Simlandy\*2

**Abstract:** C-C bond formation between heterocycles and biaryls through transition metal catalysis has led to advances in modern-day chemistry. Diving into the more specific, deeper research area, scientists have not shed much light on C-C coupling between arene and heteroarene moieties using cyclic diaryliodonium salts. Currently, our research is concentrating on synthesizing axially chiral biaryl atropisomers, which can be found in several natural products with biological activities.

The enantioselective ring opening of cyclic diaryliodonium salts with different heteroatoms has been well explored to date;1 however, the reactivity of various carbon-based nucleophiles remains elusive to chemists. Given the abundance of indole motifs in various biomolecules and the well-known generation of point chirality at the C3 position of indole via dearomative arylation,2 We aimed to develop a protocol using Friedel-Crafts biarylation to introduce an axially chiral biaryl motif at the C3 position of an indole. This method becomes well-tolerated with various substituted indoles and different types of cyclic diaryliodonium salts, where the torsional strain in the cyclic diaryliodonium salt plays a crucial role in enabling the reaction. Scheme/diagram:



**Figure 1**:<sup>3</sup> Synthesis of double axially chiral indole derivatives via Friedel-Crafts biarylation

Keywords: Cu-Catalysis, Fused N-hetrocycles, Organic synthesis

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Research Area: Asymmetric Synthesis & Catalysis

