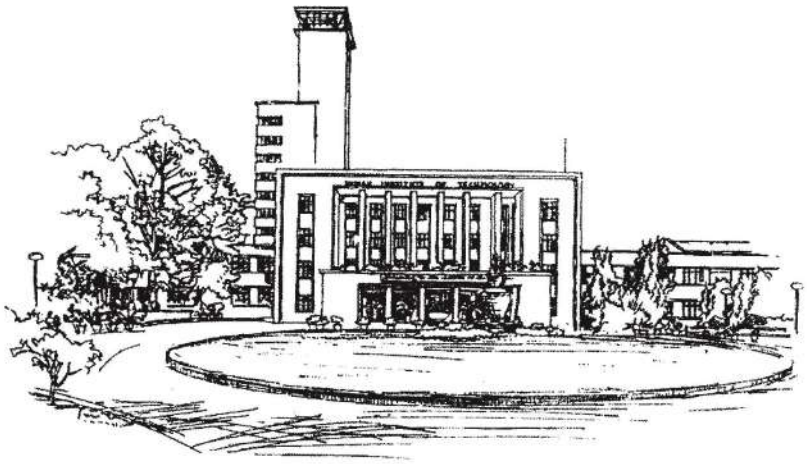
Indian Institute of Technology Kharagpur

WELCOME

ETCS-2024



2nd International Conference on

EMERGING TRENDS IN CATALYSIS & SYNTHESIS

07-09 March, 2024

Organized by
Department of Chemistry
IIT Kharagpur

Programme and Abstract

About The ETCS-2024 Conference

The ‘Emerging Trends in Catalysis & Synthesis’, in short ETCS, is an International Conference started at the Department of Chemistry, IIT Kharagpur in 2020 (**ETCS 2020**). This conference is a themed based conference focusing on the various aspect of catalysis and synthesis. The department of Chemistry, IIT Kharagpur is the first department in chemistry among the chains of all IITs. IIT Kharagpur is one of the leading and oldest IIT among chain of IITs in India. The first version of this conference was realized after a long initial planning of three years dated back to 2016. It was first a two-day conference involving around 24 invited talks, 50 posters, and 200 participants. Now, the second version of this international conference (**ETCS 2024**), have been expanded to a three-day event spanning between 7th March to 9th March, 2024. Intense scientific discussion among eminent researchers across the world from both academia and industry are prime focus of this conference. More than 42 invited lectures, 24 flash talks, and 110 poster presentations are planned for this event. More than 90 faculty participants from outside IIT Kharagpur, about 10 delegates from industries, about 150 PhD scholars, and more than 100 UG and PG students from various institutions and Universities are expected to participate in this conference. The scientific program will include a broad spectrum of inorganic and organic chemistry covering total synthesis, organometallics and catalysis, photocatalysis, organocatalysis, peptide chemistry, asymmetric catalysis, supramolecular chemistry, and computational chemistry. It will also empower the researchers to identify possible areas where collaborative work may be carried out for better understanding of a complex system or designing new catalysts, reactions, and materials.

ABOUT THE VENUE

The Indian Institute of Technology Kharagpur (IIT Kharagpur) is a institutution established by the government of India in 1951. It is the first IITs established in India and is recognized as an Institute of National Importance. In 2019 it was awarded the status of Institute of Eminence. The institute was initially established to train scientists and engineers after India attained independence in 1947. However, over the years, the institute's academic capabilities diversified with offerings in management, law, architecture, humanities, etc. IIT Kharagpur has an 8.5 square kilometres (2,100 acres, one of the largest campus in India) campus and has about 25,000 residents. The students and alumni of IIT Kharagpur are informally referred to as KGPians. On the grounds that West Bengal had the highest concentration of industries at the time, Bidhan Chandra Roy, the Chief Minister of West Bengal, persuaded Jawaharlal Nehru (India's first prime minister) to establish the first institute in West Bengal. The first Indian Institute of Technology was thus established in May 1950 as the Eastern Higher Technical Institute. It was located in Esplanade East, Calcutta, and in September 1950 shifted to its permanent campus at Hijli, Kharagpur. Hijli had been used as a detention camp during the British colonial rule in India, to keep Indian freedom fighter’s captive. The name "Indian Institute of Technology" was adopted beforethe formal inauguration of the institute on 18th August 1951 by Maulana Abul Kalam Azad.

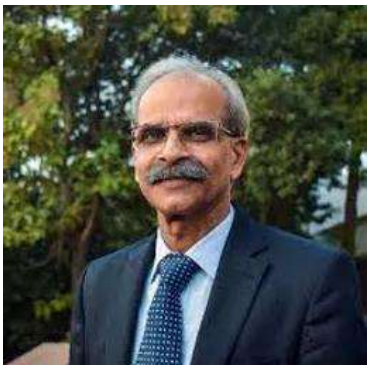
PLACE AND CLIMATE

The best time to visit Kharagpur is during the spring. This time of the year offers a pleasant weather in West Bengal and draws in tourists. This is the absolute time span over the year to plan a family holidays and even if you are with your coluges to enjoy the peaceful nature. The minimum temperature goes down to 15 °C and the maximum temperature generally hold in between 24 °C to 28 °C.

PLACES TO VISIT

Tourist visits the following places in West Bengal (Near Kharagpur): Historical Nehru Museum of Science and Technology, Kharagpur, Digha, Mandarmoni, Jhargram, Purulia, Temples in Bishnupur, Birla Planetarium, Belur Moth, Fort William, Victoria Memorial, Chandipur Beach, Digha Beach, Indian Museum, Science City, Eden Garden, Birla Industrial and Technological Museum, Kalighat Temple, The Botanical Garden, The Alipore Zoo, Nicco Park, Aquatica, Millenium Park.

Patron



Prof. Virendra Kumar Tewari
Director, IIT Kharagpur

Chairperson

Prof. Joykrishna Dey
HoD-Chemistry, IIT Kharagpur

Conveners

Dr. Modhu Sudan Maji
Associate Professor
Department of Chemistry
IIT Kharagpur

Dr. Santanu Panda
Assistant Professor
Department of Chemistry
IIT Kharagpur

Programme Schedule

07th March, 2024 (Thursday)		
(8:00-9:00)	Registration	
(9:00-9:30)	Inauguration, Lamp Lighting, Welcome Remarks [Deputy Director; Dean, Faculty of Sciences; Associate Dean, International Relations; Head of the Department, Chemistry; Convener]	
Session 1: Dedicated to Zoetis (Kalidas Auditorium) **Chairperson:** Prof. Dipakranjan Mal, Ex-Professor, IIT Kharagpur		
IL-01 (9:30-10:00)	Prof. Vladimir Gevorgyan, University of Texas	
IL-02 (10:00-10:30)	Prof. Manas K. Ghorai, IIT Kanpur	
IL-03 (10:30-11:00)	Prof. Johannes F. Teichert, TU Chemnitz, Germany	
Tea/Coffee Break (11:00-11:30)		
Session 2: Dedicated to Syensqo (Kalidas Auditorium) **Chairperson:** Dr. Kaustav Chakraborty, Syensqo, India		
IL-04 (11:30-12:00)	Prof. Andy Lawrence, University of Edinburgh	
IL-05 (12:00-12:30)	Prof. Stellios Arseniyadis, Queen Mary University of London	
IL-06 (12:30-13:00)	Prof. Monika Raj, Emory University	
Lunch Break & Networking & Photo Session (13:00-14:30)		
Session 3 & 4 (14:30-16:30)	**Session 3: (Maitrayee)** **Chairperson:** Prof. K. C. Majumdar, Ex-Professor, University of Kalyani	**Session 4: (Gargi)** **Chairperson:** Prof. Debashis Ray, IIT Kharagpur
IL-07, 08 & 09 (14:30-15:00)	IL-07: Prof. Todd Marder, Julius-Maximilians-University of Würzburg	IL-08: Prof. Ajay Kumar Srivastava, CDRI Lucknow IL-09: Prof. Madhab C. Das, IIT Kharagpur
IL-10 & 11 (15:00-15:20)	IL-10: Prof. Subhas Chandra Pan, IIT Guwahati	IL-11: Prof. Jaideep Saha, NIPER Mohali
IL-12 & 13 (15:20-15:40)	IL-12: Prof. Indranil Chatterjee, IIT Ropar	IL-13: Prof. Chandan K. Jana, IIT Guwahati
IL-14 & 15 (15:40-16:00)	IL-14: Prof. Tabrez Khan, IIT Bhubaneswar	IL-15: Prof. Rajarshi Samanta, IIT Kharagpur
IL-16 & 17 (16:00-16:20)	IL-16: Prof. Jeyakumar Kandasamy, Pondicherry University	IL-17: Prof. Bidraha Bagh, NISER Bhubaneswar
FL-01 & 02, IL-18 (16:20-16:30)	FL-01: Anton Paar FL-02: Thermo Fisher Scientific	IL-18: PI Industries
Tea/Coffee Break (16:30-17:00)		

Session 5: Dedicated to TCG Lifesciences (Kalidas Auditorium) **Chairperson:** Dr. Uttam Khamrai, TCG Lifesciences, India	
IL-19 (17:00-17:30)	Prof. Buddhadeb Chattopadhyay, CBMR Lucknow
IL-20 (17:30-18:00)	Prof. Rafal Kowalczyk, Wroclaw University of Science and Technology
IL-21 (18:00-18:30)	Prof. Alakesh Bisai, IISER Kolkata
IL-22 (18:30-19:00)	Prof. Pazhamalai Anbarasan, IIT Madras
Session 6: (Kalidas Auditorium) **Chairperson:** Prof. Nikhil K. Singha, IIT Kharagpur	
FL-(03-08) (19:00-19:30)	Flash Lectures
Cultural Program & Dinner (19:45-21:45)	
08th March, 2024 (Friday)	
Session 7: Dedicated to PI Industries (Kalidas Auditorium) **Chairperson:** Dr. Ajay Singh Yadav, PI industries, India	
IL-23 (09:00-09:30)	Prof. Parthasarathi Das, IIT(ISM) Dhanbad
IL-24 (09:30-10:00)	Prof. Andy A. Thomas, Texas A&M University
IL-25 (10:00-10:30)	Prof. Martín Fañanás-Mastral, CiQUS, Spain
IL-26 (10:30-11:00)	Prof. Nitin T. Patil, IISER Bhopal
Tea/Coffee Break (11:00-11:30)	
Session 8: Dedicated to RSC (Kalidas Auditorium) **Chairperson:** Dr. Lijina MP, RSC, India	
IL-27 (11:30-12:00)	Prof. Santanu Mukherjee, IISc Bangalore
IL-28 (12:00-12:30)	Prof. Vinh Nguyen, UNSW Sydney
IL-29 (12:30-13:00)	Prof. David C. Powers, Texas A&M University
Lunch Break (13:00-14:00)	
Poster Sessions: (14:00-15:30) **Chairpersons:** Prof. Alakananda Hazra, Visva-Bharati University & Prof. Sanjib Kumar Patra, IIT Kharagpur	

Session 9 & 10 (15:30-16:50)	**Session 9: (Maitrayee)** **Chairperson:** Prof. Swagata Dasgupta, IIT Kharagpur	**Session 10: (Gargi)** **Chairperson:** Prof. Srabani Taraphder, IIT Kharagpur
IL-30 & 31 (15:30-15:50)	IL-30: Prof. Krishna Pada Bhabak, IIT Guwahati	IL-31: Prof. Nilanjana Majumdar, CDRI Lucknow
IL-32 & 33 (15:50-16:10)	IL-32: Prof. Sandip Murarka, IIT Jodhpur	IL-33: Prof. Lisa Roy, ICT-IOC Bhubaneswar
IL-34 & 35 (16:10-16:30)	IL-34: Prof. Chinmoy K. Hazra, IIT Delhi	IL-35: Prof. Amit Kumar, IIT Patna
IL-36 & 37 (16:30-16:50)	IL-36: Prof. Devarajulu Sureshkumar, IISER Kolkata	IL-37: Prof. Shivnath Mazumder, IIT Jammu

Session 11: (Gargi Auditorium) **Chairperson:** Prof. Partha Pratim Jana, IIT Kharagpur	
FL-(09-14) (16:55-17:30)	Flash Lectures

Tea/Coffee Break (17:30-17:50)	
Session 12: (Gargi Auditorium) **Chairperson:** Prof. Braja Gopal Bag, Vidyasagar University	
FL-(15-26) (17:50-19:00)	Flash Lectures
Dinner (19:30)	
09th March, 2024 (Saturday)	
Session 13: (Kalidas Auditorium) **Chairperson:** Prof. N. D. Pradeep Singh, IIT Kharagpur	
IL-38 (09:00-09:30)	Prof. Debabrata Maiti, IIT Bombay
IL-39 (09:30-10:00)	Prof. Seung Hwan Cho, POSTECH, Pohang, Republic of Korea
IL-40 (10:00-10:30)	Prof. David A Nagib, The Ohio State University
Tea/Coffee Break (10:30-11:00)	
Session 14: (Kalidas Auditorium) **Chairperson:** Prof. Kumar Biradha, IIT Kharagpur	
IL-41 (11:00-11:30)	Prof. Shoubhik Das, University of Bayreuth
IL-42 (11:30-12:00)	Prof. René Michael Königs, RWTH Aachen
IL-43 (12:00-12:30)	Prof. Abhishek Dey, IACS Kolkata
(12:30-13:00)	**Lucky Draw,** **Best Poster Award,** **Vote of Thanks: Prof. Santanu Panda** **Concluding Remarks: Prof. Modhu Sudan Maji**
Lunch (13:00-14:00)	
Departure	

Flash Lectures:

Session 6: (Kalidas Auditorium) [07th March, 2024] **Chairperson:** Prof. Nikhil K. Singha, IIT Kharagpur	
FL-03 (19:00-19:05)	Prof. Thirupathi Barla, IISER Berhampur
FL-04 (19:05-19:10)	Mr. Samrat Kundu, IIT Kharagpur
FL-05 (19:10-19:15)	Mr. Kanak Kanti Das, IIT Kharagpur
FL-06 (19:15-19:20)	Prof. Soumitra Maity, IIT(ISM) Dhanbad
FL-07 (19:20-19:25)	Prof. Srinivasan Easwar, Central University Of Rajasthan
FL-08 (19:25-19:30)	Prof. Biplab Maji, IISER Kolkata

Session 11: (Gargi Auditorium) [08th March, 2024] **Chairperson:** Prof. Partha Pratim Jana, IIT Kharagpur	
FL-09 (16:55-17:00)	Prof. Parthasarathi Subramanian, IIT Kanpur
FL-10 (17:00-17:05)	Prof. Gopinath Purushothaman, IISER Tirupati
FL-11 (17:05-17:10)	Ms. Swagata Paul, IIT Kharagpur
FL-12 (17:10-17:15)	Mr. Ganesh Karan, IIT Kharagpur
FL-13 (17:15-17:20)	Prof. Shanti Gopal Patra, NIT Silchar
FL-14 (17:20-17:25)	Prof. Akshai Kumar Alape Seetharam, IIT Guwahati

Session 12: (Gargi Auditorium) [08th March, 2024] **Chairperson:** Prof. Braja Gopal Bag, Vidyasagar University	
FL-15 (17:50-17:55)	Prof. Indu Bhusan Deb, IICB Kolkata
FL-16 (17:55-18:00)	Prof. Debayan Sarkar, IIT Indore
FL-17 (18:00-18:05)	Mr. Arya Bhattacharyya, IIT Kharagpur
FL-18 (18:05-18:10)	Prof. Avik Kumar Bagdi, University of Kalyani
FL-19 (18:10-18:15)	Prof. Koena Ghosh, Presidency University
FL-20 (18:15-18:20)	Prof. Paresh Nath Chatterjee, NIT Durgapur
FL-21 (18:20-18:25)	Prof. Ganesh Venkataraman, IIT Kharagpur
FL-22 (18:25-18:30)	Prof. Basudev Sahoo, IISER Thiruvananthapuram
FL-23 (18:30-18:35)	Prof. Suman De Sarkar, IISER Kolkata
FL-24 (18:35-18:40)	Prof. Arunabha Thakur, Jadavpur University
FL-25 (18:40-18:45)	Prof. Ranjan Jana, IICB Kolkata
FL-26 (18:45-18:50)	Prof. Kiran Kumar Pulukuri, IISER Tirupati

Bio-Sketch of Convenor

Prof. Modhu Sudan Maji

Affiliation: Associate Professor
Department of Chemistry, IIT Kharagpur
Kharagpur 721302, WB, India.
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Prof. Modhu Sudan Maji born in 1982 and did his schooling from his native place Howrah, WB. He completed BSc in Chemistry (honors) from University of Calcutta in 2003, and stood second in the University. During his MS from IISc, Bangalore, he worked on ´´An Exploratory Approach Towards the Bioactive Marine Natural Product Tetrodotoxin`` with Prof. Goverdhan Mehta. In 2009, he completed his PhD under the guidance of Prof. Armido Studer from University of Muenster, Germany. Following this he received prestigious Alexander von Humboldt Fellowship and completed 3.2 years of post-doctoral research with Prof. Magnus Rueping of RWTH Aachen University, Germany. After another short post-doctoral research stay with Prof. Martin Oestreich of Technical University Berlin, Germany, he joined the Department of Chemistry of IIT Kharagpur as assistant professor in December 2013; where he is currently working as associate professor. His major research topics are organo-catalysis, new catalyst development and natural product total synthesis. He has published 54 research papers in renowned journals. Under his guidance seven students completed PhD, and twenty-seven master students completed their thesis work. Currently he is leading a research group of nine PhD students, one post-doctoral fellow, and four MSc students.

Research Interests:

1. Development of synthetic methods and their application in total synthesis of alkaloids
2. Catalyst design and asymmetric synthesis
3. Functionalization of peptides

Awards and Honours:

[1] He received prestigious *Faculty Excellence Award* from IIT Kharagpur for his overall contribution at the associate professor level in the year 2020. [2] He is also recipient of *'SwarnaJayanti Fellowships'* (2020-2021). [3] *Merck Young Scientist Award* (2021). [4] *AVRA Young Scientist Award* (2021). [5] *Thieme Chemistry Journals Award"* (2022). [6] *Alexander von Humboldt Fellowship* (2010). [7] *INSA Medal for Young Scientists*, Indian National Science Academy (INSA), New Delhi, India (2022). [8] Chemical Research Society of India (CRSI) Bronze Medal for the year 2024. [9] *INSPIRE Faculty Award* from the Department of Science and Technology, India (2014-2019). [10] *D. K. Mitra Gold Medal Awards* from Ramakrishna Mission Residential College, Kolkata (2003) for securing highest marks in Chemistry and also secured second position in the University of Calcutta.

International Conference on Emerging Trends in Catalysis & Synthesis (IC-ETCS 2024)

Bio-Sketch of Convenor

Dr. Santanu Panda

Assistant Professor
Department of Chemistry
Indian Institute of Technology Kharagpur, WB, India.

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Dr. Santanu Panda obtained his PhD on 2013 in organocatalysis and total synthesis of natural products under Prof. Antony Pearson, Case Western Reserve University, Cleveland, USA. After finishing his PhD, he moved to Dallas and joined Prof. Joseph Ready's group as a postdoc. During his postdoc, he was exposed to transition metal-catalyzed cross coupling and organoboron chemistry. In July 2018, he joined IIT Kharagpur as an assistant professor. His group is very active in organoboron chemistry, total synthesis of natural products, and organophotoredox chemistry.

Awards / Honors / Membership:

- 2023 Merck Young Scientist Award as Winner
- 2022 CRS (Chirantan Rasayan Sanstha) Bronze Medal
- 2018 Ramanujan Fellowship from SERB
- Best Poster Award at UTSW Biochemistry Retreat at Dallas Botanical Garden, Dallas On 2017.
- Invited seminar to the annual UTSW Biochemistry department seminar series at UT Southwestern Medical Center, Dallas.
- Graduate outstanding teaching assistant award 2013, Department of Chemistry, Case Western Reserve University, USA.

Representative Publications:

Org. Chem. Front. **2024**, *11*, *854-863*
Angew. Chem. Int. Ed. **2023**, *62*, e202309136
Org. Lett. **2023**, *25*, 314-319
Chem. Commun. **2023**, *59*, 14447-14450
Chem. Eur. J. **2023**, e202303056
Chem. Asian J. **2023**, e202300911
Synthesis **2023**, *55, 3799-3808*
Chem. Sci. **2022**, *13*, 9678-9684
Org. Chem. Front. **2022**, *9*, 838-852
Chem. Rec. **2022**, *22*, e202100290
Chem. Eur. J. **2022**, *28*, e202200556
Eur. J. Org. Chem. **2022**, *2022*, *e202200581*
Chem Asian J. **2022**, *17*, e20220083
Chem. Commun. **2021**, *57*, 441-459
Adv. Synth. Catal. **2021**, *363*, 2444-2463
Coord. Chem. Rev. **2021**, *448*, 214165
Org. Biomol. Chem. **2021**, *19*, 7276-7297
Asian J. Org. Chem. **2021**, *11*, e202100092
Chem. Eur. J. **2020**, *26*, 1922-1927
Chem. Eur. J. **2020**, *26*, 14270-14282
Org. Biomol. Chem., **2020**, *18*, 8939-8974

Invited Lecture

Bio-Sketch of Speaker

Vladimir GEVORGYAN
University of Texas at Dallas
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Group Website: https://labs.utdallas.edu/gevorgyan-group/
University of Texas Southwestern Medical Center
E-MAIL: Vladimir.Gevorgyan@UTSouthwestern.edu

EDUCATION

1991-1994	Postdoctoral Research Fellow, Tohoku University, Sendai, Japan
1984	Ph.D. in Chemistry; Latvian Institute of Organic Synthesis, Riga, Latvia
1978	B.Sc. in Chemistry; The Kuban State University, Krasnodar, Russia

ACADEMIC CAREER

2019-present	Robert A. Welch Distinguished Chair of Chemistry, UTD, USA
2019-present	Professor, University of Texas Southwestern Medical center, USA
2012-2019	Distinguished Professor of Liberal Arts and Sciences, UIC, USA
2006-2019	Chair of Organic Division, Chemistry Department, UIC, Chicago, USA
2003-2012	Professor at Chemistry Department UIC, Chicago, USA
1999-2003	Associate Professor at Chemistry Department UIC, Chicago, USA
1997-1999	Associate Professor at Tohoku University, Sendai, Japan
1996	Assistant Professor at Tohoku University, Sendai, Japan
1995	Visiting Professor at I. Co. C. E. A. CNR (Italian Academy of Sciences) with Prof. Chryssostomos Chatgilialoglu, Bologna, Italy
1991-1994	Postdoctoral Research Fellow with Prof. Y. Yamamoto Tohoku University, Sendai, Japan
1986-1990	Group Leader at the Latvian Institute of Organic Synthesis, Riga Latvia
1985	Research Scientist at the Latvian Institute of Organic Synthesis, Riga Latvia

AWARDS AND LECTURESHIPS

2022	Israeli Chemical Society, Honorary Member
2021	Honorary Professor of Kuban State University
2018	Markovnikov Medal, Moscow State University
2016	Foreign Member of Latvian Academy of Sciences
2016	Excellence in Synthesis Lectureship, UTSW
2015	Lilly Lectureship at Imperial College London, London
2014	Visiting Professor at Sorbonne Universities, Paris
2012	University Scholar, University of Illinois
2012	Distinguished Professor of Liberal Arts and Sciences, UIC
2012	Honorary Professor of St. Petersburg State University
2011	Abbott Symposium on Organic Synthesis Lecturer, UIC
2010	Organic Synthesis Series Lecturer, Wayne State University
2009	Negishi-Brown Lecturer at 4th Purdue Negishi-Brown Symposium
2008	UIC Researcher of the Year Award
2006	Gakushuin University Visiting Scientist Travel Award
1993	CIBA - GEIGY International Foundation Postdoctoral Fellowship
1992	J.S.P.S. International Postdoctoral Fellowship

RESEARCH INTERESTS

Gevorgyan group has been working in development of regio- and chemoselective transition metal-catalyzed annulation reactions and their application in the synthesis of multifunctional, polysubstituted aromatic compounds; development of novel transition metal-catalyzed methodologies for the synthesis of heterocyclic compounds; development of novel direct and directed C-H functionalization methods; and development of robust methodologies amendable for synthesis of small molecules libraries for wide biological screening. Lately, the group focuses on development of photoexcited chemistry of transition metals. In all projects, the emphasis is placed on conceptual novelty and potential application of the newly developed methods.

Hybrid Pd-radical Chemistry: New Mechanism, New Possibilities

Vladimir Gevorgyan

University of Texas at Dallas, USA
e-mail: vlad@utdallas.edu

We uncovered new reactivity of hybrid Pd-radical species, generated at room temperature under visible light without use of exogenous photosensitizers. This led to the development of novel transformations, including new types of Heck reaction, aliphatic C–H functionalization methods, as well as new cascade transformations. A set of both directed and direct functionalization methods have been developed.

The scope of these transformations will be demonstrated and the mechanisms will be discussed.

Bio-Sketch of Speaker

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Prof. Ghorai obtained his B.Sc. (Hons.) from University of Calcutta (1989), M.Sc. from IIT Kharagpur (1991), and Ph.D. from NCL, Pune (1998) with Prof. Ganesh Pandey. He worked as a postdoctoral research associate with Prof. Michael Schmittel at the University of Wuerzburg Germany (1998–2000), as an Alexander von Humboldt fellow in the University of Siegen (2000–2001), and as a postdoctoral research associate with Prof. JoAnne Stubbe at MIT, USA (2001–2002). He joined the Department of Chemistry at IIT Kanpur as an assistant professor in 2002. He became an associate professor in 2007, full professor in 2012 and HAG-professor in 2019. He was USV Chair Professor at IIT Kanpur (2015-18). Presently he is N. C. Nigam Chair Professor at IIT Kanpur. He is a Fellow of National Academy of Sciences (FNASc.), Fellow of Academy of Sciences (FASc) and Fellow of West Bengal Academy of Science and Technology (FAST). His research interests are synthetic and mechanistic investigation of small ring aza-heterocycles and carbacycles, Memory of Chirality (MOC), enolate anion and dianion chemistry, organocatalysis, and material chemistry.

DROC and ROC of Small Ring Aza Heterocycles: Synthesis of Biologically Significant Complex N/O-Heterocycles

Manas K. Ghorai*

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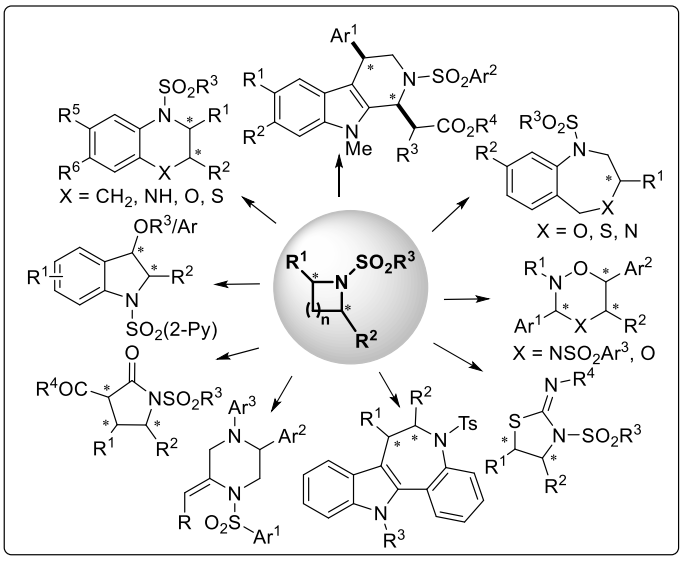
Abstract:

We have demonstrated that in the presence of a Lewis acid, aziridines and azetidines undergo nucleophilic ring-opening transformations with an appropriate nucleophile following an S_N2-type pathway. By exploiting and exploring our protocols of domino-ring-opening-cyclization (DROC) and ring-opening-cyclization (ROC), several novel strategies for the synthesis of non-racemic *N/O*-heterocycles of contemporary interest have been developed. Those compounds include tetrahydro-*β*-carbolines, *γ*-lactams, tetrahydrobenzodiazepines, oxadiazinanes, dioxazinanes, iminothiazolidines, tetrahydrobenzoazepinoindoles, hexahydropyrroloindoles, oxazolidines, imidazolines, indolines, tetrahydroquinoxalines, tetrahydroquinolines, tetrahydropyrimidines, morpholines, dihydropyrroles, piperazines, spiropiperidino indolenines, 1,4-oxazines, etc., and many more such intricate molecular frameworks with immense synthetic, biological and pharmacological significance. The progressive development of this chemistry over more than two decades, in particular during the last five years, in terms of further mechanistic investigations, enhanced enantio- and diastereoselectivity, kinetic and dynamic kinetic resolution, and important applications in asymmetric organic synthesis as well as other fields will be presented.



Scheme 1. Synthetic exploration of domino ring-opening cyclization (DROC) and ring-opening cyclization (ROC) of small ring Aza/oxa-heterocycles.

References: [a] S. Tarannum, S. Sk, S. Das, I. A. Wani, M. K. Ghorai, *J. Org. Chem.* **2020**, *85*, 367-379. [b] S. Pradhan, N. Chauhan, C. K. Sahi, A. Bhattacharyya, M. K. Ghorai, *Org. Lett.* **2020**, *22*, 7903-7908. [c] S. Pradhan, C. K. Sahi, S. Bhattacharyya, M. K. Ghorai, *Chem. Commun* **2018**, *54*, 8583-8586. [d] I. A. Wani, S. Sk, A. Mal, A. S. Gupta, M. K. Ghorai, *Org. Lett.* **2022**, *24*, 7867-7872, [e] B. Singh, M. Kumar, G. Goswami, I. Verma, M. K. Ghorai, *J. Org. Chem.* **2023**, *88*, 4504-4518. [f] B. Singh, S. Kashyap, S. Singh, S. Gupta, M. K. Ghorai, *J. Org. Chem.* **2024**, 89, 2247-2263.

Bio-Sketch of Speaker

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- **EDUCATION**

2006-2011	PhD studies (with Prof. Dr. Ben L. Feringa) Stratingh Institute, Synthetic Organic Chemistry, Rijksuniversiteit Groningen, the Netherlands
2004-2005	Exchange Student (in the group of Prof. Dr. Michel Etienne) Université Paul Sabatier, Toulouse, France
2001-2006	Studies in chemistry (diploma thesis with Prof. Dr. Gerhard Hilt), Philipps-Universität Marburg, Germany
2001	Civil service, Hamburg
2000	High school diploma, Wilhelm-Raabe-Schule, Lüneburg

- **CURRENT POSITION**

2021 –	Professor for Organic Chemistry Institute of Chemistry, Technische Universität Chemnitz, Germany

- **PREVIOUS POSITIONS**

2016 – 2021	Assistant Professor Institute of Chemistry, Technische Universität Berlin, Germany
2013 – 2016	Independent Research Group Leader (funded by a Liebig-Grant of the Funds of the German Chemical Industry), in the vicinity of Prof. Dr. Martin Oestreich Institute of Chemistry, Technische Universität Berlin, Germany
2011– 2013	Postdoctoral Researcher (with Prof. Jeffrey W. Bode) Laboratorium für Organische Chemie, ETC Zürich, Switzerland

- **FELLOWSHIPS AND AWARDS**

Awards

2019	Forschungspreis by the Dr.-Otto-Röhm-Gedächtnisstiftung, Germany
2018	Nomination for the Young Investigator Workshop by the European Association for Chemical and Molecular Sciences (EuCheMS)
2014	Thieme Chemistry Journal Award, Germany
2010	Invited Participation at the Roche Symposium Leading Chemists, Basel, Switzerland

Fellowships

2017 –	Emmy Noether-Programme of the German Research Foundation (DFG), Germany
2016	Exploration Grant of the Boehringer Ingelheim Stiftung, Germany
2016	Postdoctoral fellowship of the Daimler and Benz Foundation, Germany
2013 – 2018	Liebig-Stipendium of the Fonds der chemischen Industrie, Germany
2011 – 2013	Postdoctoral Fellowship of the Leopoldina - Nationale Akademie der Wissenschaften (German National Academy of Sciences), Germany
2004 – 2006	Fellow of the Studienstiftung des deutschen Volkes (German National Merit Foundation), Germany

Copper hydride catalysis driven by H_2 – reactivity-driven methods and selectivity-driven catalyst design

Prof. Johannes F. Teichert*
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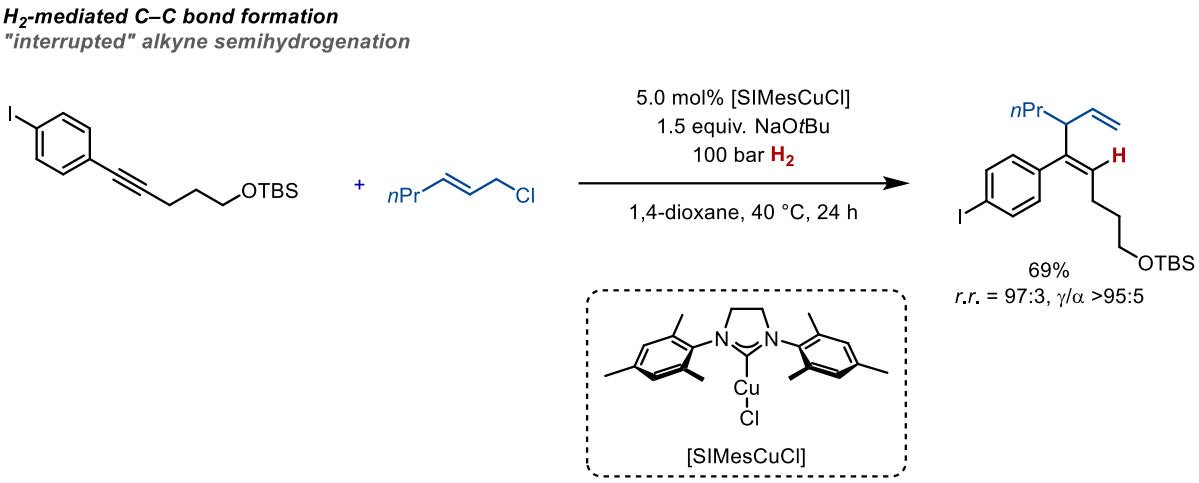
Copper hydride complexes are versatile reagents in organic synthesis and catalysis.[1–3] In order to replace the commonly employed stoichiometric hydrosilane reducing agents, we have disclosed approaches to access the so-called "copper hydride catalysis" with H_2 as terminal reducing agent.[4–8]
In this talk, new approaches to H_2-driven C–C bond forming reactions are discussed.[9] This methodology allows for an elegant synthetic access to versatile building blocks while relying on a readily available 3d metal catalyst,[10] rarely employed in this kind of methods. (For similar approaches using noble metals, see for example[11,12])
The second part of the presentation will focus more closely on ligand design. We have recently shown that the combination of copper/N-heterocyclic carbene complexes and hydrogen-bond organocatalysts enables the realization of hitherto unknown reactivity of copper hydride complexes.[13] In this vein, we are now able to control reactivity by supramolecular interaction, which allows the reduction of formally "hard" electrophiles with the typically "soft" copper hydride reducing agents.



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Bio-Sketch of Speaker

Prof. Andrew L. Lawrence
Professor, School of Chemistry
University of Edinburgh
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Introduction: Prof. Andy Lawrence is a synthetic organic chemist with research interests in the chemical synthesis of natural products, exploring new strategies and concepts in chemical synthesis, and developing new synthetic methodology. Andy joined the University of Edinburgh in 2013 and is now full Professor (Chair of Organic Synthesis).

Academic Background:

MChem: University of Oxford (St John's College) (2002-06) (First class)

DPhil: University of Oxford (St John's College) (2006-10); Supervisor- Prof. Sir Jack Baldwin and Prof. Robert Adlington

Post-Doctoral Research: Australian National University, Canberra, Australia (2010–11) With Prof. Mick Sherburn

Independent Fellowship: Australian National University, Canberra, Australia (2012–13)

Awards / Honors / Membership:

i. Korea Advanced Institute of Science & Technology Lectureship Award 2024.

ii. Science and Technology in Science (STS) Forum Young Leader 2023.

iii. Blavatnik Awards for Young Scientists in the UK Chemistry Finalist 2023.

iv. BMOS-RSC Young Investigator Distinction Award 2018.

v. RSC Hickinbottom Award 2017.

vi. Thieme Chemistry Journals Award 2016.

Website: https://lawrence-group.org/

Rethinking Enantioconvergent Reactions

Professor Andrew L. Lawrence

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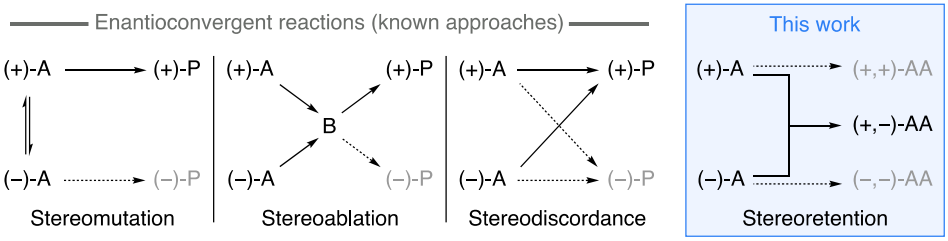
Enantioconvergent reactions are preeminent in contemporary asymmetric synthesis as they convert both enantiomers of a racemic starting material into a single enantioenriched product, thus avoiding the maximum 50% yield associated with resolutions. All currently known enantioconvergent processes necessitate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



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Bio-Sketch of Speaker

Stellios Arseniyadis
Reader in Organic Chemistry (Associate Professor)
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Homepage: https://arseniyadislab.sbcs.qmul.ac.uk/

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

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

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

Dr. S. Arseniyadis *
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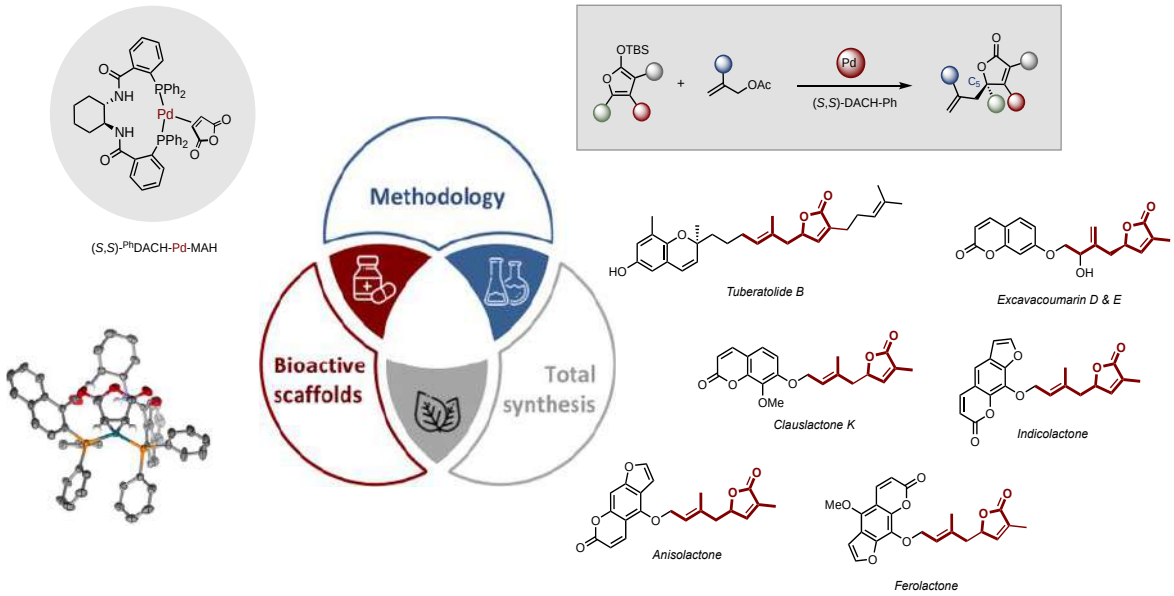
For the past two decades, the group has been focused on developing new synthetic tools with a special emphasis given to structural and functional diversity as well as chirality. In this context, we've been particularly interested in the development of new palladium-catalysed asymmetric allylic alkylations applied to various pro-chiral heterocyclic scaffolds and ultimately apply the methods in natural product synthesis.[1] This has led to the development of bench stable, single component chiral palladium pre-catalysts exhibiting improved reactivity and selectivity across the field. I'll present some of these results.[2]



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[1] For selected examples of Pd-AA and Pd-AAA reactions developed in the group, see: (a) F. Richard *et al*. *Nat. Synth*. **2022**, 1, 641. (b) M. Dolé Kerim *et al*. *J. Org. Chem*. **2020**, *85*, 12514. (c) T. Katsina *et al. Org. Lett*. **2019**, *21*, 9348. (d) S. Aubert *et al*. *Org. Lett*. **2019**, *21*, 2231. (e) T. Song *et al. Org. Lett*. **2019**, *21*, 603. (f) T. Song *et al. Chem. Eur. J*. **2018**, *24*, 8076. (g) M. Nascimento de Oliveira *et al. Chem. Eur. J*. **2018**, *24*, 4810. (h) M. Nascimento de Oliveira *et al. Org. Lett*. **2017**, *19*, 14. (i) H. Elhachemia *et al. Chem. Commun*. **2016**, *52*, 14490. (j) J. Fournier *et al*. *Angew. Chem. Int. Ed*. **2013**, *52*, 1257. (k) J. Fournier *et al*. *Angew. Chem. Int. Ed*. **2012**, *51*, 7562.

[2] T. Keenan *et al*. *Nat. Commun*. **2023**, *14*, 8058.

Bio-Sketch of Speaker

Dr. Monika Raj
Professor
Department of Chemistry
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M.: 630-337-9658

Dr. Raj is a Professor in the Department of Chemistry, Emory University, Atlanta, United States. Much of Dr. Raj's research focuses on understanding the roles proteins play in various physiological and pathological processes and utilizes this knowledge to identify novel therapeutic targets and drugs to treat diseases. To achieve these goals, Dr. Raj focuses on the development of novel chemical probes, cyclic peptides, synthetic strategies, and imaging tools that draw from core disciplines of organic and biological chemistry. Dr. Raj is also interested in identifying posttranslational modifications (PTMs), imaging enzymes responsible for these PTMs, and determining their role in various signaling pathways.

Academic Background:

2024-present	Professor of Chemistry, Emory University, Atlanta, Georgia
2020-2024	Associate Professor of Chemistry, Emory University, Atlanta, Georgia
2017-2020	James E. Land Professor, Assistant Professor of Chemistry, Auburn University
2014-2017	Assistant Professor of Chemistry, Seton Hall University, NJ
2011-2014	Postdoctoral Associate, New York University, NY
2010-2011	Postdoctoral Associate, University of Pennsylvania, Philadelphia
2005-2009	Doctor of Philosophy, IIT Kanpur, Kanpur, India

Awards / Honors / Membership:

2023	Distinguished Faculty Lecture, Emory College of Arts and Science
2023	Kavli Fellow, National Academy of Sciences
2022	McLean Lecture in the Dept. of Chemistry and Biochemistry at Detroit Mercy
2020	Sloan Research Fellow, Alfred P. Sloan Foundation
2019	NIH Maximizing Investigators' Research Award (R35 MIRA)
2019	Early Career Lectureship, Japan Peptide Society (JPS),
2019	Early Career Lectureship, American Peptide Society (APS)
2019	Rising Star Award, Chemical Protein Synthesis (CPS), German Science Foundation
2018	NSF CAREER Award

As an accomplished academic, Dr. Raj has authored 50 publications and holds 9 US patents. Furthermore, under her guidance, 10 students have been awarded Ph.D. degrees, and Dr. Raj is currently supervising 10 research fellows in their pursuit of Ph.D. degrees and 5 postdocs. Additionally, Dr. Raj has mentored 30 undergraduate students in their dissertation work.
Website: https://raj.emorychem.science/

Chemical Tools for Biological Discoveries

Monika Raj*
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Abstract:
In the Raj lab, we develop novel chemical probes and sensors for global profiling of undruggable proteome, selective detection of posttranslational modifications (PTMs), and biological metabolites. This research program leads to the discovery of novel protein biomarkers, affordable diagnostic tools for the early detection of cancer, and endogenous protein partners thus facilitating the synthesis of biotherapeutics. In the first part of my talk I'll focus on our efforts towards the identification of proteins and PTMs at a single molecule level in a cell or an organism to understand biological processes, disease analysis and biomarker discovery. We have developed multiple bioconjugation approaches for the selective labeling of lysine,[1] methionine, asparagine, mono-methyl lysine,[2-3] di-methyl lysine[4] and monomethyl-histidine posttranslational modifications (PTMs) to fill the present gap in the range of available techniques to sequence and identify proteins and PTMs at the single molecule and single cell level with high sensitivity and high accuracy. We showed the utility of our chemical methods in identifying methyl lysine PTMs at the single-molecule level by using fluorosequencing technology. In the 2nd part of the talk, I will focus on our efforts of developing turn-on and ratiometric chemical sensors for detecting and measuring the concentrations of aliphatic aldehydes inside the live cells.[5] These sensors would aid in the identification of early disease warning signals.

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3. Nwajiobi, O.; Verma, A.; Raj, M. *J. Am. Chem. Soc.* **2022**, *144*, 4633-4641.
4. Emenike, B.; Donovan, J.; Raj, M. *J. Am. Chem. Soc.* **2023**, *154*, 16417-16428
5. Wills, R.; Farhi, J.; Czabala, P.; Shahin, S.; Spangle, J.; Raj, M. *Chem. Sci*. **2023**, *14*, 8305-8314.

Acknowledgement: NIH, NSF, American Cancer Society (ACS)

Professor Dr. Dr. h.c. Todd B. Marder, FRSC(UK)
Senior Professor
and
Co-Head, Institute for Sustainable Chemistry & Catalysis with Boron
Julius-Maximilians-Universität Würzburg (Germany)

Institut für Anorganische Chemie and
Institute for Sustainable Chemistry & Catalysis with Boron
Julius-Maximilians Universität Würzburg
Am Hubland, 97074 Würzburg, Germany
E-mail: todd.marder@uni-wuerzburg.de

Marder received his B.Sc. from M.I.T. and Ph.D. from UCLA, was a postdoc at the University of Bristol (UK), and a Visiting Research Scientist at DuPont Central Research. He joined the faculty at the University of Waterloo, Canada in 1985, moved to the University of Durham (UK) in 1997 as Chair of Inorganic Chemistry, and to the University of Würzburg, Germany in 2012 as Chair I of Inorganic Chemistry where he is now a Senior Professor. Awards include: Royal Society of Canada Rutherford Memorial Medal for Chemistry (Canada), RSC Awards in Main Group Element Chemistry and in Organometallic Chemistry (UK), 2 JSPS Invitation Fellowships (Japan), Humboldt Research Award (Germany), Royal Society Wolfson Research Merit Award (UK), 1000-Foreign Talents Award for Foreign Experts (China) which he declined, and Docteur Honoris Causa, Université de Rennes 1 (France). He is a Fellow of the RSC (UK), Member of the Bavarian Academy of Sciences (Germany), Fellow of the American Association for the Advancement of Science (AAAS) (USA), and Fellow of the European Academy of Sciences.

He has published >430 papers (>33,000 citations, h-index = 101 Web of Science, h-index = 101 Google Scholar) and presented >430 invited lectures worldwide.

He has held Visiting or similar Professorships in the UK, France, Hong Kong, China, Japan, India, and Australia, and holds an Honorary Professorship at Durham University (UK), an Adjunct Professorship in Chemistry at the Hong Kong University of Science and Technology, a Guest Professorship at Shandong University, and a Visiting Professorship at Northeast Normal University (China). He has served on the editorial boards of *Chinese Journal of Chemistry, Organometallics, Inorganic Chemistry, Journal of Organometallic Chemistry, Polyhedron, Inorganica Chimica Acta, Applied Organometallic Chemistry, Canadian Journal of Chemistry, Chinese Journal of Chemistry, Crystal Engineering.* Over 45 of his former co-workers hold or have held academic positions around the world.

His research interests include: metal-boryl compounds, diboron(4) compounds, homogeneous catalysis (especially metal-catalyzed borylation and cross-coupling processes), organic, organoboron, and organometallic materials for applications in linear and nonlinear optics, organic electronics, bioimaging, photodynamic therapy, sensing of biomolecules, and fluoroarene-arene interactions in crystal engineering and liquid crystal phase behavi

Metal-Catalyzed and Metal-Free Borylation – Synthesis of Boronate Esters

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Organoboronate esters are key reagents for organic synthesis with numerous applications in pharmaceutical, agrochemical, and materials chemistry. This lecture will highlight some of our contributions to the synthesis of mono-, and polyboronate esters via catalytic processes involving transition metals, both thermal and photocatalytic processes, as well as metal-free processes. Examples include the borylation of aromatic and benzylic C-H bonds and aromatic, aliphatic, and acyl C-X bonds (X = F, Cl, Br, I), as well as additions to alkenes and alkynes, especially those involving activation of B-B bonds in diboron(4) reagents.

References: Selected recent papers: [a] J. Hu, M. Tang, J. Wang, Z. Wu, A. Friedrich, T.B. Marder, "Photocatalyzed Borylcyclopropanation of Alkenes with a (Diborylmethyl)iodide Reagent," *Angew. Chem. Int. Ed.*, **62**, e202305175 (2023). [b] H.H. Al Mamari, J. Borel, A. Hickey, E. Courtney, J. Merz, X. Zhang, A. Friedrich, T.B. Marder, G.P. McGlacken, "Regioselective Iridium-Catalyzed C8-H Borylation of 4-Quinolones *via* transient *O*-Borylated Quinolines," *Chem. Eur. J.*, **29**, e202301734 (2023). [c] L. Tendera, F. Fantuzzi, T.B. Marder, U. Radius, "Nickel boryl complexes and nickel-catalyzed alkyne borylation," *Chem. Sci.*, **14**, 2215-2228 (2023). [d] S. Jos, C. Szwetkowski, C. Slebodnick, R. Ricker, K.L. Chan, W.C. Chan, U. Radius, Z. Lin, T.B. Marder, W.L. Santos, "Transition Metal-Free Regio- and Stereo-Selective trans Hydroboration of 1,3-Diynes: A Phosphine-Catalyzed Access to (E)-1-Boryl-1,3-Enynes," *Chem. Eur. J.*, **28**, e202202349 (2022). [e] L. Kuehn, L. Zapf, L. Werner, M. Stang, S. Würtemberger-Pietsch, I.Krummenacher, H. Braunschweig, E. Lacôte, T.B. Marder U. Radius, "NHC induced Radical Formation *via* Homolytic Cleavage of B–B Bonds and its Role in Organic Reactions," *Chem. Sci.*, **13**, 8321-8333 (2022). [f] X. Zhang, A. Friedrich, T.B. Marder, "Copper-Catalyzed Borylation of Acyl Chlorides with an Alkoxy Diboron Reagent: A Facile Route to Acylboron Compounds," *Chem. Eur. J.*, **28**, e202201329 (2022).

Recent reviews: [a] J. Hu, M. Ferger, Z. Shi, T.B. Marder, "Recent Advances in Asymmetric Borylation by Transition Metal Catalysis," *Chem. Soc. Rev.*, **50**, 13129-13188 (2021). [b] S.K. Bose, L. Mao, L. Kuehn, U. Radius, J. Nekvinda, W. Santos, S.A. Westcott, P.G. Steel, T.B. Marder, "First-Row d-Block Element-Catalyzed Carbon-Boron Bond Formation and Related Processes," *Chem. Rev.*, **121**, 13238-13341 (2021). [c] W. Ming, H. Soor, X. Liu, A. Trofimova, A. Yudin, T.B. Marder, "α-Aminoboronates: Recent Advances in their Preparation and Synthetic Applications," *Chem. Soc. Rev.*, **50**, 12151-12188 (2021). [d] Y.-M. Tian, X.-N. Guo, H. Braunschweig, U. Radius, T.B. Marder, "Photoinduced Borylation for the Synthesis of Organoboron Compounds," *Chem. Rev.* **121**, 3561-3597 (2021). [e] Y.P. Budiman, S.A. Westcott, U. Radius, T.B. Marder, "Fluorinated Aryl Boronates as Building Blocks in Organic Synthesis," *Adv. Synth. Catal.*, **363**, 2224-2255 (2021). [f] E.C. Neeve, S.J. Geier, I.A.I. Mkhalid, S.A. Westcott, T.B. Marder, "Diboron(4) Compounds: From Structural Curiosity to Synthetic Workhorse," *Chem. Rev.*, **116**, 9091-9161 (2016).

Bio-Sketch of Speaker

Dr. Ajay Kumar Srivastava
Principal Scientist/Associate Professor
Medicinal & Process Chemistry
CSIR-Central Drug Research Institute
Sitapur Road, Lucknow-226031, UP, India
e-mail: ajayk.srivastava@cdri.res.in
M.: 9652548543

Introduction: Dr. Srivastava is working as Principal Scientist in the Department of Medicinal & Process Chemistry, CSIR-CDRI, India. His current research interest includes development of NCEs through multicomponent reactions and non-catalytic processes, Process development for High valued APIs and KSMs.

Academic Background:

B.Sc.: D. D. U. University, Gorakhpur, UP, India (1998-2001)

M.Sc.: University of Delhi, Delhi, India (2001-2003)

Ph.D.: CSIR-CDRI & Jadavpur University (2003-2008); Supervisor- Dr. Gautam Panda (CSIR-CDRI) and Dr. Umashish Jana (JU)

Post-Doctoral Research: Seoul National Univeristy, Seoul, South Korea (2009–2011) With Prof. Seung Bum Park

Awards / Honors / Membership:

i. “2008 Dr. M. M. Dhar Memorial Best Thesis Award in Chemical Sciences”.

ii. B K Postdoctoral Fellowship 2009-2011, SNU

iii. Best Young Scientist Award, CSIR-IICT.

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Catalytic and Non-Catalytic Functionalizations of Alkynoic Acids Utilizing Isoyanides

Ajay Kumar Srivastava

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[b]*Chemical Sciences Division, Academy of Scientific and Innovative Research (AcSIR) Ghaziabad-201002, Uttar Pradesh, India.*

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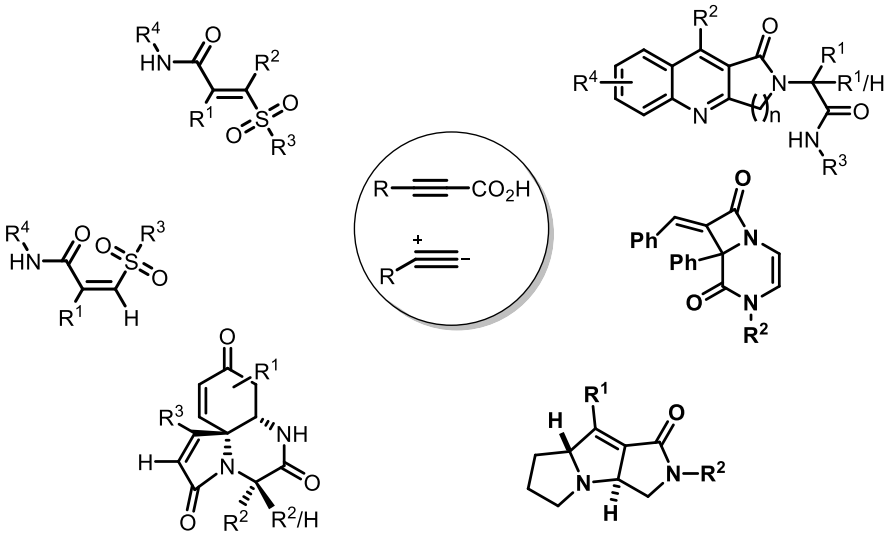
Abstract: Alkynoic acids and isocyanides serve as excellent reacting partners to develop multi-component reactions (MCRs) to construct small molecule libraries for drug development. Our group has developed efficient post-IMCR modifications to synthesize sp3-enriched heterocycles. Herein, we present synthesis of alkaloid-mimicking tricyclic skeletons via transition metal-free MCR approach and our recent findings in the area of alkyne difuctionalizations to synthesize sulfonylacrylamides in a highly regio- and stereoselective manner.



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2. A. Ghoshal, D. Yugandhar, J. B. Nanubolu, **A. K. Srivastava**, *Acs Comb Sci* **2017**, *19*, 600-608.
3. S. Tripathi, M. Kumar, M. D. Ambule, A. Saxena, R. Kant, S. K. Shukla and **A. K. Srivastava**, *Org Lett*, **2022**, 24, 7632-7636.
4. S. Tripathi, M. Kumar, A. Shivhare, R. Kant, M. M. Deshmukh, **A. K. Srivastava**, *Org Lett* **2023**, *25*, 6638-6642.
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7. A. Ghoshal, A. Yadav, **A. K. Srivastava**, *J. Org. Chem.* **2020**, 85, 14890-14904.

Bio-Sketch of Speaker

Dr. Madhab C. Das
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Web: https://www.chemiitkgp-mcdaslab.com/
@mcdlab_iitkgp

Madhab C. Das completed his Ph.D. in Supramolecular Chemistry at IIT Kanpur, India under the supervision of Professor P.K. Bharadwaj (Nov, 2009). Then, he worked with Professors Banglin Chen at the University of Texas at San Antonio, George K.H. Shimizu at University of Calgary, and Hiroshi Kitagawa at Kyoto University as postdoctoral fellow (Dec, 2009–Nov, 2013) before joining IIT Kharagpur as Assistant Professor in Dec, 2013. Since 2019, he is an Associate Professor at IIT Kharagpur. His work is focused on functional MOFs and HOFs mostly toward gas separations, proton condution, small molecule sesning, electrochemical energy storage, and heterogeneous catalysis.

The group (Framework Laboratory) designs and synthesizes own family of Porous Metal-Organic Frameworks (MOFs) materials with exceptional chemical robustness known as MOF IITKGP (IITKGP stands for Indian Institute of Technology Kharagpur).

Awards/Fellowships/Honors:

Name of Award / Fellowship/ Recognitions	*Agency*	*Year*
Humboldt (AvH) Research Fellowship for 'Experienced Researchers'	AvH Foundation, Germany	2022
Member of The National Academy of Sciences, India	NASI, Prayagraj	2022
'Stellar Reviewer' of 'Inorganic Chemistry' (*Inorg. Chem.* **2021**, *60*, 14489−14490).	ACS	2021
JSPS Post-Doctoral Research Fellowship	JSPS (Japan)	2012
A one-time merit award for the excellent research performance	University of Texas at San Antonio	2011

Strategic Design and Development of pH-Stable Metal–Organic Frameworks (MOFs) for Multipurpose Heterogeneous Catalysis

Dr. Madhab C. Das*
Department of Chemistry, Indian Institute of Technology Kharagpur, Kharagpur-721302
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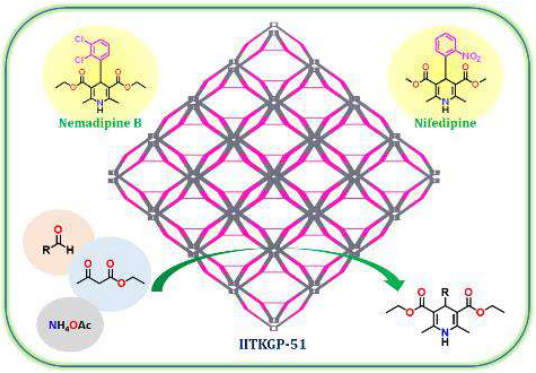
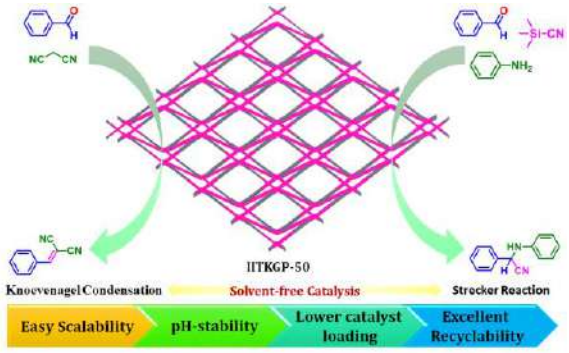
Metal-organic frameworks (MOFs) have attracted immense attention as efficient heterogeneous catalysts over other solid catalysts, however, their chemical environment instability often limits their catalytic potential. A heterogeneous catalyst must be chemically stable for its meaningful depolyment in industry. Although taking advantage of many superiorities MOFs have been explored in several catalytic reactions, the employment of MOFs for synthesizing drug molecules and natural products are not yet explored. This presentation focuses on such research gaps. The substrate binding sites and host-guest interactions are verified crystallographically and computational modeling as well in order to gain better insight into mechanistic aspects at molecular level. Besides, variation in catalytic efficacies of pH-stable MOFs by altering activation methods has been documented. The sustainable synthetic pathway under *solvent-free* conditions for a broad scope of substrates using low catalyst loading and excellent recyclability made our developed pH-stable frameworks as highly promising heterogeneous catalysts.[a-d]





References: [a] R. Sahoo, B. Pramanik, S. Mondal, and M. C. Das*, *Small* **2024**, 2309281; [b] R. Sahoo, S. Mondal, S. Chand, and M. C. Das*, *Inorg. Chem.* **2023**, *62*, 12989-13000; [c] S. Chand, S. C. Pal, M. Mondal, S. Hota, A. Pal, R. Sahoo and M. C. Das* *Cryst. Growth Des.* **2019**, *19*, 5343-5353; [d] *unpublished results*

Bio-Sketch of Speaker

Subhas Chandra Pan

Professor, *Department of Chemistry*
Indian Institute of Technology Guwahati
Guwahati-781039, Assam, India
E-Mail: span@iitg.ac.in

Introduction, Academic:

Professor Subhas Chandra Pan obtained his B.Sc. degree in Chemistry Honours in 2001 from Calcutta University and M.S. degree in 2004 from Indian Institute of Science, Bangalore. During his MS thesis he worked in Prof. Goverdhan Mehta's laboratory on the total synthesis of epoxyquinone natural products. He obtained his PhD degree in 2008 under the guidance of Prof. Benjamin List at the Max-Planck-Institut für Kohlenforschung, Mülheim an der Ruhr, Germany. After doing postdoctoral studies at Harvard University with Prof. E J Corey and at the Scripps Research Institute, Florida with Prof. Glenn C. Micalizio, he joined IIT Guwahati as Assistant Professor in 2011 and was promoted to Associate Professor in 2015 and to Full Professor in 2019.

Awards / Honors / Membership:

DAE Young Scientist Research Award 2012

Thieme Chemistry Journal Award 2018

Fellow of the Royal Society of Chemistry (FRSC), 2021.

Member of the Editorial Advisory Board (EAB) of the Journal of Heterocyclic Chemistry from September 2020 onwards.

Webpage: https://subhaschandrapan.wixsite.com/span

Synthesis of Cyclic Molecules via Sequential Catalysis and Cyclization Reactions of Vinylidene *ortho*-Quinone Methides

Prof. Subhas Chandra Pan*
Department of Chemistry, Indian Institute of Technology Guwahati, Assam, 781039
(E-mail:span@iitg.ac.in, Web: https://subhaschandrapan.wixsite.com/span)

Cyclic molecules are very important as many drugs contain cyclic structures.[1] Organocatalytic cyclization and cycloaddition[2] reactions play an important role for the synthesis of carbocyclic and heterocyclic frame works.

Our group is interested for the development of new organocatalytic/dual organo-metal catalytic cyclization reactions. The presentation will include synthesis of cyclic molecules via sequential catalysis and cyclization reactions of vinylidene *ortho*-quinone methides.[3]

References: [a] R. D. Taylor, M. MacCoss, A. D. G. Lawson, *J. Med. Chem*. **2014**, *57*, 5845.

[b] A. Moyano, R. Rios, *Chem. Rev*. **2011**, *111*, 4703.

[c] (1) R. Khuntia, S. K. Mahapatra, L. Roy, S. C. Pan, *Chem. Sci.* **2023**, *14*, 10768. (2) S. Biswas, S. K. Purkayastha, A. K. Guha, S. C. Pan, *Chem Commun.* **2023**, *59*, 12156*;* (3) A Shikari, C. Parida, S. C. Pan, *manuscript submitted;* (4) R. Meher, S.C. Pan, *manuscript submitted.*

Bio-Sketch of Speaker

Biosketch: Jaideep Saha obtained his B.Sc. in Chemistry from **Calcutta University** (India) in 2003 and M.Sc. (Chemistry) from IIT Madras (India) in 2005. He pursued his doctoral studies with Prof. Mark W. Peczuh at the **University of Connecticut** (USA) where he worked in synthetic method development for the synthesis of unnatural carbohydrates and phosphine-catalyzed transformations. He was a research intern at **Boehringer-Ingelheim Pharmaceutical Inc**. CT (USA) in the chemical development department (with Dr. Chris Senanayake and Dr. Daniel Fandrick). After completing his PhD in 2012, he moved to the **University of Pittsburgh** (USA) as a postdoctoral fellow to work with Prof. Peter Wipf. He worked on medicinal chemistry projects and synthesized selective small-molecule inhibitors of NOX-2 enzyme. At that time, he was also a Vascular Medicine Institute Fellow at the school of medicine. For his second post-doc, he moved to the **University of Oxford** (UK) as a Marie-Curie Post-doctoral Fellow in 2013 to work with Prof. Stuart Conway, where he developed small-molecule probes for targeting tumor hypoxia. This work was performed in collaboration with department of oncology.

In December 2016, he began his independent career at the **Centre of Biomedical Research** (India) as a faculty member in the division of molecular synthesis and drug discovery, where his group was involved in the development of new synthetic methodologies and the preparation of compounds for application in medicinal chemistry and drug discovery. He was involved in research supervision of PhD/post-docs, competitive fund acquisition, project management and building national and international collaboration. Currently he is an assistant professor at **National Institute of Pharmaceutical Education and Research** (NIPER), India where he is actively involved in teaching and research programs for MS and PhD students in the department of medicinal chemistry.

Recently he was awarded the Thieme Chemistry Journals Award (2022). He has been inducted as an early career advisory board member of Bioorganic & Medicinal Chemistry and Bioorganic & Medicinal Chemistry Letters (2022). He is also the recipient of a Marie-Curie Fellowship (2013), an INSPIRE faculty award from Department of Science and Technology, India (2013), a Dr. K. S. Krishnan Research Fellowship, BRNS India (2015), and a Discovery Early Career Research Award (DECRA) by Australian Research Council (ARC) in 2017.

Key publications as corresponding author in peer-reviewed journals: (i) *Angew. Chem. Int. Ed*. **2023**, *62*, e202304471; (ii) *Angew. Chem. Int. Ed*. **2021**. *60*, 8808; (iii) *Chem. Commun*. **2023**, *59*, 10028; (iv) *Org. Lett*. **2023**, *25*, 5676; (v) *Chem. Eur. J*. **2022**, *28*, e202201208; (vi) *Chem. Commun*. **2022**, *58*, 7538; (vii) *Chem. Commun*. **2022**, *58*, 2504; (viii) *J. Org. Chem*, **2022**, *87,* 613; (ix) *Adv. Synth. Catal*. **2020**. *363*, 4130; (x) *Org. Lett*. **2020**. *22*, 5115; (xi) *J. Org. Chem*. **2019**. *84*, 15255; (xii) *Org. Lett*. **2019**. 21, 5848; (xiii) *Chem. Commun*. **2019**, 55, 7069; (xiv) *J. Org. Chem*. **2019**, *84*, 710; (xv) *ACS Catal*. **2018**, 8, 5085.

Major research grants: [**national**]; (a) *Investigation on the Expansion of Application Portfolio of Oxyallyl Cation and Related Species from Complex Molecular Synthesis to Site-Selective Protein Modifications* (2021-2024), CRG-SERB (INR: 5,000,000) (Role: PI]; (b) *Exploring Dual Activation Strategies Using Transient Azaoxyallyl Cations: New Opportunity for Heterocycle Synthesis* (2021-2024), CSIR-EMR, (INR 2,860,000). (Role: PI]; (c) *Development of New Methodologies for the Synthesis of Diverse Seven-Membered Cyclic Systems via Ring Opening-Annulation Cascade Using Donor-Acceptor Cyclopropanes* (2017-2020). ECR-SERB, (INR 3,650,000); (Role: PI] [**international**]; (i) *New Stereoselective Synthesis of Sialosides and Study of Human Anti-sialoside Antibodies by the Method of Chemical Biology (2018-2021)*; agency: DST-RFBR; (ii) *Catalytic Strategies for Biomolecule Functionalization and Generation of Pseudo Natural Products*. Agency: DST-JSPS.

Expanding the synthetic landscape of oxyallyl cation-based transformations

*Dr. Jaideep Saha**

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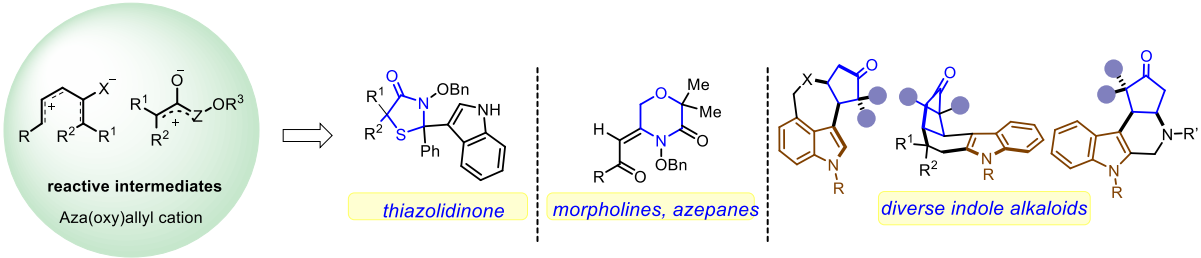
Azaoxyallyl cation, an aza-variant of oxyallyl cation has been recognized as an important synthon for the construction of important nitrogen containing heterocycles. Some important structural are necessary for this transient intermediate to display certain reactivities, conducive to the synthesis of different heterocycles or interesting synthetic building blocks. Some of these aspects and new development in our laboratory will be presented. The venerable Piancatelli rearrangement also involves oxyallyl cation during its progress toward forming cyclic enones from a furan carbinol. A novel Piancatelli-templated strategy is developed in our laboratory for accessing diverse indolyl-cyclopentenones and indole-annulated medium-sized rings, which was based on an unprecedented reaction modality of γ-aminocyclopentenone and invokes the possibility of a retro-aza-Piancatelli reaction. These findings will be presented.



References: *[a] Jaiswal, V.; Mondal, S.; Singh, B.; Singh, V.P.; Saha, J*. Angew. Chem. Int. Ed. 2023, 62, e202304471; [b] Bera, T.; Singh, B.; Jana, M.; Saha, J*.; Chem. Commun. 2022, 58, 7538; [c] Mondal, B.; Jagadeesh, C; Das, D.; Saha, J*. Chem. Commun. 2022, 58, 2504*

Bio-Sketch of Speaker

Indranil Chatterjee
Assistant Professor
Department of Chemistry
Indian Institute of Technology, Ropar
Contact Number: 8240424391
email: indranil.chatterjee@iitrpr.ac.in
Homepage: https://indranilchatterjee9.wixsite.com/icresearchgroup

Dr. Indranil Chatterjee obtained his B.Sc. from Calcutta University, India in 2006, and then he moved to IIT Kharagpur for his M.Sc. study. In 2008 he moved to Germany for his Ph.D. study at Westfälische Wilhelms-University Muenster under the guidance of Prof. Dr. Armido Studer, where his studies centred on catalytic asymmetric cycloaddition reactions. After finishing his Ph.D. study in November 2011, he joined as a Postdoctoral fellow with Prof. Paolo Melchiorre in ICIQ, Tarragona, Spain in March 2012. His area of research mainly focused on new organocatalytic cascade reactions. After that from 2014 to 2016 he did another Post-Doc with Prof. Martin Oestreich at the Technische Universität Berlin, concentrating his research on Lewis acid catalysis. Since December 2016 he is holding a position of Assistant Professor at the Indian Institute of Technology Ropar, India.

Details of fellowship/awards/honours :

(i) National Scholarship in Secondary and Higher Secondary exam. (2000 & 2002).

(ii) Ph.D. scholarship of the International Graduate School of Chemistry (GSC-MS), University of Muenster, Germany (2008-2011)

(iii) Postdoctoral Fellowship at ICIQ, Tarragona, Spain (2012-2014)

(iv) Cluster of Excellence UniCat Fellowship for Postdoctoral Research at Technical University Berlin, Germany (2014-2016)

(v) Institute Best Teaching Award (2020).

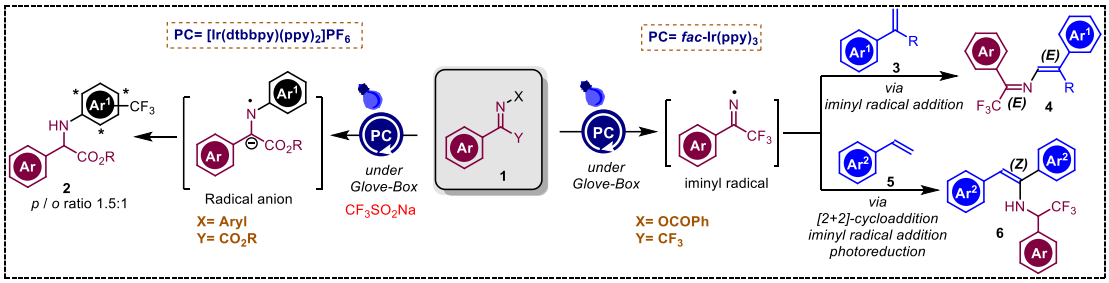
(vi) Thieme Chemistry Journal Award, 2022.

Generation of *N*-Centered Radicals under Visible Light Photoredox Catalysis

Dr. Indranil Chatterjee*
Assistant Professor, IIT Ropar
Indranil.chatterjee@iitrpr.ac.in

Herein, we have disclosed C–N and C–C bond formation strategies via *N*-centered radicals. We have utilized easily synthesizable oxime-esters and iminoesters as the precursor under blue LED irradiation. Fluoroalkylation using Langlois reagent (CF_3SO_2Na) is a very common synthetic technique,[1] we have exploited it for synthesizing pharmaceutically valuable trifluoroarylated amino acids **2**. In this case, reductive trifluoromethylation of α-iminoesters occurs via umpolung strategy to generate *N*–centred radical under photoredox catalysis, which rearranges to form *C*–centred radical followed by radical-radical coupling of trifluoromethyl radical delivering the desired trifluoromethylated product **2**.[2]

On the other hand, oxime-esters have been used as the source of iminyl radicals.[3] Photocycloaddition is an age-old process.[4] Our another thought-process combines these altogether to attain a cycloaddition of olefins followed by iminyl addition under photocatalyzed blue LEDs irradiation. Successfully we have discovered a multitasking Ir-catalysis combining both energy-transfer and photoredox process. α, α'-disubstituted olefins **3** generates the *E*-selective imine addition product **4**, while *Z*-selective aminated stilbene derivatives **6** are obtained using simple unsubstituted styrenes **5**.[5]



Scheme 1: Photoredox mediated various reactivities of *N*-centred radicals

References

1. (a) D. A. Nagib and D. W. C. MacMillan, *Nature*, 2011, **480**, 224–228. (b) J. Xie, X. Yuan, A. Abdukader, C. Zhu and J. Ma, *Org. Lett.*, 2014, **16**, 1768–1771.
2. H. Paul, S. K. Ariyan, S. Pradhan and I. Chatterjee (manuscript under preparation).
3. (a) G. Tan, M. Das, H. Keum, P. Bellotti, C. Daniliuc and F. Glorius, *Nat. Chem.*, 2022, **14**, 1174–1184. (b) S.-Q. Lai, B.-Y. Wei, J.-W. Wang, W. Yu and B. Han, *Angew. Chem., Int. Ed.*, 2021, **60**, 21997–22003.
4. S. Poplata, A. Tröster, Y. Q. Zou, and T. Bach, *Chem. Rev.*, 2016, **116**, 9748–9815.
5. B. Paul, S. Das and I. Chatterjee (manuscript under preparation)

Bio-Sketch of Speaker

Prof. Chandan K. Jana

Professor
Department of Chemistry
Indian Institute of Technology Guwahati, Guwahati, 781039, India
E-Mail: ckjana@iitg.ac.in web: http://www.iitg.ac.in/ckjana/

Chandan K. Jana completed his M.S. in 2005 from the Indian Institute of Science Bangalore. In 2008, he received his Ph.D. degree from the group of Prof. A. Studer at the University of Muenster, Germany, as a member of the International Graduate School of Chemistry. He was a postdoctoral fellow with Prof. K. Gademann at EPFL and the University of Basel, Switzerland (2009–2011). In 2011, he started his independent research career as an Assistant Professor in the Department of Chemistry at the Indian Institute of Technology Guwahati, where he became Professor in 2019. His research and teaching focus on organic chemistry.

Academic/Positions

Since 08/2019	Professor at the Department of Chemistry, IITG
02/2015 – 08/2019	Associate Professor at the Department of Chemistry, IITG
06/2011 – 02/2015	Assistant Professor at the Department of Chemistry, IITG
04/2009 – 05/2011	Post-doctoral research with Prof. K. Gademann, University of Basel, Basel, Switzerland and EPFL, Lausanne, Switzerland
10/2005 – 10/2008	Ph.D. thesis with Prof. A. Studer at the Westfälische Wilhelms-University of Muenster, Germany
07/2002 – 09/2005	Master of Science thesis in chemical science with Prof. N. Jayaraman
05/1999 – 04/2002	Bachelor of Science (B.Sc.) in chemistry, University of Calcutta, India.

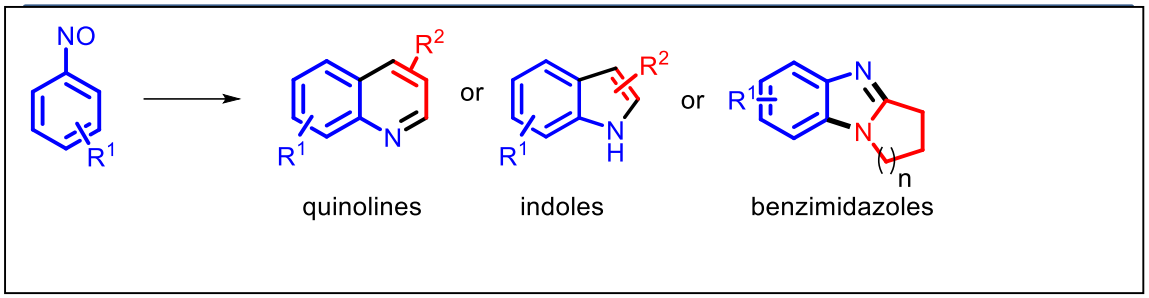
Awards /Fellowships

04/2023	SERB - Science and Technology Award for Research (SERB-STAR), Government of India
07/2012	DAE Young Scientist Research Award, Government of India,
04/2009 – 05/2011	Swiss National Postdoctoral fellowship
10/2005 – 10/2008	Ph.D. fellowship of the International Graduate School of Chemistry (GSC-MS), University of Muenster, Germany
07/2002 – 09/2005	M S scholarship of Indian Institute of Science (IISc), Bangalore, India
09/2004	National scholarship of University of Calcutta, India

Arene Functionalization of Nitrosoarenes to Aromatic Heterocycles

Prof. Chandan K. Jana*
Department of Chemistry, Indian Institute of Technology Guwahati, Guwahati-781039
(E-mail: ckjana@iitg.ac.in; Web: www.iitg.ac.in/ckjana)

Nitrosoarenes participate in a wide variety of reactions to incorporate nitrogen and/or oxygen functionality in a molecule. In most cases, the arene moiety of the nitrosoarene is sacrificed in order to get the desired hetero functionality. However, the reactions of nitrosoarenes that functionalize the arene moiety incorporating it into the product are underdeveloped. Our group aimed to develop reactions that functionalize the arene moiety of the nitrosoarene. The methods developed in our group for the synthesis of important fused aromatic heterocycles via arene functionalization of nitrosoarene will be discussed.



Scheme 1. Nitrosoarene to aromatic fused heterocycles

References:

[a]A. Purkait, S. Saha, S. Ghosh, C. K. Jana* *Chem. Commun*. **2020**, 56, 15032.

[b] S. K. Roy, A. Purkait, SK M.T. Aziz, C. K. Jana* *Chem. Commun*. **2020**, 56, 3167.

[c] A. Purkait, S. K. Roy, H. K. Srivastava, C. K. Jana* *Org. Lett*. **2017**, 19, 2540.

Bio-Sketch of Speaker

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Dr. Khan is an Associate Professor at the School of Basic Sciences, IIT Bhubaneswar. His research interest revolves around the development of novel catalytic/noncatalytic synthetic methods for functionalized carbo-/heterocycles for application in bioactive natural products.

Education:
2003: M. Sc. Mumbai University (Organic Chemistry Specialization)
2009: Ph. D. Univ. of Mumbai (Synthetic Organic Chemistry) (Mentor: Prof. S. H. Mashraqui).
Professional Experience:
2009-2010 Dr. D.S. Kothari Postdoctoral Fellow with Prof. G. Mehta, IISc Bangalore
2010-2012 Dr. D.S. Kothari Postdoctoral Fellow with Prof. G. Mehta, University of Hyderabad
2012-2013: Fulbright-Nehru Postdoctoral Fellow with Prof. K.C. Nicolaou, The Scripps Research Institute, CA, US
Sept. 2013-March 2014: Research Investigator with Biocon-Bristol Myers Squibb Research Centre (BBRC), Bangalore, India
April 2014-Oct. 2022- Asst. Prof. @ IIT Bhubaneswar
Oct. 2022-Present: Assoc. Prof. @ IIT Bhubaneswar

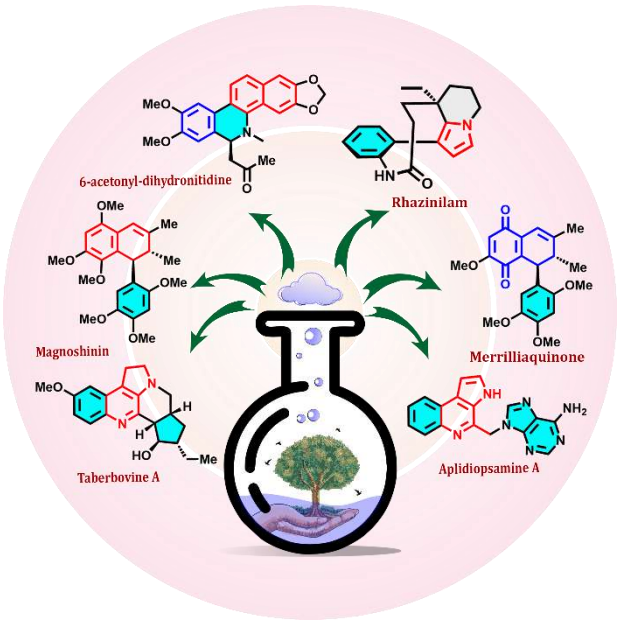
Award and Honors:
Dr. D. S. Kothari Postdoctoral Fellowship (2009-2012)
Fulbright-Nehru Postdoctoral Fellowship (2012-2013)
SERB EMR Funding (2016-18)
CSIR EMR Funding (2018-21)
SERB CRG (2019-22)
SERB CRG (2024-27)

Catalytic/Non-catalytic Synthetic Strategies for Natural /Unnatural Products While Aiming Sustainable Chemistry

Tabrez Khan
Organic Synthesis Laboratory, School of Basic Sciences, Indian Institute of Technology Bhubaneswar
(tabrez@iitbbs.ac.in)

Abstract:

Very often natural product synthesis demands the development of methodologies for carbocycles as well as heterocyclic scaffold synthesis with specific regio-, chemo-, or stereoselectivity. In this context, some of the methodologies that have been developed in our laboratory and applied for the total synthesis of some bioactive natural products will be discussed.[1-6] Also, in our synthetic journey how experimental and spectroscopic methods played an important role in some cases in understanding the reaction mechanism will be demonstrated.



References and Notes:

1) V. Kumar, A. Awasthi, A. Metya, T. Khan, *J. Org. Chem.* **2019**, *84*, 11581-11595.
2) V. Kumar, A. Awasthi, A. Salam, T. Khan, *J. Org. Chem.* **2019**, *84*, 11596-11603.
3) V. Kumar, A. Salam, D. Kumar, T. Khan, *ChemistrySelect* **2020**, 5, 14510-14514.
4) D. Kumar, A. Salam, T. K. Sahu, S. S. Sahoo, T. Khan, *J. Org. Chem.* **2021**, 86, 15096-15116.
5) A. Salam, D. Kumar, T. K. Sahu, R. Khan and T. Khan, *Eur. J. Org. Chem.* **2022**, e202101452 (1-8).
6) T. K. Sahu, A. Vishwakarma, V. Kumar, R. Khan and T. Khan *ChemRxiv* Dec. **2023**: https://doi.org/10.26434/chemrxiv-2023-j53bc

Bio-Sketch of Speaker

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EDUCATION:
PhD (2010), IICT Hyderabad (Mentor: Prof. T. K. Chakraborty)
MSc (2004), Jadavpur University, Kolkata (Mentor: Prof. Rina Ghosh)
BSc (2002), Jadavpur University, Kolkata

CAREER:
Associate Professor (Aug 2019-present)
Assistant Professor (Sep 2013-Aug 2019)
Postdoc (MPI Dortmund; Mentor: Prof. A. P. Antonchick; June 2010- Sep 2013)

AWARDS AND HONORS:
Thieme Chemistry Journals Award (Thieme, Stuttgart, Germany, 2023)
Associateship for the Indian Academy of Sciences (2019-2022)
"Emerging Investigator" by *New J Chem* (RSC, 2021)
"Young Investigators" in Asia in Homogeneous Catalysis by *Chem Asian J* (Wiley, 2018)
Max-Planck Postdoc Fellowship, MPI, Germany (2010)

AREA OF RESEARCH:
I) Straightforward synthesis of azaheterocycles and natural products via C-H bond functionalizations using metallocarbenes and nitrenes.
II) Synthesis of axially chiral heterobiaryls using quinoid carbene chemistry
III) Step-economic construction of *N*-PAHs and photophysical properties screening.

Insertion of Quinoid Carbene: Applications in Heterobiaryls to Natural Products

*Dr. Rajarshi Samanta**

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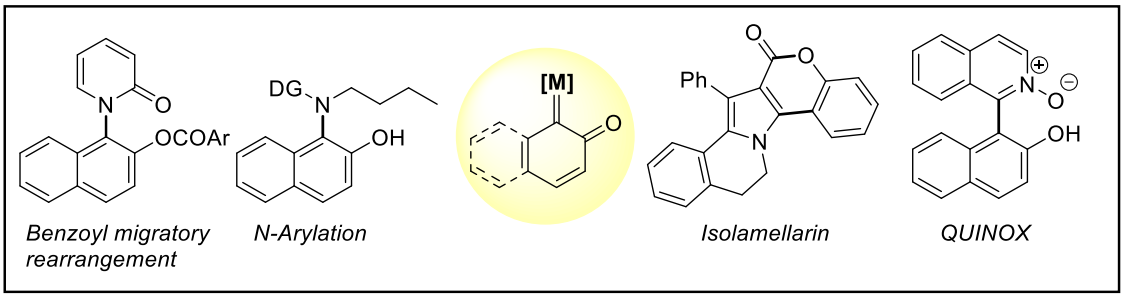
The diazo quinone or quinone diazide compounds have been extensively utilized to introduce phenol/naphthol moieties into hydrocarbons or nitrogen-containing heterocycles under transition metal catalysis.[1] The reactions proceed via C–H/X-H insertion or migratory insertion of metal carbenes. In this presentation, the racemic synthesis of important phosphine ligands like QUINAP, METHOX, PINAP, PHENAP will be discussed.[2] Construction of indolocoumarin using the migratory insertion of quinoid carbene will be explained.[3] Next, *N*-arylation of electron-deficient systems will be discussed.[4,5]



Scheme 1: Synthetic strategies using quinoid carbene

References:

1. *Related Review*: Bera, S.; Sarkar, S.; Samanta, R. *New J. Chem*. **2021**, *45*, 10135-10149.
2. Biswas, A.; Pan, S.; Samanta, R. *Org. Lett*. **2022**, *24*, 1631-1636.
3. Sarkar, S.; Samanta, R. *Org. Lett*. **2022**, *24*, 4536-4541.
4. Bera, S.; Roy, S.; Pal, S. C.; Anoop, A.; Samanta, R. *ACS Catal*. **2021**, *11*, 10847-10854.
5. Pan, S.; Kundu, S.; Samanta, R. *Org. Lett*. **2023**, *25*, 2873-2877.

Bio-Sketch of Speaker

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Dr. Jeyakumar Kandasamy has completed Master's degree from the University of Madras, Chennai and Ph.D. from IIT Madras with Prof. Dillip Kumar Chand. He worked with Prof. Timor Baasov (Technion-Israel) and Prof. Peter H. Seeberger (Max-Planck Institute of Colloids and Interfaces, Germany) as a postdoctoral fellow. In June 2014, he joined IIT(BHU)-Varanasi as an Assistant Professor in the Department of Chemistry and was promoted to associate Professor on 14.08.2019. Recently, he moved to Pondicherry University as an Associate Professor. His research focuses are carbohydrate synthesis, the development of reaction methodology, and medicinal chemistry. He is the recipient of the Euroglycoscience Award: European Young Investigator Workshop-France. 2011, Schulich Postdoctoral Fellowship (Technion, Israel): -Oct. 2008 -Sep-2011. He also qualified for the national exams Council of Scientific and Industrial Research (CSIR-JRF): 2004 Graduate Aptitude Test in Engineering (GATE): -2004 with 95 percentiles. Published nearly 70 research papers in well-reputed journals and guided 10 students to Ph.D. Handled SERB, DST, and MPIKG research projects.

Palladium-catalyzed Heck-type Coupling Reactions: Applications in Stereocontrolled Synthesis of *C*-Aryl glycosides and More!

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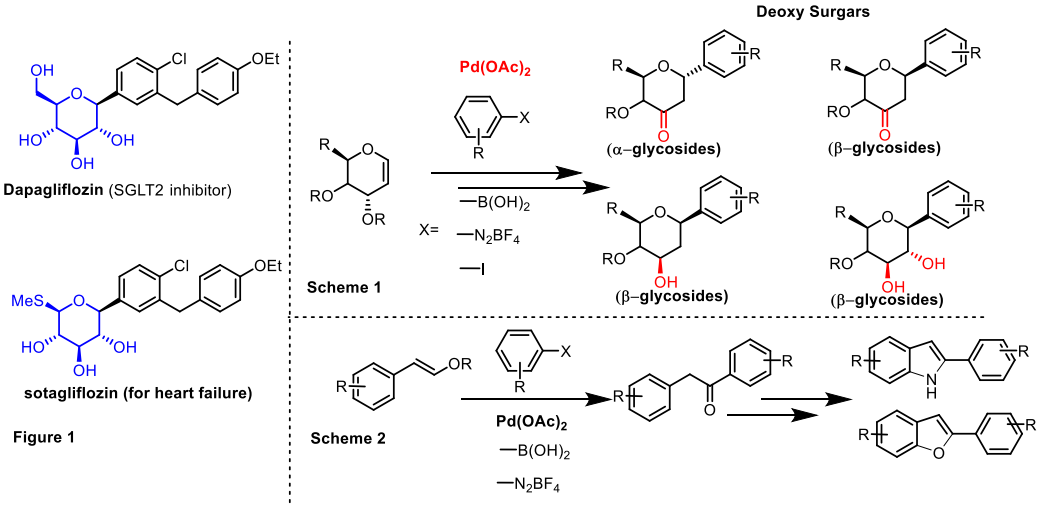
Heck coupling reaction plays a key role in the construction of complex organic molecules and natural products. Aryl *C*-glycoside is one of the distinct motifs found in various bioactive molecules and natural products [1]. Recently, several aryl glycosides have been approved for the treatment of diabetes mellitus and heart failure (Figure 1). The synthesis of aryl-C-glycoside received tremendous interest in synthetic organic chemistry owing to their biological significance. In this context, here we disclose the synthesis of aryl C-glycosides and 2-deoxy aryl-*C*-glycosides from different glycals and aryldiazonium salts/arylboronic acids/aryl iodides in the presence of palladium acetate (Scheme 1) [2]. We have extended our investigations towards the preparation of α-aryl acetophenones using vinyl ethers through Heck coupling (Scheme 2).



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Bio-Sketch of Speaker

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Dr. Bagh is working as a Reader-F in the School of Chemical Sciences, National Institute of Science Education and Research. His current research interest includes the development of base metal catalyzed protocols for important organic transformations such as hydrosilylation, transfer hydrogenation, aerobic oxidation, peroxidative oxidation and □-alkylation.

Academic Background:

B.Sc.: Visva-Bharati (2001-04) (First class)

M.Sc.: IIT Guwahati (2005-07)

Ph.D.: Univ. of Saskatchewan, Canada (2007-2012); Supervisor- Prof. Jens Müller

Post-Doctoral Research: University of Toronto, Canada (2012–2014) With Prof. Douglas Stephan, University of Amsterdam, Netherlands (2015–2017) With Prof. Jarl Ivar van der Vlugt and University of Berb, Switzerland (2017) With Prof. Martin Albrecht.

Awards / Honors / Membership:

i. Gold Medal (“Taube Metal”) for PhD thesis, University of Saskatchewan, Canada (Awarded to the best thesis among all PhD and masters candidates defended in 2012).

ii. Early Career Research Award, SERB, India, 2019.

Website: https:// www.niser.ac.in/users/bidraha

Development of Base Metal Catalysts for the Hydrosilylation of Challenging Functionalities

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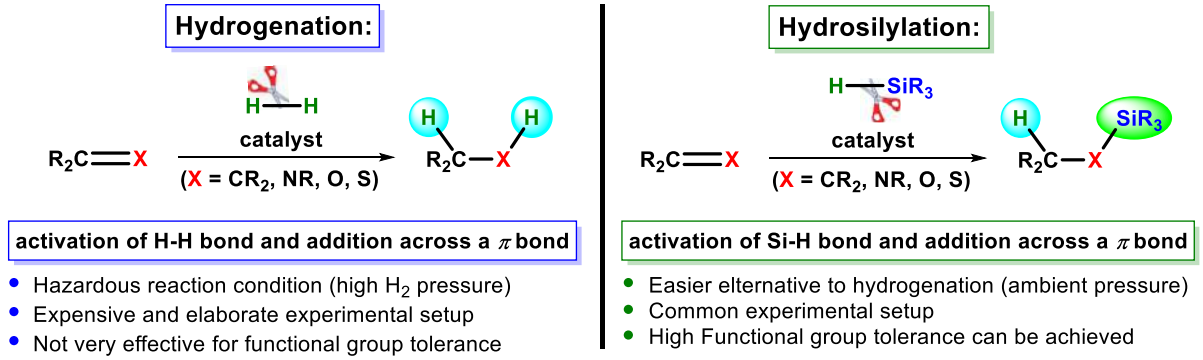
Reduction of unsaturated moieties is one of the fundamental reaction in organic transformations and catalytic hydrogenation is considered as the best reduction technique. However, hydrogenation requires expensive and elaborate experimental setup. In addition, the use of pressurized H_2 gas is detrimental. Hence, hydrosilylation have received a significant attention as easy alternative. Hydrosilation is the activation of Si-H bond followed by the addition across a multiple bond (Scheme 1). Transition metal catalyzed hydrosilylation of carbonyls is an efficient method for the selective reduction of carbonyl compounds to their corresponding alcohols using silanes as reducing agents. This transformation typically involves the use of noble metals such as platinum, rhodium, or iridium complexes. This method offers mild reaction conditions, high chemoselectivity, and excellent functional group tolerance, making it a valuable tool in synthetic organic chemistry for the synthesis of a wide range of alcohol derivatives. Sustainable base metal catalyzed hydrosilylation carbonyls is also well-established. However, much developments need to be done for the base metal catalyzed hydrosilylation of challenging unsaturated functionalities such as ester, carboxylic acid, alkyne and nitro group. In this context, I will discuss our contribution in the area of the base metal catalyzed hydrosilylations of esters, terminal alkynes and nitroarenes.[1-5]



Scheme 1. Hydrogenation and hydrosilylation as common reduction methods.

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Bio-Sketch of Speaker

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Buddhadeb graduated (2003) with M.Sc. in Organic Chemistry from Visva-Bharati University (Santiniketan) and earned Ph.D. degree in Synthetic Organic Chemistry from the University of Kalyani (2009), West Bengal. Buddhadeb spent around six years in USA for his postdoc from 2009 to 2014 (University of Illinois at Chicago, USA and Michigan State University, Michigan, USA). In August 2014, he started his independent career at Centre of Biomedical Research (CBMR) Lucknow. Since 2019, he is serving in the same institute as Associate Professor, Chemistry. His research interest includes catalyst/ligand engineering employing various noncovalent interactions for the C–H bond activation/borylation chemistry and synthesis of medicinally important high-valued N-heterocyclic molecules via metal-nitrene/carbene chemistry. Buddhadeb is a recipient of Ramanujan Fellowship (**2014**), DST-Young Scientist Award (**2015**), Thieme Chemistry Journal Award (**2017**), SERB-STAR Award (**2019**), SERB-TETRA Award (**2022**). Dr. Chattopadhyay's research contribution has been recognized by the **National Academy of Sciences (NASI), FNASc (2023)**.

Representative publications:

(1) Bisht, R.; Chattopadhyay, B. *J. Am. Chem. Soc.* **2016**, *138*, 84-87.

(2) Hoque, E.; Bisht, R.; Haldar, C.; Chattopadhyay, B. *J. Am. Chem. Soc.* **2017**, *139*, 7745-7748.

(3) Das, S. K.; Roy, S.; Khatua, H.; Chattopadhyay, B. *J. Am. Chem. Soc.* **2018**, *140*, 8429-8433.

(4) Roy, S.; Khatua, H.; Das, S. K.; Chattopadhyay, B. *Angew. Chem. Int. Ed.* **2019**, *58*, 11439-11443.

(5) Hoque, E.; Hassan, M. M. M.; Chattopadhyay, B. *J. Am. Chem. Soc.* **2021**, *143*, 5022–5037.

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Catalyst Engineering for C–H Bond Functionalization

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Abstract: The direct C–H bond functionalization using transition metal catalysts is one of the key emergent methods that is currently drawing remarkable attention owing to the rapidly expanding abundant chemical feedstocks to achieve high-valued materials. In this context, catalyst engineering concept through ligand design strategy is one of the most demanding concepts for the direct C–H bond functionalization chemistry. Innovative catalyst design help to deliver the sustainable green chemistry by minimizing extra steps and hazardous toxic materials for a particular reaction. Importantly, direct C-H activation is such innovative idea which originated to eliminates lots of serious problems, now taken a special place towards the sustainable development. Several natural products/chemicals that required multi-step sequences now have been performed with shorter route with improve process through the C-H activation methodology. We have been working in the area of C–H bond activation and borylation chemistry, where site selectivity is primarily controlled by the catalyst engineering concept. In this talk, I will briefly discuss some of our efforts regarding the catalyst engineering concept for the direct CH bond borylation.

Selected References:

(1) Bisht, R.; Chattopadhyay, B. *J. Am. Chem. Soc.* **2016**, *138*, 84-87.

(2) Hoque, E.; Bisht, R.; Haldar, C.; Chattopadhyay, B. *J. Am. Chem. Soc.* **2017**, *139*, 7745-7748.

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Bio-Sketch of Speaker

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Scopus ID: **35290490800**
Web of Science ID: **R-6820-2019**
Google Scholar: **JVO46DgAAAAJ**

Education

- 2018 – Habilitation in Chemistry, Faculty of Chemistry, Wrocław University of Science and Technology, Poland
- 2006 – PhD in Chemistry, Supervisor: Prof. Jacek Skarżewski, Faculty of Chemistry, Wrocław University of Technology, Poland
- 2002 – MSc in Chemistry, Faculty of Chemistry, Wrocław University of Technology, Wrocław, Poland

Fellowships

- 2009-2010 – Institute of Organic Chemistry, RWTH Aachen University, Prof. Carsten Bolm
- 2002 – Ghent University, Prof. Christian V. Stevens

Research

- Asymmetric Catalysis*
- C-H Functionalization of Csp2-H and Csp3-H Bonds

Cooperation

- Prof. Łukasz Albrecht (Lodz University of Technology)
- Prof. Debabrata Maiti (IIT Mumbai)
- Prof. Geraldine Masson (Institut de Chimie des Substances Naturelles (ICSN), Gif-sur-Yvette)

Selected Publications

1. Mała, Ż. A.; Janicki, M. J.; Góra, R. W.; Konieczny, K. A.; Kowalczyk, R. *Mechanochemical Assisted Chemoselective and Stereoselective Hydrogen-Bonding Catalyzed Addition of Dithiomalonates to Enones.* *Advanced Synthesis and Catalysis* **2023**, **365** (19), 3342–3352.
2. Kowalczyk, R. Mechanochemistry and High-Pressure Techniques in Asymmetric Organocatalysis. In *Asymmetric Organocatalysis: New Strategies, Catalysts, and Opportunities*: Volume 1-2; 2022; Vol. 1–2, pp 393–432.
3. Mała, Ż. A.; Janicki, M. J.; Niedźwiecka, N. H.; Góra, R. W.; Konieczny, K. A.; Kowalczyk, R. Stereoselectivity Enhancement During the Generation of Three Contiguous Stereocenters in Tetrahydrothiophenes. *ChemCatChem* **2021**, *13* (2), 574–580.
4. Dajek, M.; Pruszczyńska, A.; Konieczny, K. A.; Kowalczyk, R. *Cinchona Squaramide-Catalyzed Intermolecular Desymmetrization of 1,3-Diketones Leading to Chiral 1,4-Dihydropyridines.* *Advanced Synthesis and Catalysis* **2020**, *362* (17), 3613–3620.

How does Hydrogen Bonding drive Palladium-catalyzed *meta*-C-H Alkenylation of Nitroarenes?

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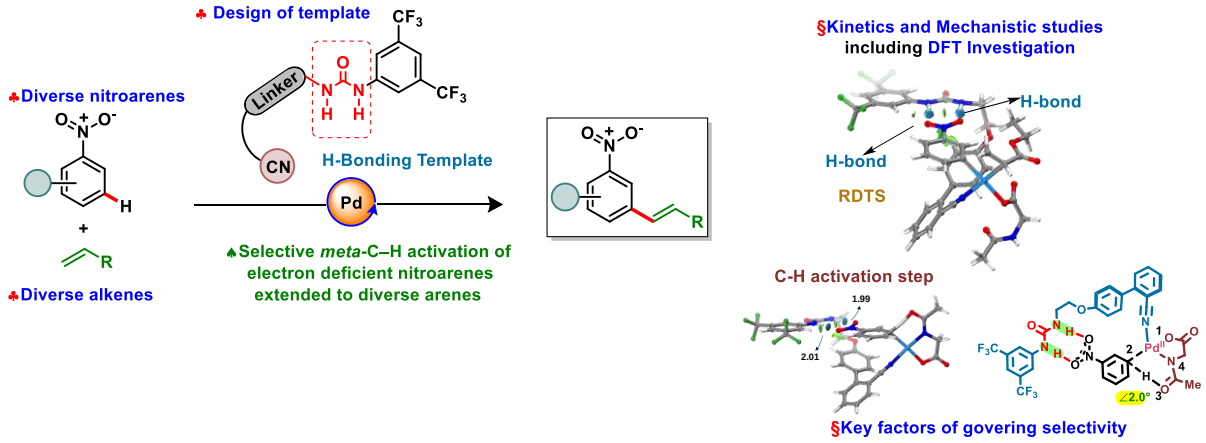
Web: https://bioorganic.pwr.edu.pl/people/rafal-kowalczyk)

This presentation will introduce a breakthrough in synthetic chemistry, addressing the persistent challenge of regioselective distal functionalization of nitroarenes. A novel approach involves a palladium-catalyzed *meta*-C-H alkenylation utilizing urea-based templates with an elongated biphenyl linker. Strong hydrogen bonding with the nitro group and coordination with the palladium center through a cyano-based directing group enables the activation of the remote *meta*-C-H bond of nitrobenzene (Scheme 1).

Computational investigations underscore the crucial role of hydrogen bonding in regulating regioselectivity. Successful palladium-catalyzed distal meta-alkenylation is demonstrated across diverse substrates, supported by control experiments, NMR analysis, and DFT-based mechanistic studies confirming hydrogen bonding interactions.



Scheme 1. Olefination of arenes governed by hydrogen-bonding template

Kinetic studies reveal the 1,2-migratory insertion as the rate-determining step, intricately governed by the hydrogen-bonding template. The extended biphenyl spacer-based hydrogen bond donor template, in synergy with the ligand, holds promise for broader synthetic applications. The results provide key insights into the complexities of the reaction, paving the way for advancements in regioselective C-H functionalization methodologies employing non-covalent interactions.

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Bio-Sketch of Speaker

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Professor of Chemistry & SERB-STAR Fellow
IISER Kolkata, Mohanpur, Nadia 741 246, WB
Previously at **IISER Bhopal** (2009-2020)
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Alakesh obtained his Ph.D. from IIT Kanpur in Sept. 2006 working with Prof. Vinod K. Singh. Immediately afterward, he moved to the University of California, Berkeley, CA, where he held postdoctoral position with Prof. Richmond Sarpong (Sept. 2006 – Dec. 2009). During his stay at Berkeley, he completed the total synthesis of '*lycopodium alkaloids*' lyconadin A, that received considerable attention from the synthetic community. In Dec. 2009, he left Berkeley and joined Department of Chemistry, IISER Bhopal as an Assistant Professor of Chemistry, later he was promoted to an Associate Professor followed by Professor (Jan., 2018) and continued his Academic journey till May, 2020. Meanwhile, he moved to the Department of Chemical Sciences, IISER Kolkata in May, 2019.

The research focus of the AB research group includes the total synthesis of architecturally interesting and biologically active natural products that provide an ideal platform for the invention of new strategies and highly selective organic transformations. His total synthesis has been highlighted twice in '*Organic Chemistry Portal*' as '*The Bisai Synthesis of (-)-Physovenine*' (**2018**) and '*The Bisai Synthesis of Lycoramine*' (**2023**).

The research of the AB Group has been appreciated in various forms, to name a few notable ones: **A. Srikrishna** Memorial Lecture (2023, UoH); **CDRI Award** (2022, CSIR-CDRI) (Excellence in Drug Research); '**Special Call**' on 'Reagentless Chemistry' (2022, SERB); **Silver Medal**, Chirantan Rasayan Sanstha (2021, VU); **D. Nasipuri** Memorial Lecture Award (2021, ICS); **Bronze Medal**, Chemical Research Society of India (2021); **Fellow**, Indian Chemical Society (FICS-2020); **SERB-STAR** Award (STAR-2020); **CRSI** Young Scientist Award (2018); **DST** Young Scientist Research Grant (2013); **BRNS** Young Scientist Award & Grant (2011).

Architecturally Intriguing Bioactive Natural Products as the Inspiration for New Strategies/Methodologies

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Department of Chemical Sciences, IISER Kolkata, Mohanpur, WB
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Nature produces a variety of complex natural products in entioenriched form (see, Figure).[1-2] Since these are isolated from Nature in limited quantity (mostly in mg scale), total synthesis endeavors play a crucial role in bioactivity evaluation by providing access to significant quantity.[3] This also provides platform for the invention of oxidative strategies for chemical synthesis, such as C-C, C-N, and N-N bond forming reactions.[4-5] Since these processes avoid a protection and deprotection groups, the development of methodologies following aerobic oxidations are welcome to synthesize value added organic molecules, particularly for the synthesis of natural products and in pharmaceutical industries.

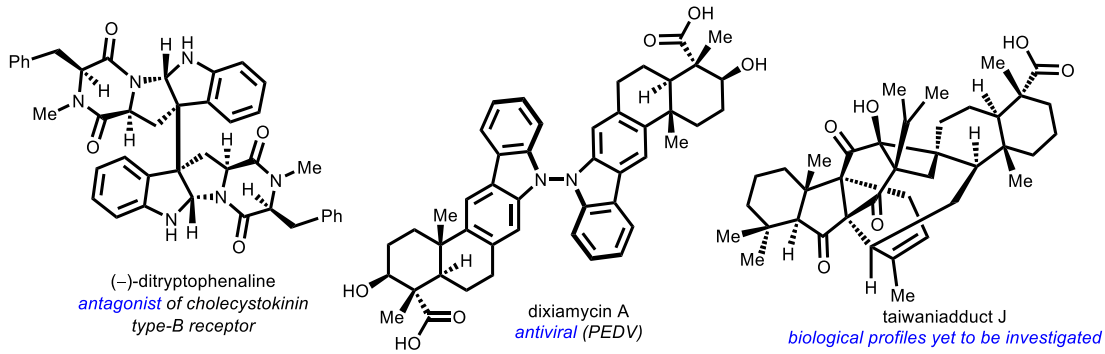

Figure. Architecturally intriguing indole alkaloids of biological relevance.

In the above context, naturally occurring alkaloids with impressive diversity of biological activities drew our interest for the development of strategies to form C-C, C-N, and N-N bonds under oxidative conditions.[1a] Interestingly, a variety of alkaloids of this family show interesting biological activities, such as antibacterial and cytotoxic activities.[1a] Towards this direction, we explored novel oxidative strategies under mild condition that will be discussed in this talk.[6]

References & Notes:

1. (a) N. Kumar, M. K. Das, S. Ghosh, A. Bisai, *Chem. Commun.* **2017**, *53*, 2170. (a) N. Babu, A. Roy, M. Singh, A. Bisai, *Org. Lett.* **2018**, *20*, 6327. (b) M. K. Das, N. Kumar, A. Bisai, *Org. Lett.* **2018**, *20*, 4421.
2. (b) S. Bhunia, S. Chaudhuri, A. Bisai, *Chem. Eur. J.* **2017**, 23, 11234. (c) N. Babu, L. K. Kinthada, P. P. Das, A. Bisai, *Chem. Commun.* **2018**, *54*, 7963. (d) S. Sharma, A. Roy, K. Shaw, A. Bisai, A. Paul *J. Org. Chem.* **2020**, *54*, 14926.
3. (a) A. Roy, M. K. Das, S. Chaudhuri, A. Bisai, *Chem. Commun.* **2018**, *54*, 940. (b) S. Chaudhuri, S. Bhunia, A. Roy, M. K. Das, A. Bisai, *Org. Lett.* **2018**, *20*, 288.
4. (a) K. Shaw, S. Sharma, A. Khatua, A. Paul, A. Bisai, *Org. Biomol. Chem.* **2021**, *19*, 9390. (b) A. Khatua, P. Shyamal, S. Pal, A. Mondal, A. Bisai, *Chem. Commun.* **2022**, *58*, 3929.
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6. (a) R. Nandi, S. Kundu, V. R. Gavit, M. Munda, S. Niyogi, A. Bisai *Chem. Sci.* **2022**, *13*, 11666. (b) R. Nandi, S. Niyogi, S. Kundu, V. R. Gavit, M. Munda, R. Murmu, A. Bisai *Chem. Sci.* **2023**, *14*, 8047.

Bio-Sketch of Speaker

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Professor

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

Research Interest:

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

Awards and Recognitions:

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

Stereodivergent Functionalization of C-H bonds with Cyclopropenes

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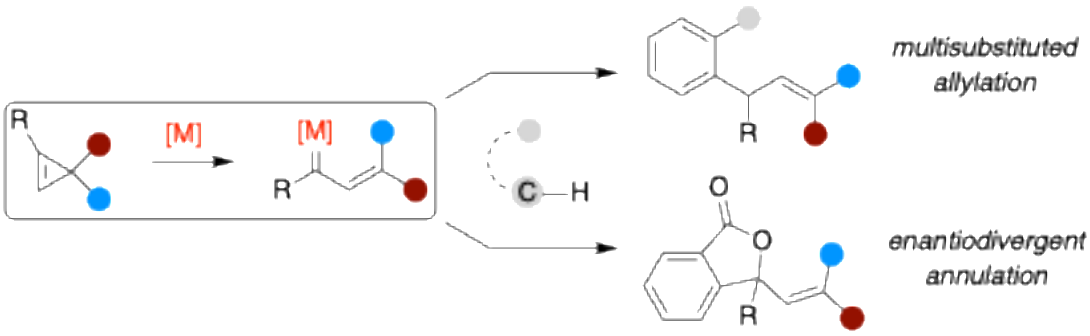
Metallocarbenes show versatile reactivity in organic synthesis and offers access to diverse complex frameworks in single step. Most often these metallocarbenes are generated from reactive α-diazocarbonyl compounds in the presence of suitable transition metal.[1] In the quest of finding suitable alternative,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



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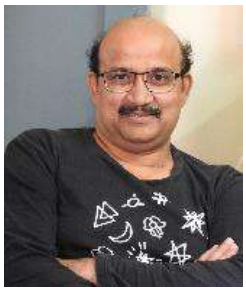
Bio-Sketch of Speaker



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

Expanding Discovery Chemistry Toolbox: From Concept to Practice

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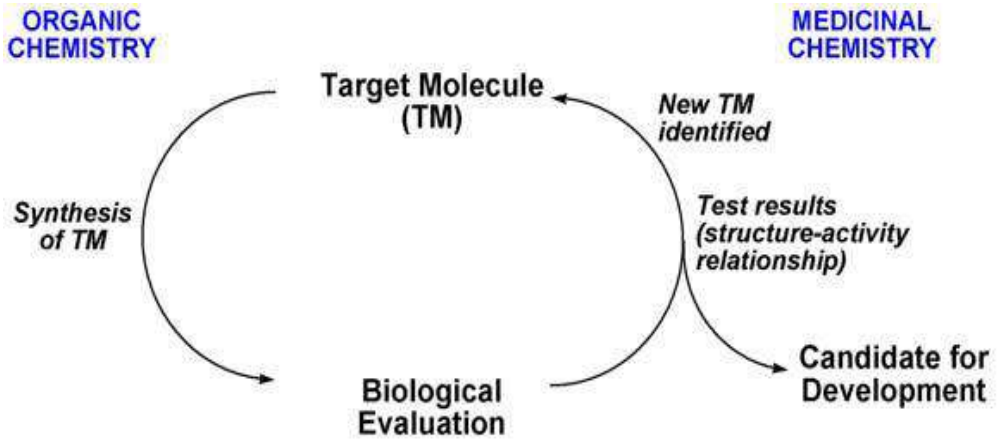
Abstract:
The pharmaceutical industry remains solely reliant on synthetic methodology to prepare drugs or drug like molecules for their discovery/process program. The expansion of synthetic methodology in recent years has greatly facilitated the preparation of molecules that would once have been considered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



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Bio-Sketch of Speaker

Andy A. Thomas, PhD

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Appointment

August 2020 –	**Texas A&M University** **Assistant Professor, Department of Chemistry**

Education

August 2011 – May 2017	**University of Illinois at Urbana-Champaign** **Ph. D. in Chemistry** Advisor: Prof. Scott E. Denmark
May 2010 – August 2011	**University of North Carolina at Charlotte** **Masters of Science in Chemistry** Advisor: Prof. Craig A. Ogle
August 2006 – May 2010	**University of North Carolina at Charlotte** **Bachelors of Science in Chemistry** Thesis: *Investigations of Lithium Tetramethylcuprate* Advisor: Prof. Craig A. Ogle

Recent Research Articles at TAMU

(Undergraduate co-authors are underlined)

- Gonzalez, R.; Hsu, H.-H.; **Thomas, A. A.***, Improved Synthesis of Lithium Dendrites for the Synthesis of (Trimethylsilyl)methyllithium [*Being Checked at Org Syn*]
- Wu, D.; Martin, R. T.; Piña, J.; Kwon, J.; Crockett, M. P.; **Thomas, A. A.**; Gutierrez, O.; Park, H. H.; Hedrick, J. L.; Campos*, L. M., A Generalized Approach to Activate CO_2 for Carbonation Polymerization and Functional Transformations. [*Accepted Angew Chem.*]
- Aguirre, L. S.; Litwiller, L; Lugo, A.; **Thomas, A. A.***, Phosphine Urea Ligands for Mild Cross-Coupling Reactions. [*Accepted Helv. Chim. Acta]*
  - (Special issue honoring Prof Scott E. Denmark 70th Birthday)
- Arriaga, D. K.; Kang, S.; **Thomas, A. A.***, Solvent Effects on the Rate of Olefin Ozonolysis: Development of a Homogeneous Flow Ozonolysis Protocol. *J. Org. Chem.* **2023,** *88*, 13720-13726.
  - (Highlighted in *Org. Process Res. Dev.* **2023**, *11*, 1848-1857)
- Arriaga, D. K.; **Thomas, A. A.***, Capturing Primary Ozonides for a *syn*-dihydroxylation of olefins. *Nat. Chem.* **2023**, *15*, 1262-1266.
  - (Highlighted in *Org. Process Res. Dev.* **2023**, *9*, 1535-1545)
- Crockett, M. P.; Piña, J.; Gogoi, A. R.; Lalisse, R. F.; Nguyen, A. V.; Gutierrez, O.; **Thomas, A.A.***, Breaking the tert-Butyllithium Contact Ion Pair: A Gateway to Alternate Selectivity in Lithiation Reactions. *J. Am. Chem. Soc.* **2023**, *145*, 10743-10755.
- Crockett, M. P.; Aguirre, L. S.; Jimenez, L. B.; Hsu, H.-H.; **Thomas, A. A.***, Preparation of Highly Reactive Lithium Metal Dendrites for the Synthesis of Organolithium Reagents. *J. Am. Chem. Soc.* **2022**, *144*, 16631-16637.
  - (Highlighted in C&EN News, Science Magazine, Spotlights in JACS)
- Arriaga, D. K.; **Thomas, A. A.***, Antibiotics the easy way. Nat Synth. **2022** (News & Views)

Reimagining Ancient Reactions for the 21st Century

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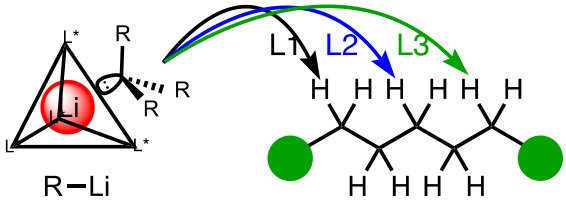
Abstract



The ability to prepare highly functionalized molecules in general and predictable ways is central to modern drug design and discovering new treatments for human disease. The aim of our program is to create new methods to solve the longstanding synthetic challenge of asymmetrically constructing biologically active small molecules. Classical synthetic approaches based on CH activations are ubiquitous but limited by the inherent directing effects of embedded heteroatoms. This presentation will discuss our recently discovered scheme to access highly basic ion pairs with organolithiums which provides a new pathway to override intrinsic heteroatom directing effects. In addition, we will describe our progress in developing new methods for carbon-oxygen bond formation reactions that utilizes primary ozonide intermediates.

Bio-Sketch of Speaker

Martín Fañanás-Mastral

Biographical sketch

Martín Fañanás Mastral graduated in Chemistry from the University of Oviedo in 2002. He performed his PhD studies at the same university under the supervision of Prof. José Barluenga and Prof. Fernando Aznar, working on the development of cascade reactions of Fischer carbene complexes and their application in organic synthesis. He received his PhD in 2007 and his doctoral thesis was awarded with the "Extraordinary Doctorate Award". He performed a predoctoral stay at the group of Prof. Steven Ley at the University of Cambridge (UK), where he worked in the total synthesis of the natural product Bengazole A.

In 2009 he joined the group of Prof. Ben L. Feringa at the University of Groningen (The Netherlands) as postdoctoral researcher. There he worked on the development of enantioselective catalytic allylic substitution reactions, cross-coupling of organolithium reagents and catalytic oxidation processes.

In 2014 he moved to the Centro Singular de Investigación en Química Biológica y Materiales Moleculares (CiQUS), at the University of Santiago de Compostela, as Ramón y Cajal researcher. In 2020 he was promoted to Associate Professor.

He leads a research group at CiQUS and his research is based on the development of novel transition metal catalyzed reactions which allow to perform highly atom-efficient and sustainable transformations oriented towards enantioselective C-C bond formation, alkane functionalization and synthesis of biologically active phosphorous compounds.

Martín Fañanás Mastral has been awarded with the "Thieme Chemistry Journal Award" (2015), the Spanish Royal Society of Chemistry "Young Researchers Award" (2016) and with the "Lilly Young Researcher Award" (2018). In 2019, he received an ERC-Consolidator Grant awarded by the European Research Council.

CATALYTIC STEREOSELECTIVE HYDROCARBON DIFUNCTIONALIZATION

Martín Fañanás-Mastral

Centro Singular de Investigación en Química Biolóxica e Materiais Moleculares (CiQUS), Universidade de Santiago de Compostela, 15782 Santiago de Compostela, Spain

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The development of efficient, safe, clean and operationally simple transformations is a primary challenge in modern synthetic chemistry. Traditionally, transition metal catalyzed C-C bond forming reactions have been developed using pre-made organometallic reagents. These procedures are inherently limited to the availability and reactivity profiles of the reagent itself and entail the formation of a stoichiometric amount of inorganic salt as a reaction by-product. The goal of our research program is to discover and study new metal-catalyzed reactions with the aim to develop highly selective synthetic methodologies based on the use of readily accessible materials. In this context, we have recently developed new synthetic transformations based on the use of simple unsaturated hydrocarbons as transient functionalized organometallic intermediates in multicomponent reactions.[1-4] From simple and readily available materials we can obtain complex structures with a high level of selectivity.

In this lecture, different catalytic strategies to accomplish difunctionalization of unsaturated hydrocarbons based on selective carboboration processes will be presented.

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2. E. Rivera-Chao, M. Mitxelena, J. A. Varela, M. Fañanás-Mastral, *Angew. Chem. Int. Ed.* **2019**, *58*, 18230-18234.

3. E. Rivera-Chao, M. Fañanás-Mastral, *Angew. Chem. Int. Ed.* **2021**, *60*, 16922-16927

4. A. Chaves-Pouso, A. M. Álvarez-Constantino, M. Fañanás-Mastral, *Angew. Chem. Int. Ed.* **2022**, *61*, e202117696.

Bio-Sketch of Speaker

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Academic Qualifications:

- Ph.D. (**1997-2002**): University of Pune, India
- M.Sc. (**1995-1997**): North Maharashtra University, Jalgaon, India
- B.Sc. (**1992-1995**): North Maharashtra University, Jalgaon, India

Professional Experience:

- Professor (10/2023 - Present): Department of Chemistry, IISER Bhopal, Bhopal
- Associate Professor (07/2017 - 10/2023): Department of Chemistry, IISER Bhopal, Bhopal
- Senior Scientist (08/2013-06/2017): CSIR-NCL, Pune
- Senior Scientist (03/**2011-08**/2013): CSIR-IICT, Hyderabad
- QRS (09/2008-**03/2011**): CSIR-IICT, Hyderabad
- Research Fellow (01/2008-**07/2008**): The Scripps Research Institute, USA
- Research Fellow (06/2006-**12/2007**): Institute of Chemical and Engineering Sciences, Singapore
- Assistant Professor (04/2005-**03/2006**): Tohoku University, Japan
- JSPS Postdoctoral Fellow (11/2002-**03/2005**): Tohoku University, Japan
- Postdoctoral Fellow (03/2002-**11/2002**): University of Goettingen, Germany

Research Keywords: Organic Synthesis, Metal Catalysis, Organocatalysis, Enantioselectivity, Organometallics, Total Synthesis etc.

Awards and Honours:

- Recipient of the J. C. Bose Fellowship, CNR Rao National Prize for Chemical Sciences, SERB Distinguished Investigator Award, CRSI Bronze Medal, INSA Young Scientist Medal, Alkyl Amines – ICT Foundation Day Young Scientist Award, Avra Young Scientist Award etc.

- Fellow of the Indian National Science Academy (FNA), National Academy of Sciences (FNASc), Maharashtra Academy of Sciences (FMASc) and Royal Society of Chemistry (FRSC).

Editor of an Elsevier journal - Tetrahedron Letters (Since 2024)

Ligand-Enabled Redox Gold Catalysis

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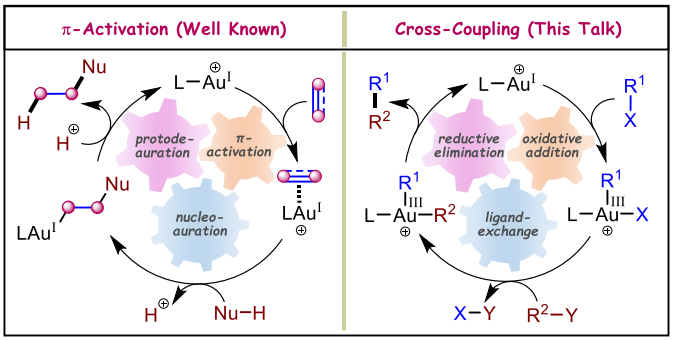
Traditionally, gold complexes have been recognized as Lewis acid catalysts for the activation of C-C multiple bonds (Scheme 1, LHS). Over the years, there has been a considerable shift, and Au(I)/Au(III) redox catalysis is now recognized as an established technique for achieving cross-coupling reactivities (Scheme 1, RHS). The pioneering work by Zhang and Toste group revealed the role of external oxidants to overcome the high redox potential of Au(I)/Au(III) couple (E^0 = +1.41 V) and to facilitate two-electron redox cycle in gold catalysis.[1] Later, the Glorius group introduced the merged gold/photoredox strategy to circumvent the need for a stoichiometric oxidant in these processes.[2] Recently, ethynylbenziodoxolones (EBXs) has also been used for accessing redox gold catalysis serving dual role as oxidant and alkyne surrogate.[3]

All the above strategies were not amenable to the use of aryl halides, and thus their use in gold-catalyzed cross-coupling reactions remains forbidden. In recent years, ligand-enabled gold-catalyzed organic reactions have emerged as a valuable tool, allowing for the use of aryl halides as cross-coupling partners. In this talk, I will discuss our most recent work in the area of alkene functionalization employing cross-coupling reactivities.[4]

Scheme 1. Fundamental Reactivity Modes in Gold Catalysis



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[3]. S. Banerjee; V. W. Bhoyare; N. T. Patil,* *Chem. Commun.* **2020**, *56*, 2677.
[4]. [a] V. W. Bhoyare, E. Daiann Sosa Carrizo, C. C. Chintawar, V. Gandon,* N. T. Patil* *J. Am. Chem. Soc.* **2023**, *145*, 8810. [b] S. P. Sancheti, Y. Singh, M. V. Mane,* Nitin T. Patil* *Angew. Chem. Int. Ed.*, **2023**, e202310493. [c] V. W. Bhoyare, A. G. Tathe, V. Gandon,* Nitin T. Patil* *Angew. Chem., Int. Ed.*, **2023**, e202312786. [d] C. C. Chintawar, V. W. Bhoyare, M. V. Mane and Nitin T. Patil,* *J. Am. Chem. Soc.*, **2022**, *144*, 7089. [e] C. C. Chintawar, A. K. Yadav, N. T. Patil,* *Angew. Chem. Int. Ed.* **2020**, *59*, 11808. [f] A. G. Tathe, Urvashi, A. K. Yadav, C. C. Chintawar, N. T. Patil,* *ACS Catal.* **2021**, *11*, 4576.

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Santanu obtained his B.Sc. (Chemistry Hons.) from Ramakrishna Mission Residential College, Narendrapur (2000) and M.Sc. (Chemistry) from Indian Institute of Technology, Kanpur (2002). After earning his Ph.D. (*summa cum laude*) in 2006 working with Professor Albrecht Berkessel at Universität zu Köln, Germany, he worked as a postdoctoral fellow with Professor Benjamin List at Max-Planck Institut für Kohlenforschung in Mülheim an der Ruhr, Germany (2006-2008) and with Professor E. J. Corey at Harvard University, USA (2008-2010). In 2010, he returned to India to take up an Assistant Professor position at the Department of Organic Chemistry in Indian Institute of Science, Bangalore. He was promoted to Associate Professor in 2015 and Professor in 2021.

Santanu's research interests revolve around various aspects of asymmetric catalysis, with a particular emphasis on desymmetrization and remote stereocontrol using different classes of organocatalysts. In addition, his research group is also works on transition metal-catalyzed enantioselective allylic, allenylic and propargylic substitution reactions.

Santanu is a recipient of the Thieme Chemistry Journals Award (2011), the Indian National Science Academy (INSA) Medal for Young Scientist (2014), Chemical Research Society of India (CRSI) Bronze Medal (2019), A. V. Rama Rao (AVRA) Young Scientist Award for the year 2019 and the Science and Technology Award for Research by Science and Engineering Research Board (SERB-STAR) for the year 2021. In 2018, he became a Fellow of the Royal Society of Chemistry, London (FRSC). He is an Associate Editor of *Organic & Biomolecular Chemistry* (RSC) since 2019. He served as a member of the Editorial Advisory Board of the *Journal of Organic Chemistry* (ACS) during 2018-2023 and is currently a member of the *SYNLETT* (Thieme) Advisory Board.

Breaking Symmetry: Development & Application to Complex Targets

Prof. Santanu Mukherjee*

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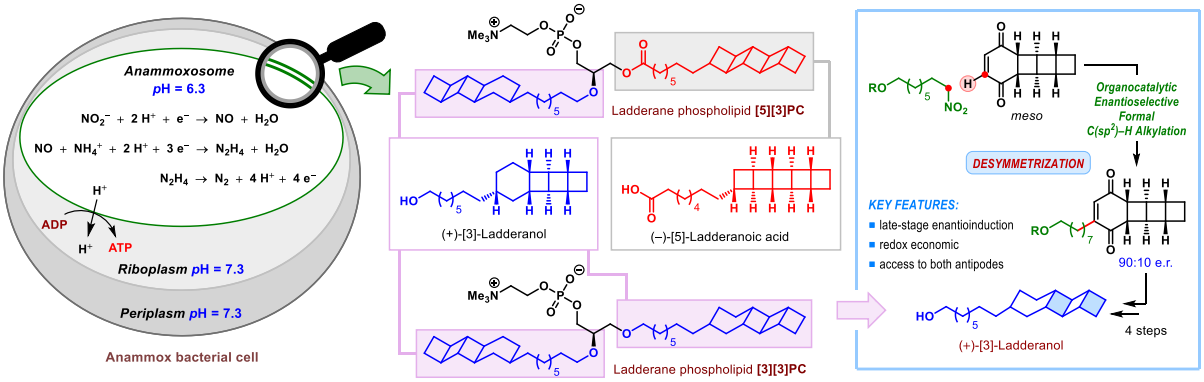
Human minds are fascinated by symmetrical objects, and we admire the challenges in constructing symmetrical architectures whenever we find one around us. In contrast to the physical world, we live in, creating symmetry in the molecular world is a relatively simple task. It is the daunting asymmetry in molecules that often challenges the chemists.

Breaking symmetry to generate asymmetry, commonly termed as *desymmetrization*, is a remarkably powerful strategy for building molecular complexity. Successful implementation of this strategy holds the potential to forge multiple stereogenic centers in a single step. In fact, stereocenters can also be created away from the reaction site.

During the past few years, we have developed a number of organocatalytic enantioselective desymmetrization reactions including formal C(sp^2)–H alkylations[1] and alkenylation[2] to the *de novo* construction of arenes[3] and heteroarenes.[4] The topic of this talk will be primarily confined to a few of these enantioselective desymmetrization reactions and their applications for the synthesis of complex targets.[5]



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7. Ghosh, B.; Balhara, R.; Jindal, G.; Mukherjee, S. *Angew. Chem. Int. Ed.* **2021**, *60*, 9086.
8. Ray, S.; Mondal, S.; Mukherjee, S. *Angew. Chem. Int. Ed.* **2022**, *61*, e202201584.

Assoc. Prof. Dr. Vinh Nguyen

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Education and training

2010 – 2013	Alexander von Humboldt Postdoctoral Research Fellow *Prof Dieter Enders' group – RWTH Aachen*
2006 – 2010	**Ph.D.** in Organic Chemistry (Supervisor: Prof. Michael Sherburn) *The Australian National University (ANU)*
2002 – 2006	**B.Eng.** in Industrial Chemistry (Honours 1st class) *University of New South Wales, Sydney (UNSW Sydney)*

Employment history

University of New South Wales, Sydney, Australia

2022 – present	Associate Professor
2018 – 2021	Senior Lecturer and ARC Future Fellow
2015 –2018	Lecturer and ARC DECRA Fellow

Curtin University, Perth, Australia

2013 – 2015	Curtin Early Career Research Fellow – Group leader

Academic awards and recognitions (selected)

2019-2022	Australian Research Council Future Fellowship
2016	Athel Beckwith medal and lectureship for outstanding early career organic chemist
2015-2018	Australian Research Council Discovery Early Career Researcher Award (DECRA)
2014	Thieme Journal Award 2014

Publications (selected)

Tuong A. To, **Thanh V. Nguyen**,* *Angew. Chem. Int. Ed.* **2023**, e202317003: "*Olefination of Aromatic Carbonyls via Site-Specific Activation of Cycloalkanone Ketals*". [https://doi.org/10.1002/anie.202317003]

Tuong A. To, Chao Pei, Rene M. Koenigs,* **Thanh V. Nguyen**,* *Angew. Chem. Int. Ed.* **2022**, *61*, e2021173: "*Hydrogen Bonding Networks Enable Brønsted Acid-Catalyzed Carbonyl-Olefin Metathesis*". [https://doi.org/10.1002/anie.202117366]

Reece D. Crocker, Domenic P. Pace, Bolong Zhang, Demelza J. M. Lyons, Mohan M. Bhadbhade, Wallace W. H. Wong,* Binh K. Mai,* **Thanh V. Nguyen**,* *J. Am. Chem. Soc.* **2021**, *143*, 20384–20394: "*Unusual Alternating Crystallization-Induced Emission Enhancement Behavior in Non-Conjugated ω-Phenylalkyl Tropylium Salts*". [https://doi.org/10.1021/jacs.1c10038]

Mohanad A. Hussein, Uyen P. N. Tran, Vien T. Huynh, Junming Ho, Mohan Bhadbhade, Herbert Mayr, **Thanh V. Nguyen**,* *Angew. Chem. Int. Ed.* **2020**, *59*, 1455-1459: "*Halide Anion Triggered Reactions of Michael Acceptors with Tropylium Ion*". [https://dx.doi.org/10.1002/anie.201910578]

Uyen P. N. Tran, Giulia Oss, Domenic P. Pace, Junming Ho,* **Thanh V. Nguyen**,* *Chem. Sci.* **2018**, *9*, 5145-5151: "*Tropylium-Promoted Carbonyl-Olefin Metathesis Reactions*". [http://dx.doi.org/10.1039/C8SC00907D]

Some Catalytic Applications of Superacids and Superbases

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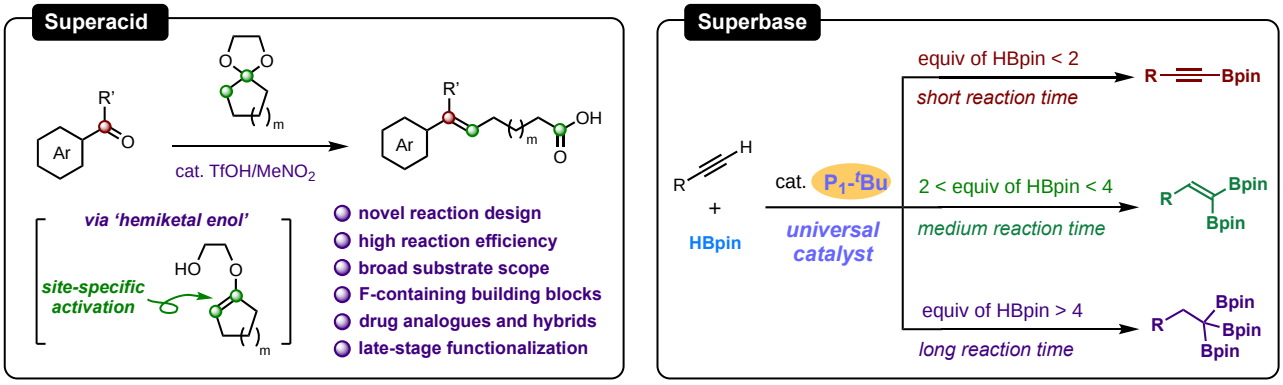
In this seminar, I would like to discuss two stories of how some Brønsted superacids and superbases promote interesting reactions for olefination of carbonyl compounds,[1,2] and multiboration of alkynes,[3,4] respectively.



[1] To, T. A.; Pei, C.; Koenigs, R. M. and Nguyen, T. V. *Angew. Chem. Int. Ed.* **2022**, *61*, e202117366.
[2] To, T. A. and Nguyen, T. V. *Angew. Chem. Int. Ed.* **2024**, *63*, e202317003.
[3] Doan, H. S.; Ton, N. H. N.; Mai, K. B. and Nguyen, T. V. *ACS Catal.* **2022**, *12*, 12409–12418.
[4] Doan, H. S.; Mai, K. B. and Nguyen, T. V. *ACS Catal.* **2023**, *13*, 8099–8105.

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David was born in Allentown, PA and pursued undergraduate education at Franklin and Marshall College. He earned a Ph.D. from Harvard University with Prof. Tobias Ritter and pursued postdoctoral research at the Massachusetts Institute of Technology and Harvard University with Prof. Daniel Nocera. He joined the Texas A&M faculty in 2015 and was promoted to Associate Professor in 2021. His research program focuses on the chemistry of sustainably generated reactive intermediates in catalysis and has been recognized by an NSF CAREER award, a DOE Early Career Award, NIH MIRA, a 2020 Sloan Fellowship, and an Alexander von Humboldt Award. His efforts in the classroom have been recognized by Montague-Center for Teach Excellence and Association of Former Students College-Level Teaching Awards.

Traceless Activation Strategies for Nitrene Transfer Chemistry

Dr. David C. Powers *
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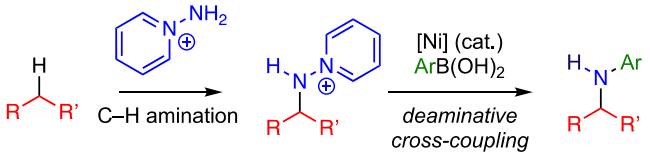
Nitrene transfer catalysis provide the opportunity to streamline the synthesis of nitrogen-containing organic small molecules via direct C–H amination and olefin aziridination reactions. In practice, the impact of intermolecular nitrene transfer methods is currently limited by typical requirement that the amine precursors bear activating groups, such as *N*-sulfonyl substituents, that are both challenging to remove and not useful synthetic handles for subsequent derivatization. This talk will introduce traceless nitrogen activation strategies that enable efficient access to a diverse array of products derived from formal nitrene transfer. In the first portion of the talk, a C–H aminopyridylation, cross-coupling strategy will be described that enables application of selective C–H amination chemistry to the preparation of diverse *N*-functionalized products. In contrast to many available C–H amination reactions, which provide access to protected amines, this method installs an easily diversifiable synthetic handle that serves as a lynchpin for C–H amination, deaminative N–N functionalization sequences. The second portion of the talk will describe extension of these methods to the preparation of *N*-arylaziridines, which are typically unavailable by direct nitrene transfer due to the inherent reactivity (and thus short lifetimes) of unstabilized nitrenes. Mechanistic investigations indicate aziridine cross-coupling proceeds via a noncanonical mechanism involving initial aziridine opening promoted by the bromide counterion of the Ni catalyst, C–N cross-coupling, and finally aziridine reclosure. Together, these results provide new opportunities to achieve selective incorporation of generic nitrene equivalents in organic molecules.



Scheme 1. C–H aminopyridylation, depyridylative cross-coupling schemes enable formal nitrene transfer to C–H bonds. Related methods provide access to *N*-aryl aziridines, β-phenethylamines, simple secondary amines, and products of olefin aziridine hydroxylation.

References: [a] Roychowdhury, P.; Herrera, R. G.; Tan, H.; Powers, D. C. Traceless Benzylic C–H Amination via Bifunctional *N*-Aminopyridinium Intermediates. *Angew. Chem. Int. Ed.* **2022**, *61*, e20220066. [b] Tan, H.; Samanta, S.; Maity, A.; Roychowdhury, P.; Powers, D. C. *N*-Aminopyridinium Reagents as Traceless Activating Groups in the Synthesis of *N*-Aryl Aziridines. *Nat. Comm.* **2022**, *13*, 3341. [c] Roychowdhury, P.; Waheed, S.; Sengupta, U.; Herrera, R. G.; Powers, D. C. Synthesis of Secondary Amines via Self-Limiting Alkylation of *N*-Aminopyridinium Salts. *ChemRXiv* **2023**, DOI: 10.26434/chemrxiv-2023-jm56l.

Bio-Sketch of Speaker

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Krishna P. Bhabak

Professional Experience

Jun, 2021 - Present	Associate Professor, Department of Chemistry, IIT Guwahati, Assam, India
Apr, 2015 - Jun, 2021	Assistant Professor, Department of Chemistry, IIT Guwahati, Assam, India
Feb, 2013 - Apr, 2015	Assistant Professor, Department of Chemistry, Presidency University, Kolkata, India.
Nov, 2012 - Feb, 2013	Post-doctoral Researcher, University of Oxford, United Kingdom
Jul, 2010 - Oct, 2012	Post-doctoral Researcher (Alexander von Humboldt Fellow), Humboldt University, Berlin, Germany

Education

Aug, 2006 - Jul, 2009	Ph.D., Department of Inorganic & Physical Chemistry, IISc Bangalore, India (Supervisor: Prof. G. Mugesh)
Aug, 2003 - Apr, 2006	M.S. in Chemical Science, IISc, Bangalore, India
Aug, 2000 - Jul, 2003	B.Sc. (Chemistry Hons.), Ramakrishna Mission Residential College, Narendrapur, University of Calcutta, India

Awards/Fellowships

Jan, 2013	INSPIRE Faculty Award by Department of Science and Technology (DST), India
Dec, 2010	Best Thesis Award by Eli Lilly and Company Outstanding Thesis Award 2010 in Asia
Mar, 2010	Alexander von Humboldt Fellowship for Post-doctoral Researcher by Alexander von Humboldt Foundation, Germany

Research summary

The major research interests of the group are in the field of (i) developing fluorogenic and non-fluorogenic donors of hydrogen sulfide (H_2S) and studying their biological implications; (ii) targeted delivery of anti-cancer/anti-inflammatory compounds/drugs using fluorogenic drug delivery systems; (iii) design and synthesis of potential bio-active organochalcogen compounds.

Development of Stimuli-responsive Fluorogenic Prodrug for the Simultaneous Delivery of Diclofenac and Hydrogen Sulfide

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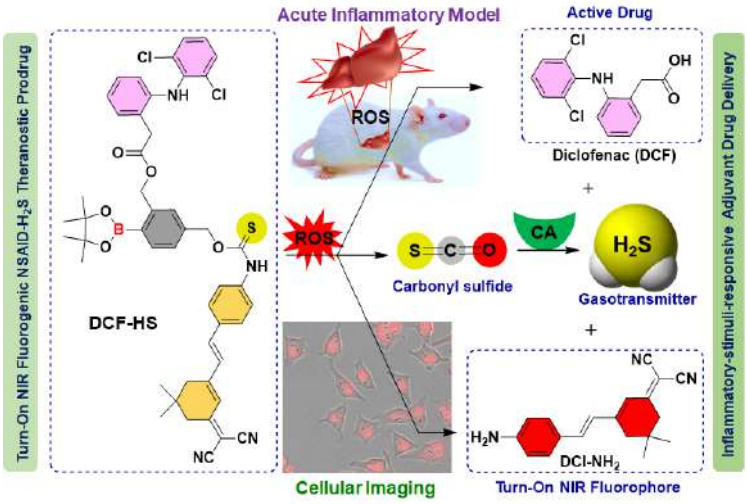
Prolonged use of the commonly prescribed non-steroidal anti-inflammatory drugs (NSAIDs) is often associated with undesired side effects including gastrointestinal ulcers.[1-2] We describe herein the design and synthesis of an inflammatory-stimuli-responsive turn-on fluorogenic prodrug **DCF-HS** for the simultaneous delivery of diclofenac (**DCF**, NSAID) and hydrogen sulfide (H_2S).[3] Upon the activation of **DCF-HS** by reactive oxygen species (ROS), **DCF** (active drug) and the NIR fluorophore **DCI-NH$_2$** was released along with carbonyl sulfide (COS). A second activation of COS by the enzyme carbonic anhydrase (CA) generated H_2S. The prodrug was synthesized using multi-step organic synthesis. Activation of the prodrug by H_2O_2 and the drug release was studied using UV-Vis and fluorescence spectroscopy and reverse phase HPLC method. Compatibility of the prodrug activation was studied next in in a representative cancer cell line (HeLa) and a macrophage cell line (RAW 264.7). The anti-inflammatory activity of **DCF** from the prodrug **DCF-HS** was studied in the lipopolysaccharide (LPS)-induced macrophage cell line and compared to that of the parent drug **DCF**. Finally, the anti-inflammatory potential of the prodrug was validated in the inflammation-induced Wister rat models.



Scheme 1. Stimuli-responsive activation of the prodrug **DCF-HS** for the simultaneous release of diclofenac and H_2S with turn-on NIR fluorescence.

References

1. S. Bindu, S. Mazumder and U. Bandyopadhyay, *Biochem Pharmacol*, **2020**, *180*, 114147.

2. A. Sufian, D. Bhattacherjee, P. Barman, A. Srivastava, R. P. Thummer and K. P. Bhabak, *Chem Commun*, **2022**, *58*, 7833.

3. A. Sufian, M. Badirujjaman, P. Barman, and K. P. Bhabak (*manuscript submitted*)

Bio-Sketch of Speaker

Dr. Nilanjana Majumdar
Senior Scientist

Medicinal & Process Chemistry
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Dr. Nilanjana Majumdar started her chemistry journey from ***Visva-Bharati University in West Bengal, India***. She completed her undergraduate education there with 1st class 1st in B.Sc. (Chemistry Hons.). In 2003, she went to ***IIT Kharagpur*** to pursue Masters. For Ph.D., she moved to ***United States*** in 2006 and worked under the supervision of ***Professor William D. Wulff in Michigan State University***. After graduation in 2012, she moved to ***Tokyo, Japan*** for first postdoctoral experience in ***Professor Masakatsu Shibasaki***'s group with ***JSPS fellowship***. After three years in Japan, she worked in ***Professor Benjamin List***'s group for one year in ***Max-Planck Institut für Kohlenforschung, Germany***. In April, 2018, she joined CSIR-Central Drug Research Institute (CSIR-CDRI), Lucknow as Senior Scientist in Medicinal & Process Chemistry Division.

Awards/achievements:

2022 Dr. Mridula Kamboj Award for Drugs, Diagnostics, Vaccines and Related Basic Research-2021
2021 CDRI Incentive Award for Technology 2021, Title: Process for the Preparation of Umifenovir (Antiviral)
2019 DST-SERB Early Career Research Award
2013 Japan Society for the Promotion of Science (JSPS) Fellowship
2003 1st class 1st in Bachelor of Science (B.Sc. Chemistry Hons.) (Visva-Bharati University)

Representative publications:

Adhikari, A.; Pandit, S.; Kant, R.; Majumdar, N. *ACS Catal.* **2023**, *13*, 6261−6267.
Majumdar, N. *ACS Catal.* **2022**, *12*, 8291−8324.
[3] Adhikari, A. S.; Majumdar, N. *Org. Lett.* **2023**, *25*, 8611–8616.
[4] Adhikari, A. S.; Majumdar, N. *Eur. J. Org. Chem.* **2024**, e202301225.
[5] Pandit, S.; Adhikari, A. S.; Majumdar, N. *Org. Lett.* **2022**, *24*, 7388−7393.
[6] Pandit, S.; Pandey, V. K.; Adhikari, A. S.; Kumar, S.; Maurya, A. K.; Kant, R.; Majumdar, N. *J. Org. Chem.* **2022**, *88*, 97–105.

Unactivated Carboxylic Acids in Catalytic Asymmetric Ring Opening Reactions

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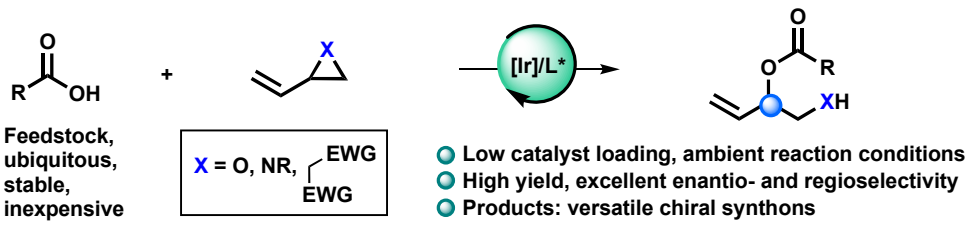
Abstract: Carboxylic acids are considered as feedstock chemicals as they are widely available, highly stable and inexpensive. They can be excellent choice of substrates in catalytic asymmetric reactions but can be quite challenging as well. Free carboxylic acids are generally not compatible for various transformations, e.g. they can be difficult substrates for nucleophilic or electrophilic reactions. Here, efficient and convenient use of free carboxylic acid substrates will be illustrated in catalytic asymmetric ring opening reactions for the preparation of important class of products that may act as useful chiral synthons.



Selected References:

Adhikari, A.; Pandit, S.; Kant, R.; Majumdar, N. *ACS Catal.* **2023**, *13*, 6261−6267.
Majumdar, N. *ACS Catal.* **2022**, *12*, 8291−8324.
[3] Adhikari, A. S.; Majumdar, N. *Org. Lett.* **2023**, *25*, 8611–8616.
[4] Adhikari, A. S.; Majumdar, N. *Eur. J. Org. Chem.* **2024**, e202301225.
[5] Pandit, S.; Adhikari, A. S.; Majumdar, N. *Org. Lett.* **2022**, *24*, 7388−7393.

Bio-Sketch of Speaker

Dr. Sandip Murarka

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Sandip Murarka did his B.Sc. in Chemistry (Hons.) from Midnapore College, Vidyasagar University (2005), and M.Sc. from IIT Bombay (2007). Subsequent to a M.S. from Rutgers University, U.S.A (2009); he moved to Germany to pursue his PhD from WWU Münster under the supervision of Prof. Armido Studer. After completion of his Ph.D. (2013), he worked as a Max-Planck postdoctoral research fellow in the laboratory of Prof. Herbert Waldmann at Max Planck Institute of Molecular Physiology, Dortmund (2013-2016). Following a year long stay (2016-2017) as a Team Leader in a reputed pharmaceutical company, Syngene International Limited, he decided to move back to academia. In May 2017, he joined Indian Institute of Technology Jodhpur, India as an Assistant Professor and got promoted to the post of Associate Professor in June 2022. His current research activities include study of novel activation modes and development of chemoselective and sustainable transformations towards the synthesis of biologically relevant and interesting molecular architectures.

Research Interests:

4. Radical Chemistry
5. Photoinduced Synthetic Transformations
6. Transition Metal Catalyzed Cross-Couplings
7. Metal-free Synthetic Transformations
8. Medicinal Chemistry

Awards and Honours:

1. Early Career Advisory Board Member of RSC Journal ‘Organic Chemistry Frontiers’ (2024).
2. Merck Young Scientist Award (Runner-up) (2023).
3. ‘Thieme Chemistry Journal Award’ by the editorial boards of the journals Synthesis, Synlett, and Synfact (2022).
4. Early Career Advisory Board Member of Wiley-VCH Journal ‘ChemistrySelect’ (2022).
5. Fellow of Indian Chemical Society (2020).
6. Early Career Research Award (ECRA) from Science and Engineering Research Board (SERB) (2018).
7. INSPIRE Faculty Award from the Department of Science & Technology (DST), India (2016).

Bio-Sketch of Speaker

Dr. Lisa Roy
Assistant Professor

Institute of Chemical Technology Mumbai –
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E-mail: L.Roy@iocb.ictmumbai.edu.in
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Dr. Roy is working as an Assistant Professor at Institute of Chemical Technology - IOC Bhubaneswar campus. Her current research interests include: reactivity study of metalloenzyme and model complexes, organo-catalysts, and metal-organic-frameworks/covalent-organic-frameworks to computationally design novel catalytic systems for sustainable energy and resources.

Academic Background:

- B.Sc (Hons.) in Chemistry (2007) from University of Calcutta
- M. Sc. in Chemistry (2009) from University of Calcutta
- Ph.D (Science) in Chemistry (2015) from Indian Association for the Cultivation of Science, Kolkata. (Degree received from University of Calcutta).
- Postdoctoral Researcher (2015 – 2017), Max Planck Institute for Chemical Energy Conversion, Germany with Prof. Frank Neese, and Prof. Shengfa Ye

Awards and Honors:

- Early Career Advisory Board Member of ChemPhysChem since Jan 2023 and ChemPlusChem since Jan 2021 (Chemistry Europe Society, Wiley VcH)
- Received SERB POWER (Promoting Opportunities for Women in Exploratory Research) Grant from SERB, India 2021
- Visiting Researcher at the Max Planck Institute for Coal Research, Germany (July 2019)
- DST INSPIRE Faculty Fellowship (2017) in Chemical Sciences Division
- Offered Postdoctoral Fellowship at The Hebrew University of Jerusalem (2017) (not availed)
- Max-Planck Postdoctoral Fellowship July 2015 – Oct 2017

Computational Mechanistic Insights on Homogeneous Water Oxidation Versus Catalyst Deactivation

Dr. Lisa Roy*
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Increased demand for a carbon-neutral sustainable energy scheme augmented by climatic threats motivates the design and exploration of novel approaches that reserve intermittent solar energy in the form of chemical bonds in molecules and materials. In this context, inspired by biological processes, artificial photosynthesis has garnered significant attention as a promising solution to convert solar power into chemical fuels from abundantly found H_2O. Among the two redox half-reactions in artificial photosynthesis, the four-electron oxidation of water according to $2H_2O \rightarrow O_2 + 4H^+ + 4e^-$ comprises the major bottleneck and is a severe impediment towards sustainable energy production.[1] As such, devising new catalytic platforms, with traditional concepts of molecular, materials and biological catalysis and capable of integrating the functional architectures of the natural oxygen-evolving complex [2] in photosystem II would certainly be a value-addition towards this objective.[3] In this talk, we would discuss about our recent endeavours with density functional theory to explore the reactivity conduits of molecular electro-catalysts with nickel and copper consisting of tetra-anionic tetradentate amide ligands.[4,5] We would try to understand why nickel complexes demonstrate complex borderline chemistry between homogeneous and heterogeneous pathways, showing competition between water oxidation and molecular species degradation, while copper complexes display robust and efficient molecular water oxidation behaviour.[6] Lastly, we discuss design strategies to expedite O-O interaction, leading to predominant homogeneous water oxidation under all conditions.

References: [1] Matheu, R.; Garrido-Barros, P.; Gil-Sepulcre, M.; Ertem, M. Z.; Sala, X.; Gimbert-Suriñach, C.; Llobet, A. *Nat. Rev. Chem.* 2019, 3, 331–341.

[2] Cox, N.; Pantazis, D. A.; Neese, F.; Lubitz, W. *Acc. Chem. Res.* 2013, 46, 1588–1596.

[3] Singh, A. K.; Roy, L. *ACS Omega* 2024 (In Press)

[4] Garrido-Barros, P.; Funes-Ardoiz, I.; Drouet, S.; Benet-Buchholz, J.; Maseras, F.; Llobet, A. *J. Am. Chem. Soc.* 2015, 137, 6758–6761.

[5] Garrido-Barros, P.; Grau, S.; Drouet, S.; Benet-Buchholz, J.; Gimbert-Surinach, C.; Llobet, A. ACS Catal. 2019, 9, 3936–3945.

[6] Singh, A. K.; Roy, L. *Eur. J. Inorg. Chem.* 2023, e202300412.

Curriculum Vitae

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Education

10/2010 - 09/2013 Doctoral Degree, Westfälische Wilhelms-Universität Münster, Germany, **Major:** Organic Chemistry; *Advisor*: Prof. Martin Oestreich

09/2008 - 08/2010 Post-Graduate Degree, Indian Institute of Technology Bombay; **Major:** Chemistry (one-year project under Prof. I. N. N. Namboothiri)

07/2004 - 07/2007 Under-Graduate Degree, Ramakrishna Mission Residential Collage, Narendrapur, University of Calcutta; **Major:** Chemistry

Professional appointments & experiences

7/2023 - Present Associate professor, Department of Chemistry, IIT Delhi, India

3/2019 – 7/2023 Assistant professor, Department of Chemistry, IIT Delhi, India

8/2018 - 3/2019 Post-doc, KAUST, Saudi Arabia (*Advisor*: Prof. Prof. Magnus Rueping)

12/2014 - 7/2018 Post-doc, KAIST, South Korea (*Advisor*: Prof. Sukbok Chang)

10/2013 - 9/2014 Post-doc, University of Strasbourg, (*Advisor*: Prof. Françoise Colobert

Awards

11/2023 Awarded the *Merck Young Scientist Award 2023 (Runner-up)*.

06/2023 Dr. Hazra's *Introducing Angewandte Author Profile* was published by the Angewandte Chemie International Edition Journal.

01/2023 Selected as one of Thieme Chemistry Journal's *Awardees* for 2023.

Publications After Joining IIT Delhi

6) Tyagi, A.; Hazra, C. K.* Direct Access to Hydrazides and Amides from Carboxylic Acids via Acyloxyphosphonium ion. *Org. Chem. Front.* **2024**, DOI: 10.1039/D3QO02062B.

5) Singh, S.; Kumar, A.; Nebhani, L.;* Hazra, C. K.* Sustainable Sulfonic Acid Functionalized Tubular Shape Mesoporous Silica as a Heterogeneous Catalyst for Selective Unsymmetrical Friedel–Crafts Alkylation in One Pot. *JACS Au*. **2023**, DOI: 10.1021/jacsau.3c00563.

4) Taneja, N.; Sharma, P.; Yadav, N.; Musib, D.; Hazra, C. K.* Non-directed, site-Selective Arylation of Quinone Imine Ketals Derived from Arylamines: One-pot Access to meta-Substituted Anilines. *Org. Lett.* **2023**, doi: 10.1021/acs.orglett.3c02181.

3) Yadav, N.; Taneja, N.; Musib, D.; Hazra, C. K.* Practical Access to *meta*-Substituted Anilines by Amination of Quinone Imine Ketals Derived from Anisidines: Efficient Synthesis of *Anti*-Psychotic Drugs. *Angew. Chem. Int. Ed.* **2023**, *e*202301166, doi: 10.1002/anie.202301166.

2) Tyagi, A.; Taneja, N.; Khan, J.; Hazra, C. K.* I_2-Mediated C–S and C–I Bond Formation: A Highly Sustainable Route for the Synthesis of *β*-Ketosulfones and Branched Sulfones. *Adv. Synth. Catal.* **2023**, doi: 10.1002/adsc.202300057.

1) Mahato, R.; Hazra, C. K.* Pentafluorophenol (C_6F_5OH) Catalyzed Pictet-Spengler Reaction: A facile and Metal-free Approach Towards (Spirocyclic)Tetrahydro-*β*-carbolines. *Chem. -Eur. J.* **2023**, e202203924. doi: 10.1002/chem.202203924.

Supervision of Master/M.Tech/PhD/post-doc students: Currently, two MSc, two Mtech, two interns, and eleven PhD students are working under my supervision

Organocatalytic Transformation of Feedstock Molecules to Value-Added Products and its Mechanistic Investigation

Dr. Chinmoy Kumar Hazra*

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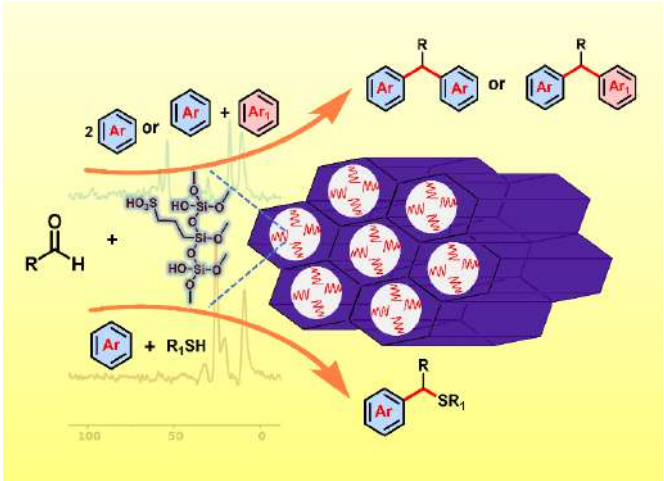
Rapid progress in the research of metal-free transformations has been observed in the past decades; however, there's still plenty of room to be solved. In this talk, some of my past and current research experience in this field will be shared with you, especially for young graduate students. First part: This talk starts with the Brønsted acid-catalyzed Friedel-Crafts reaction to convert cheap chemicals into value-added products. Unsymmetrical di-and triarylmethanes are generally synthesized through metal-catalyzed cross-coupling or Friedel–Crafts arylation using multistep harsh reaction conditions with pre-functionalized starting materials. These reaction protocols use pyrophoric materials such as Grignard reagents and metal hydrides, as well as toxic, hazardous, and problematic solvents like benzene, DMF, and THF. As an alternative, we will use a cheap, commercially available Brønsted acid-catalytic system, I will describe a one-pot three-component approach for the synthesis of unsymmetrical polyarylated alkanes from renewable feedstock chemicals. The developed method could also be scaled up and applied for a short and efficient synthesis of a phenanthrene-based anti-breast cancer agent, which reduced the conventional six-step cross-coupling approach to the one-step Friedel–Crafts approach. Also, the method will apply to the late-stage functionalization of natural products such as thymol, menthol, eugenol, etc. Second part: Reversing the conventional site-selectivity of C−H activation provides efficient retrosynthetic disconnections to otherwise unreactive bonds. In this part, I will focus on the Brønsted acid-catalyzed reaction that selectively performs meta-amination/arylation of anisidines with amines/arenes in a one-pot procedure. I will also focus on the scalability and functional group tolerance, including late-stage functionalization of pharmaceutical compounds and natural products. The control experiments and detailed computational analysis will be discussed for a better understanding of the mechanism and the origin of metal selectivity. Also, the synthesis of challenging drugs will be highlighted. Some ongoing projects will be discussed if time permits. The large-scale synthesis of pharmaceutically active ingredients through metal-free protocol will be discussed briefly.



References: [a] A. Tyagi, C. K. Hazra*, *Org. Chem. Front*. **2024**, DOI: 10.1039/D3QO02062B.; [b] S. Singh, A. Kumar, L. Nebhani*, C. K. Hazra*, *JACS Au*. **2023**, DOI: 10.1021/jacsau.3c00563; [c] N. Taneja, P. Sharma, N. Yadav, D. Musib, C. K. Hazra*, *Org. Lett.* **2023**, doi: 10.1021/acs.orglett.3c02181; [d] N. Yadav, N. Taneja, D. Musib, C. K. Hazra* *Angew. Chem. Int. Ed.* **2023**, *e*202301166, doi: 10.1002/anie.202301166.

Bio-Sketch of Speaker

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Associate Professor
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Cell Number: +91-7761897841
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Group Homepage: https://www.aklab-iitp.com/

Career profile:

- Associate Professor, IIT Patna **5th Dec. 2019**
- Assistant Professor, IIT Patna: **2014-4th Dec. 2019**
- Research Investigator-Biocon-Bristol Myers Research Center, Bangalore: **2012- 2013**
- Postdoctoral Fellow-University of Konstanz, Germany: **2010-2012**
- Postdoctoral Fellow -City University of New York, USA: **2008-2009**
- Ph. D. IIT Kanpur, India: **2008**
- M. Sc. Delhi University: **2002**

Honours and awards:

- Editorial Board Member: **Journal of Carbohydrate Chemistry from 2024**
- CRSI-Bronze Medal Award **2023**
- Council Member, CRSI-**2023-2026**
- Executive Member ACCTI- **2023-2026**
- Life-member- CRSI, India
- Life-member-ISCB, India
- Life-member, ACCT, India

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

Representative Publications:

1. *Chem.Commun.* **2022**, *58,11304*
2. *J. Org. Chem.* **2021**, *86, 9744*
3. *Org. Letter*, **2020**, *22, 5, 1908*
4. *Org. Letter*, **2020**, *22,4,1605*
5. *J. Org. Chem.* 2019, *84, 589*
6. *Org.Lett.* **2018**, *20, 4964*
7. *Org.Lett.* **2018**,*20,4964*
8. *Chem.Commun.* **2018**, *57, 7207*
9. *J. Org. Chem.* 2018, *83, 12247*
10. *J. Org. Chem.* 2016, *81, 6617*

Chemistry of Imidates for Functionalization Reactions

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Abstract:

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

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

References:

1. Lyons, T.W.; Sanford, M. S. *Chem. Rev*. **2010**, *110*, 1147.

2. (a) Y. Kumar, Y. Jaiswal and A. Kumar *Org.Lett*. **2018**,*20*,4964. (b) **Kumar, Y.,** Jaiswal, Y., Kumar, A. *J. Org. Chem.* **2016**, *81*, 12247. **(c) Kumar, Y.,** Shaw, M., Thakur, R., Kumar A. *J. Org. Chem.* **2016**, *81*, 6617.

Bio-Sketch of Speaker

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IISER Kolkata
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e-Mail: suresh@iiserkol.ac.in
Homepage: http://www.iiserkol.ac.in/~suresh/

Career Profile:

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

Significant Awards/Achievements:

Early Carrier Research Award (2017) from SERB, Government of India.
Ramanujan Fellowship (2016) from SERB/DST, Government of India.
JSPS Fellowship (2013) for Foreign Researchers (Pathway to University Positions in Japan).
JSPS Fellowship (2011) at Institute of Microbial Chemistry, Tokyo, Japan.
AvH Fellowship (2008) at Max-Planck Institute for Khölenforschung, Germany.

Representative Publications:

1. Organophotoredox Catalysis: Switchable Radical Generation from Alkyl Sodium Sulfinates for Sulfonylation and Alkylative Activation of C–C Bonds of Cyclopropenes. Chandu, P.; Biswas, B.; Pal, K.; **Sureshkumar**, **D***. *J. Org. Chem.* **2024**, *Accepted*.
2. Organophotocatalyzed Mono- and *bis*-Alkyl/Difluoroalkylative Thio/Selenocyanation of Alkenes. Pal, K.; Chandu, P.; Das, D.; Jinilkumar, A. V.; Mallick, M.; **Sureshkumar**, **D***. *J. Org. Chem.* **2023**, *88*, 17527-17537.
3. Organophotocatalyzed Alkyl/Arylsulfonylation of Vinylcyclopropanes. Chandu, P.; Mallick, M.; Srinivasu, V.; **Sureshkumar**, **D***. *Chem. Eur. J.* **2023**, e20233187.
4. Diastereoselective Hydroacylation of Cyclopropenes by Visible-Light Photocatalysis. Biswas, B.; Chandu, P.; Garai, S.; **Sureshkumar**, **D***. *Org. Lett.* **2023**, *25*, 7863-7867.
5. Diastereoselective Organophotocatalytic Hydrosulfonylation of Cyclopropenes. Chandu, P.; Biswas, B.; Garai, S.; **Sureshkumar**, *. *Green Chem.* **2023**, *25*, 9086-9091.
6. Palladium-catalyzed Direct C(sp^2)–H Cyanomethylation of Arylamides using Chloroacetonitrile. Garai, G.;
7. **Sureshkumar**, **D***. *J. Org. Chem.* **2023**, *88*, 12755-12764.
8. Visible-Metal-Free Photoredox Four-Component Strategy to 1,3-Functionalized BCP Derivatives. Srinivasu, V.; Das, D.; Chandu, P.; Ghosh, K. G.; **Sureshkumar**, **D***. *Org. Lett.* **2023**, *25*, 5308-5313.
9. Photoinduced Cascade Difluoroalkylative Ring-Opening of Vinyl Cyclopropanes. Chandu, P.; Das, D.; Ghosh, K. G.; **Sureshkumar**, **D***. *Org. Lett.* **2023**, *25*, 2857-2862.
10. Diastereoselective Palladium-Catalyzed C(sp^3)–H Cyanomethylation of Amino Acid and Carboxylic Acid Derivatives. Garai, S.; Ghosh, K. G.; Biswas, A.; Chowdhury, S.; Sureshkumar, D. *Chem. Commun*. **2022**, *58*, 7793-7796.
11. Visible-Light Photoredox Catalyzed Decarboxylative Alkylation of Vinylcyclopropanes Chandu, P.; Das, D.; Ghosh, K. G.; **Sureshkumar**, **D***. *Adv. Synth. Catal.* **2022**, *364*, 2340-2345. Accepted as a "***VIP* Article**"

Multicomponent Organophotocatalyzed 1,5-Difunctionalization of Cyclooctadienes

Debabrata Das, Shishira Babu, Krishna Gopal Ghosh, Devarajulu Sureshkumar*
Department of Chemical Sciences, Indian Institute of Science Education and Research Kolkata, Mohanpur-741246.
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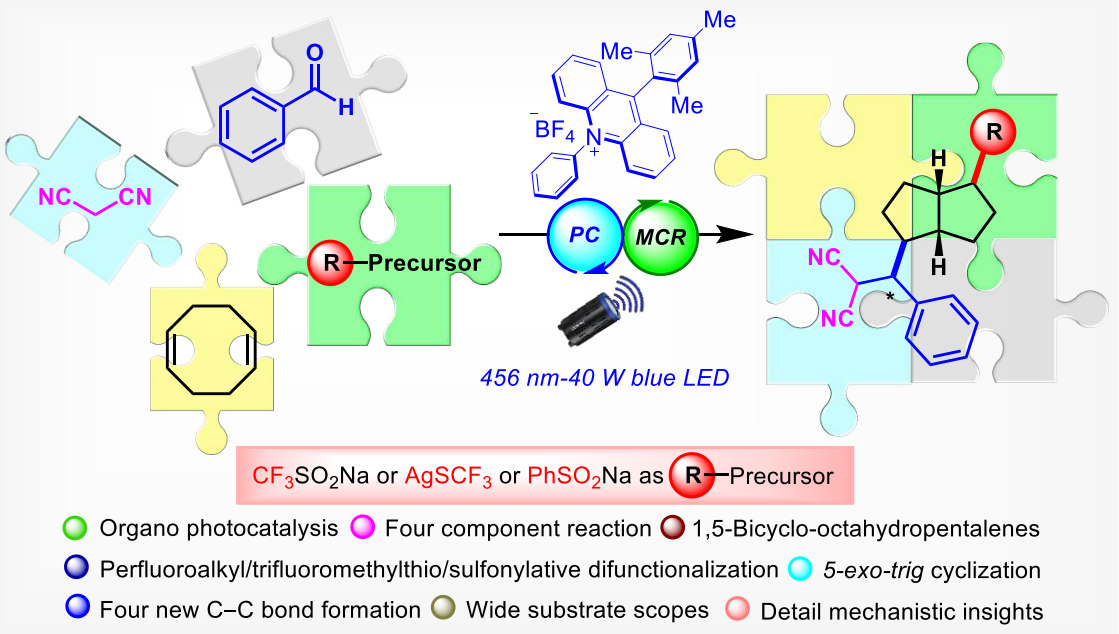
Utilizing visible light photocatalysis, a new and efficient method has been developed for the 1,5-difunctionalization of readily available 1,5-cyclooctadiene (COD), leading to the efficient synthesis of disubstituted bicyclo-octahydropentalenes. This transformation involves the formation of four new C(sp^3)-C(sp^3) bonds in a single step. Initially, photogenerated electrophilic radicals add onto COD, facilitating an intramolecular 5-exo-trig cyclization. Subsequently, a domino Giese addition occurs with *in situ* generated electron-deficient alkenes in a multicomponent manner. This innovative organo-photocatalyzed protocol offers facile access to perfluoroalkyl, trifluoromethylthio, and sulphonylated derivatives of bicyclo-octahydropentalenes, incorporating the versatile cyano-functional group moiety for further diversification. Noteworthy advantages include its scalability for gram-scale synthesis, applicability in late-stage functionalization of drug motifs, and insights gleaned from mechanistic studies.



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[a] Shishira, B. C.; Das, D.; Ghosh, K. G.; Sureshkumar, D* (*Manuscript under preparation*).

[b] Ponomarenko, M. V.; Serguchev, Y. A.; Röschenthaler, G.-V. *Journal of Fluorine Chemistry* **2010**, *131*, 270–273.

[c] Miura, W.; Hirano, K.; Miura, M. *J. Org. Chem*. **2017**, *82*, 5337–5344.

[d] Li, S.; Zhang, P.; Li, Y.; Lu, S.; Gong, J.; Yang, Z. *Org. Lett*. **2017**, *19*, 4416–4419.

[e] Wang, X.; Li, J.; Yuan, T.; You, B.; Xie, G.; Lv, X. *J. Org. Chem*. **2018**, *83*, 8984–8994.

Bio-Sketch of Speaker

Dr. Shivnath Mazumder

Associate Professor
Department of Chemistry
Indian Institute of Technology Jammu, India
Email: shivnath.mazumder@iitjammu.ac.in

Areas of Interest: Bio-Inspired Multi Electronic Catalysis
Artificial Photosynthesis
Metal-Catalyzed Coupling Reactions for Drug Discovery
Molecular Electronics
Machine Learning in Homogeneous Catalysis

Academic Positions: Associate Professor, Dept. of Chemistry, IIT Jammu (2023 – present)
Assistant Professor, Dept. of Chemistry, IIT Jammu (2018 – 2023)
Assistant Professor, Dept. of Chemistry, Hofstra Univ., USA (2016 - 2018)
Postdoctoral Scientist, Dept. of Chemistry, Wayne State Univ., USA (2013 – 2016)

Academic Qualification: PhD, Indiana University, Bloomington, USA, 2013

Memberships: Member of Royal Society of Chemistry (RSC), 2023 – Present
Member of American Chemical Society (ACS), 2017 – Present

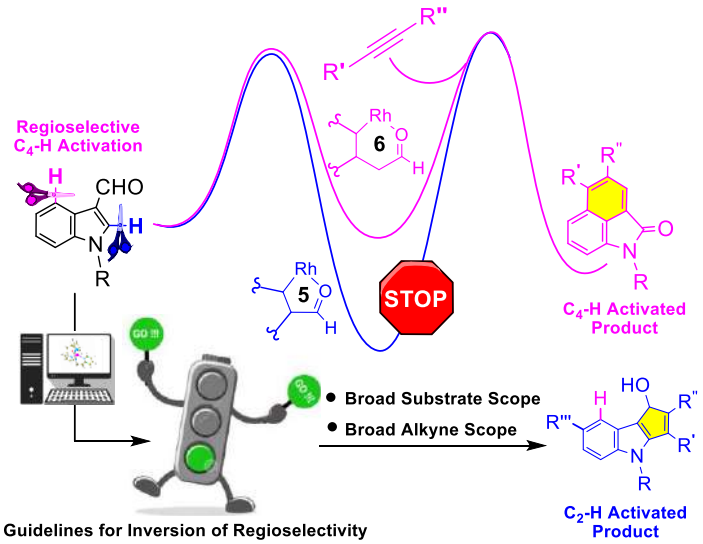
Websites: **https://iitjammu.ac.in/chemistry/faculty-list/~shivnathmazumder**
https://shivnathmazumder.wixsite.com/computationalchem

Unexpected Activation of an Inert C4–H Bond in Indolyl Aldehyde over a More Reactive C2–H Bond: Principles of Inverting the Regioselectivity Revealed by DFT Study

Dr. Shivnath Mazumder*

Department of Chemistry, Indian Institute of Technology Jammu, Jammu-181221
(E-mail: shivnath.mazumder@iitjammu.ac.in;
Web: https://shivnathmazumder.wixsite.com/computationalchem)

Rh(III)-catalyzed regioselective C–H activation/alkyne insertion/cyclization of indolyl aldehyde and acetophenone with alkynes was investigated using density functional theoretical models. Previously, it was observed that acetophenone demonstrates activation of the more reactive C2–H bond, but indolyl aldehyde showed an unexpected reactivity of the inert C4–H bond under comparable conditions. To understand this substrate-dependent outcome and to provide a set of much-awaited guiding principles to invert the regioselectivity as desired, the reaction mechanisms for C2–H and C4–H pathways were elucidated in detail and compared. We discover the key structural features that control formation of a thermodynamic sink intermediate, and we further report an *in-silico* design of optimal systems to successfully resolve the problems arising from that thermodynamic trap. A set of general guidelines have been proposed that can be adopted in an experimental laboratory to switch the selectivity towards exclusive formation of the C2–H activated product, cyclopenta[*b*]indol-1-ol, without extensive experimentation, thus saving manpower, energy, and chemical waste. To date, there has been no report of formation of this product from indolyl aldehyde.



Reference: N. Rani, S. Mazumder*, *Organometallics* **2022**, *41*, 1659.

Bio-Sketch of Speaker

Dr. Debabrata Maiti
Professor
Department of Chemistry
IIT Bombay
Powai, Mumbai - 400076
e-mail: dmaiti@iitb.ac.in
M.: 9820907155

Introduction: Dr. Maiti is working as a Professor in the Department of Chemistry, IIT Bombay, India. His research interests are focused on the development of new and sustainable synthetic and catalytic methodologies. Currently he is an Editor-in-Chief, *Synlett*

Academic Background:

B.Sc.: B.Sc. in Chemistry (Hons), University of Calcutta, India **(**1998-2001**)**
M.Sc.: IIT Bombay, India **(**2001-2003**) (**Silver Medalist**)**
Ph.D.: Department of Chemistry, Johns Hopkins University, USA (2003-2008)

Awards / Honors / Membership:

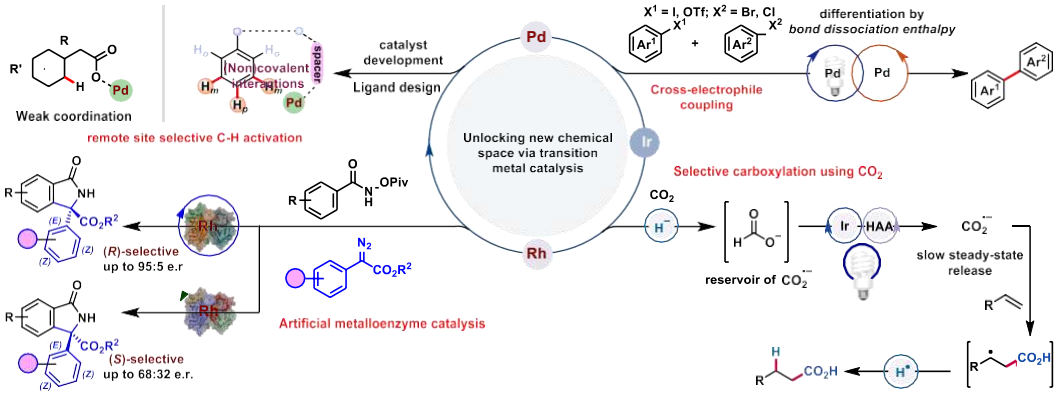
2022	**Shanti Swarup Bhatnagar Prize (SSB) for Science and Technology 2022**
2022	FASc, Fellow of Academy of Sciences
2022	IIT Bombay-Prof. SC Bhattacharya Award for Excellence in Pure Science
2022	Adjunct Professor, University Centre for Research and Development (UCRD), Chandigarh University, Chandigarh, India
2022	CRSI Bronze Medal
2022	Adjunct Professor, Vellore Institute of Technology (VIT), India
2022	IIT Bombay-IRCC Impactful Research Award
2022	IIT Bombay-IRCC Research Dissemination Award
2021	Sun Pharma Science Foundation Research Award
2021	Professor P K Bose Memorial Award
2021	The (Late) Shri G.D. Gokhale Lectureship Endowment
2021	Distinguished Adjunct Faculty, King Abdulaziz University
2020	Humboldt Research Fellowship for Experienced Researchers
2019	FRSC, Fellow of the Royal Society of Chemistry
2019	NASI Scopus Young Scientist Award-Innovation Engineering & Physical Sciences
2020	Visiting Faculty, WRHI, Tokyo Institute of Technology, Japan
2020	Visiting Faculty, CAPES, Federal University of Minas Gerais, Brazil
2017	Visiting Faculty, University of Pavia, Italy
2017	OPPI - Young Scientist Award
2015	Alkyl Amines - Young Scientist Award
2014	INSA - Young Scientist Award
2014	ISCB - Young Scientist Award
2014	AVRA - Young Scientist Award
2014	CRSI Young Scientist Award
2013	Thieme Chemistry Journal Award
2013	IIT Bombay-IRCC Young Scientist Award
2013	IAS-Young Associate
2013	NASI- Young Scientist Platinum Jubilee Award

Website: https://www.dmaiti.com

Unlocking new chemical space via selective catalysis

Debabrata Maiti
IIT Bombay, www.dmaiti.com, Email : dmaiti@iitb.ac.in

The limitations of cross-coupling such as the availability of prefunctionalized coupling partners, instability, and synthesis expense remain, posing significant barriers to unlocking new chemical space for molecular complexity. To solve these underlying problems of cross-coupling we are mainly focused on the development of techniques for direct C–H functionalization and cross- electrophile coupling. Selectively targeting a remote C–H bond in a molecule remains more challenging due to the inaccessibility of these sites in formation of energetically favorable organometallic pre-transition states. We believe that the direct release of the reactive metal catalyst in close proximity to the targeted remote C–H bond could solve this problem. We devised covalently attached template-directed methods that require precise spatial positioning of the directing group in order to selectively activate remote C–H bonds. We recently demonstrated that various non-covalent interactions are also successful in recognizing the perfect orientation of catalyst and the substrate to achieve selective C–H bond activation. In this vein, we have developed a method for the activation of methylene C–H bond in presence of methyl C–H bondsto form unsaturated bicyclic lactones utilizing the weak coordinating nature carboxylic acid towards palladium. Cross-electrophile coupling (XEC) approach would be a powerful tool for theconstruction of (hetero)biaryl moiety because of the widespread availability and stability of (hetero)aryl electrophiles. We have demonstrated a ligand controlled visible light driven monometallic cross-electrophile coupling platform for the synthesis of unsymmetrical (hetero)biaryls directly from (hetero)aryl halides and pseudohalides. In addition, our lab is pursuing the development of a paradigm in which small molecules such CO_2, SO_2 *etc.* can be converted into a wide range of chemicals and materials using renewable visible light photocatalysis.



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1. Dutta, U.; Maiti, S.; Bhattacharya, T.; Maiti, D. *Science*, **2021**, *372*, 701.
2. Goswami, N.; Sinha, S. K.; Mondal, P.; Adhya, S.; Datta, A.; Maiti, D. *Chem*, **2023**, *9*, 989.
3. Saha, A.; Guin, S.; Ali, W.; Bhattacharya, T.; Sasmal, S.; Goswami, N.; Prakash, G.; Sinha, S. K.; Chandrashekar, H. B.; Panda, S.; Anjana, S. S.; Maiti, D. *J. Am. Chem. Soc*. **2022**, *144*, 1929.
4. Das, J.; Ali, W.; Ghosh, A.; Pal, T.; Mandal, A.; Teja, C.; Dutta, S.; Pothikumar, R.; Ge, H.; Zhang, X.; Maiti, D. *Nat. Chem*. **2023**, *15*, 1626.
5. Maiti, S.; Ghosh, P.; Raja, D. K.; Ghosh, S.; Chatterjee, S.; Sankar, V.; Roy, S.; Lahiri, G. K.; Maiti, D. *Nat. Catal.* **2024**
6. Mukherjee, P.; Sairaman, A.; Deka, H. J.; Jain, S.; Mishra, S. K.; Roy, S.; Bhaumik, P.; Maiti, D. *Nat. Synth.* **2024**

Presenter Details: Prof. Debabrata Maiti received his PhD from Johns Hopkins University in 2008 underthe supervision of Prof. Kenneth D. Karlin. After postdoctoral studies at MIT with Prof. Stephen L. Buchwald, he joined the Department of Chemistry at IIT Bombay in 2011. His research interests are focusedon the development of new and sustainable synthetic and catalytic methodologies. Currently he is *Editor- in-Chief, Synlett*

Bio-Sketch of Speaker

Seung Hwan Cho
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Associate Professor
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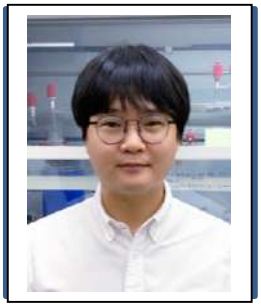
Phone: +82-54-279-2340 (Office), +82-54-279-8041 (Lab)
Fax: +82-54-279-8042



EDUCATION

Ph. D. in Organic Chemistry, KAIST (Prof. Sukbok Chang)	2006 – 2011
B. S. in Chemistry, KAIST	2001– 2005

PROFESSIONAL EXPERIENCE

Department of Chemistry, POSTECH *Assistnat & Associate Professor*	2014.07 – present
Department of Chemistry, University of California, Berkeley *Postdoctoral Fellow* (Prof. John F. Hartwig)	2012 – 2014
Department of Chemistry, KAIST *Postdoctoral Fellow* (Prof. Sukbok Chang)	2011 – 2012

EDITORIAL ADVISORY BOARD MEMBER OF JOURNALS

Green Synthesis and Catalysis (Editorial Board Member)	2022-present
ACS Catalysis (Early Career Advisory Board)	2019-2021

AWARDS AND HONORS

“Toray Research Grant for Young Investigator” (Korea Toray Science Foundation)	2022
“Hanseong Science Award” (Hanseong Sonjaehan Foundation)	2022
"Young Organic Chemist Award” (Korean Chemical Society)	2021
“KCS-Wiley Young Chemist Award” (Korean Chemical Society)	2020
“Young Korean Academy of Science and Technology	2018
“Thieme Journal Award” (Synlett/Synthesis/Synfact Award for Young Investigator)	2017
“TJ Park Cheongam Fellowship for Young Investigator” (Cheongam (POSCO) Foundation)	2017

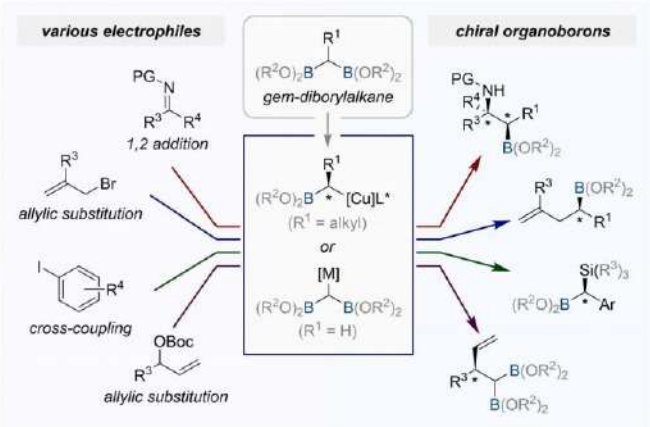
Design, Synthesis, and Application of New Organoboron Reagents

*Prof. Seung Hwan Cho**

Department of Chemistry, Pohang University of Science and Technology (POSTECH), Pohang-37673

(E-mail: seunghwan@postech.ac.kr; Web: www.chogroup.postech.ac.kr)

Chemo- and stereoselective transformations of polyborylalkanes are powerful and efficient methods to access optically active molecules with greater complexity and diversity through programmed synthetic design. In particular, gem-diboryl compounds have attracted much attention in organic chemistry as versatile synthetic handles [a] The notable advantage of gem-diboryl compounds lies in their ability to generate two key intermediates, □-borylalkyl anions and (gem-diborylalkyl)anions. These two different intermediates can be applied to various reactions to rapidly access a diverse set of organoboron compounds, which can be further manipulated to generate various synthetically valuable molecules. In this talk, I will summarize our recent contributions to the design and synthesis of halogen-substituted-gem-diboryl compounds and their application to the development of highly chemo- and stereoselective transformations.[b-e]



Scheme 1. *Chemo- and Stereoselective Transformations of 1,1-Diborylalkyl Reagents*

References: *[a] Y. Lee, S. Han, S. H. Cho, Acc. Chem. Res.* ***2021,*** *54, 3917-3929. [b] M. Kim, B. Park, M. Shin, S. Kim, J. Kim, M.-H Baik, S. H. Cho, J. Am. Chem. Soc.* ***2021****, 143, 1069. [c] C. Hwang, Y. Lee, M. Kim, Y. Seo, S. H. Cho, Angew. Chem. Int. Ed.* ***2022,*** *61, e202209079.[d] S. Han, Y. Lee, Y, Jung, S. H. Cho, Angew. Chem. Int. Ed.* ***2022,*** *61, e202210532. [e] Y. Jung, S. Y. Yoo, Y. Jin, J. Yu, S. Han, J. Yu, Y. Park, S. H. Cho,. Angew. Chem. Int. Ed.* ***2023****, 62, e202218794.*

David A Nagib

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APPOINTMENTS

The Ohio State University
College of Arts and Sciences Distinguished Professor 2022 – Present
Harold and Betty Miller Professor of Organic Chemistry 2022 – Present
Associate Professor with Tenure 2020 – 2022
Assistant Professor 2014 – 2020

University of California, Berkeley 2011 – 2014
NIH Postdoctoral Fellow with F. Dean Toste

EDUCATION

Princeton University 2006 – 2011
Ph.D. with David W. C. MacMillan
Thesis: New Trifluoromethylation Reactions via Photoredox Catalysis

Boston College 2002 – 2006
B.S. *with Honors* (& *Scholar of the College*) with Scott J. Miller
Thesis: Peptide-Catalyzed Desymmetrization of Meso-Alcohols

AWARDS AND HONORS

- **Named/Award Lectures**: Rosenfeld (**Smith**), Closs (**Chicago**), GSK (**Yale**), Sigma-Aldrich (**Columbia**), Pfizer (**Duke**), Student-Hosted (**MIT**), Woodward (**Harvard**), Organic Reactions (**Florida**), Fagnou (**Ottawa**)
- **Brown Investigator Award**, Brown Science Foundation, 2023
- **Pfizer Global Chemistry Forum**, Keynote Speaker, 2022
- **National Academy of Sciences**, Kavli Frontiers of Science Symposium, 2022
- **Arthur C. Cope Scholar** Award, American Chemical Society, 2021
- **Merck Outstanding Chemists of Color** Award, 2021
- **Lilly Young Investigator** Award, 2020
- ***JOC* Outstanding Article of the Year** Award, 2020
- **Sloan Research Fellowship**, Alfred P. Sloan Jr. Foundation, 2019

KEY PUBLICATIONS

DeMuynck, B. M.; Zhang, L.; Ralpha, E. K.; Nagib, D. A. Cyclopropanation of Unactivated Alkenes With Non-Stabilized Iron Carbenes. ***Chem***, 2024, *377*, DOI: doi.org/10.1016/j.chempr.2024.01.006

Zhang, L.; Nagib, D. A. Carbonyl Cross-Metathesis via Deoxygenative *gem*-di-Metal Catalysis. ***Nat. Chem.***, 2024, *16*, 107 – 113.

Zhang, L.; †DeMuynck, B. M.; †Paneque, A. N.; †Rutherford, J. E.; Nagib, D. A. Carbene Reactivity from Alkyl and Aryl Aldehydes. ***Science***, 2022, *377*, 649 – 654.

†Herbort, J. H.; †Bednar, T. N.; Chen, A. D.; RajanBabu, T.V.; Nagib, D. A. γ C-H Functionalization of Amines via Triple H-Atom Transfer of a Vinyl Sulfonyl Radical Chaperone. ***J. Am. Chem. Soc.***, 2022, *144*, 13366 – 13373.

†Stateman, L. M.; †Dare, R. M.; Paneque, A. N.; Nagib, D. A. Aza-Heterocycles via Copper-Catalyzed, Remote C-H Desaturation of Amines. ***Chem***, 2022, *8*, 210 – 224.

†Nakafuku, K. M.; †Zhang, Z.; †Wappes, E. A.; Stateman, L. M.; Chen, A. D.; Nagib, D. A. Enantioselective Radical C-H Amination for the Synthesis of β-Amino Alcohols. ***Nat. Chem.***, 2020, *12*, 697 – 704.

Wang, L.; Lear, J. M.; Rafferty, S.; Fosu, S.C.; Nagib, D. A. Ketyl Radical Reactivity via Atom Transfer Catalysis. ***Science***, 2018, *362*, 225 − 229.

†Wappes, E.A.; †Nakafuku, K. M.; Nagib, D. A. Directed β C-H Amination of Alcohols via Radical Chaperones. ***J. Am. Chem. Soc.***, 2017, *139*, 10204 – 10207.

Harnessing Radicals and Carbenes To Enable Unconventional Reactivity

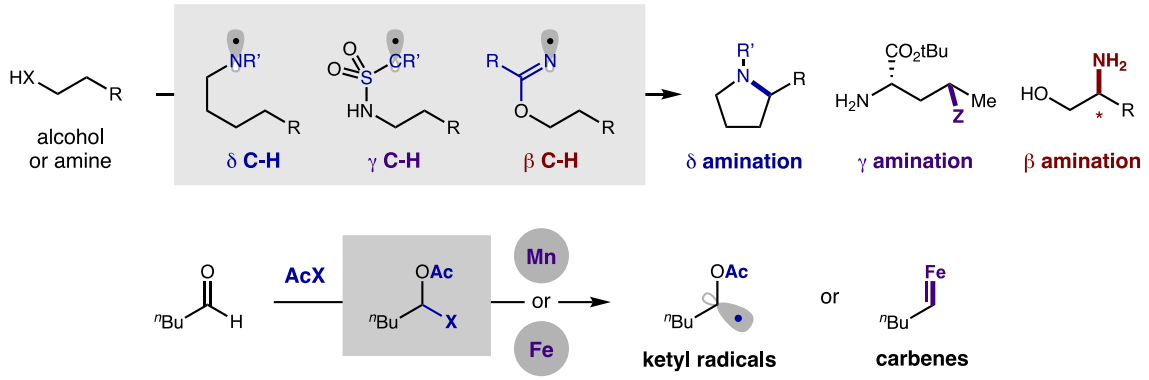
*Dr. David Nagib**

Department of Chemistry and Biochemistry, The Ohio State University, USA

(E-mail: nagib.1@osu.edu; Web: research.cbc.osu.edu/nagib.1)

Abstract:

Radical and carbene chemistry can afford opposite or orthogonal reactivity to classic two-electron pathways. By developing radical chaperone strategies that merge open (1e-) and closed shell (2e-) processes, we have harnessed this complementary reactivity and imparted new types of chemo-, regio-, and stereo- selectivity for remote, double, or reversed C-H and C-O functionalizations of alcohols, amines, and carbonyls. These carbene and radical chaperone strategies are continually being developed to streamline the synthesis of complex, medicinally relevant molecules and heterocycles. This seminar will highlight our newest, most exciting chemistry and the mosaic of champions behind these discoveries.



Key References:

Chem, *2024, 377, DOI: doi.org/10.1016/j.chempr.2024.01.006;*
Nat. Chem., *2024, 16, 107 – 113;*
Science, *2022, 377, 649 – 654;*
J. Am. Chem. Soc., *2022, 144, 13366 – 13373;*
Chem, *2022, 8, 210 – 224;*
Nat. Chem., *2020, 12, 697 – 704;*
Science, *2018, 362, 225 – 229;*
J. Am. Chem. Soc., *2017, 139, 10204 – 10207.*

Bio-Sketch of Speaker

Prof. Dr. Shoubhik Das
Department of chemistry
University of Bayreuth
Bayreuth, Germany
E-mail: shoubhik.das@uni-bayreut.de
Internet: www.shoubhikdas.uni-bayreuth.de/en

Education & Experience:

Aug, 2023 -	***Chair professor (W3), Organic chemistry***
	University of Bayreuth, Bayreuth, Germany.
Nov, 2019 -	***Assistant professor***
July, 2023	Department of Chemistry, University of Antwerp, Belgium.
Aug, 2015 -	***Independent research group leader (Liebig Fellow)***
Oct, 2019	Georg-August-Universität Göttingen, Germany.
Jan, 2013 -	***Scientist* with Prof. Dr. Paul J. Dyson**
July, 2015	EPFL, Lausanne, Switzerland
Jan, 2012 -	***Post-doctoral research* with Prof. Dr. Matthew J. Gaunt**
Dec, 2012	University of Cambridge, Cambridge, UK
9th Jan, 2012	***Ph.D. degree*** obtained in the thesis entitled *''Novel catalytic methods for hydrosilylation of carboxylic acid derivatives and related reactions''.*
Nov, 2008 -	***Ph.D.* with Prof. Dr. Matthias Beller**
Dec, 2011	Leibniz Institut für Katalyse e. V., Rostock, Germany
Nov, 2006 -	***Research chemist at GlaxoSmithKline***
Oct, 2008	Early stage drug discovery, Stevenage, UK.
July, 2006 -	***Research Chemist at Ranbaxy Pharmaceuticals***
Oct, 2006	Chemical Research Department, India.
June, 2004 -	***Master of Science (Chemistry)***
May, 2006	IIT Kharagpur, Kharagpur, India.
June, 2001-	***Bachelor of Science (Chemistry)***
May, 2004	Presidency College, Kolkata, India

Selective Awards & Fellowships:

- Member of the Editorial Board, Green Synthesis and Catalysis & Industrial Chemistry and Materials (since 2022)
- Member of the Advisory Board, Tetrahedron Green Chem. & Helvetica Chimica Acta (since 2022).
- Odysseus award, 2021 (1 M Euro).
- Francqui Lecturer award, 2020
- European young chemist award (finalist, independent researcher category), 2020.
- Invited panel member of the Swedish research council, 2020
- Belgian representative of the EuChemS, 2020
- Invited member of the 'CO_2 Capture', 2020
- JSP Fellowship, 2020.
- Your JOC Talent award, 2019.
- Liebig fellowship from Fonds der Chemischen Industrie, 2015.
- Finalist in the European Young Chemist Award, 2014.
- University of Cambridge post-doctoral fellowship, UK, 2012.
- Leibniz post-doctoral fellowship, 2011.
- One of the most talented Young chemists in 3rd EuCheMS conference, 2010.
- Annex Fellowship for PhD from Leibniz Society, Germany (2008-2011).

Photocatalysis for Sustainability: Bon Voyage from Homogeneous to Heterogeneous and Beyond

Prof. Dr. Shoubhik Das
University of Bayreuth, Bayreuth, Germany

Recently solar energy has exhibited great potential as a promising alternative to substituting the traditional energy sources because it is renewable, abundant, affordable, and everlasting. Among various solar energy conversion techniques, photocatalysis is deemed as a promising, environmentally benign, and cost-effective strategy to generate both fuels and high-value chemicals. While in this domain homogeneous photocatalysts prevail due to higher selectivity but the reutilisation of the catalyst is next to impossible. On the other hand, heterogeneous photocatalysts are recyclable but not highly selective. Therefore, to make a bridge between these two, a new strategy has been developed by synthesizing single metal atom photocatalysts that are selective as well as recyclable. Based on this, recently we have developed several photocatalytic strategies for the synthesis of fuels as well as high valued chemicals where the catalysts exhibited excellent selectivity as well as recyclability.

Bio-Sketch of Speaker

Prof. Dr. René M. Koenigs

Academic experience

RWTH Aachen University, Institute of Organic Chemistry, Landoltweg 1, 52074 Aachen, Germany

Since May 2022	Professor for Organic Chemistry
2023 – 2024	Visiting professor at IIT Bombay, India
2017 – *2020*	Visiting professor at UNSW Sydney, Australia
Oct. 2015 – Apr 2022	Assistant professor for Organic Chemistry

Main Research Areas: Organic synthesis, photochemistry, carbene transfer reactions, nitrene transfer reactions, reactive intermediates, catalysis, method development, medicinal chemistry.

Professional experience

Grünenthal GmbH, Global Drug Discovery, 52099 Aachen, Germany

May 2013 - Oct. 2015	Head of Laboratory in Lead Optimization Chemistry
Nov. 2011 - Apr. 2013	*Post-Doc* in Lead Optimization Chemistry

Education

PhD thesis

Feb. 2008 – Oct. 2011	PhD thesis under the supervision of Prof. Dr. M. Rueping, Goethe Universität, Frankfurt/M. then RWTH Aachen University (*Summa cum laude*, 1.0)

Chemistry studies

Oct. 2002 – Jan. 2008	chemistry studies at Goethe University Frankfurt/M. Diplom (*with distinction*, 1.0)
Jun. 2007 – Jan. 2008	diploma thesis under the supervision of Prof. Dr. M. Rueping

Awards and Scholarships

2023	*Australian Research Council* Future Fellowship
2021	Teaching award from the chemistry student council
2021	*RWTH Aachen FAMOS* award for excellence in leadership
2020	Research Award by the *Dr. Otto Roehm Foundation*
2018	Boehringer Ingelheim Exploration Grant
2017	Thieme Journal Award 2017
2016	RWTH Start-Up Funds

Spin states matter – fundamentals, applications and translation to drug discovery

Rene M. Koenigs

RWTH Aachen University, Institute of Organic Chemistry, Landoltweg 1, 52074 Aachen, Germany.
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Carbenes and nitrenes are versatile reactive intermediates that find widespread application in organic synthesis. Their high reactivity, however, often necessitates the use of metal complexes for stabilization of such species.[1,2]

Herein, we describe our recent approaches towards photochemical and photocatalytic carbene and nitrene transfer reactions. Strategies in accessing either singlet or triplet carbenes will be discussed and their applications in synthesis methodology will be presented.[3,4]

We commence with a discussion of nitrene intermediates and how these can be accessed under visible light irradiation without the need of conventional metal catalysts. We describe strategies, how the access of nitrene intermediates can be manipulated by single electron transfer reactions or direct photoexcitation.[5] We conclude with a discussion of a collaborative approach towards drug discovery, where fundamental discoveries can be translated into new drugs and medicines.[6]

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Abhishek Dey, PhD

Abhishek Dey has a background in electronic structure in inorganic chemistry. His research aims at emulating the reactivity of enzyme active sites in synthetic analogues using the geometric and electronic structure function relationships present in natural systems. His current area of interest includes multi-proton and multi-electron transformations that are key for clean energy and environment and development of new analytical techniques for interrogation and intuition driven innovations in electrocatalysis.

Education

Aug 2001 – May 2007 **Stanford University**
PhD, Chemistry
Palo Alto, United States

Aug 1999 – Jun 2001 **Indian Institute of Technology Kanpur**
M. Sc, Chemistry
Kanpur, India

Aug 1996 – Jun 1999 **Presidency College, Kolkata**
B. Sc., Chemistry
Kolkata, Bengal, India

Honors and Awards

Fellow, The National Academy of Science, India, 2023
Fellow, The Indian Academy of Sciences, Bangalore**,** 2023
James Hoeschele Award, Asian Society of Biological Inorganic Chemistry, 2022
CRSI Bronze Medal, Chemical Research Society of India, 2020
SERB-STAR, Department of Science and Technology, 2020
SBIC Emerging Investigator Award, Society of Biological Inorganic Chemistry, 2019
Rising Star of Asia Medal, Federation of Asian Chemical Societies, 2019
SPP/ICPP Young Investigator Award, Society of Porphyrins and Phthalocyanine, 2014
Young Associate, Indian Academy of Science, Bangalore, 2010
Young Investigator Award, ACS, Division of Inorganic Chemistry, 2007
Evelyn Laing McBain Stanford Graduate Student Fellowship, 2005

Synergistic activities

- **Associate Editor**, ACS Catalysis.
- Editorial Advisory Board Member of Journals
  Present**: Chemical Communications, Journal of Inorganic Biochemistry (JIB), Chemical Reviews, Chemical Society Reviews, Resonance, ACS Central Science**
  Past*: Inorganic Chemistry*, *Journal of Biological Inorganic Chemistry* (JBIC), *ACS Catalysis*,
- **Council Member,** Chemical Research Society of India, 2023-2026
- Council member: Asian Society of Biological Inorganic Chemistry (**AsBIC**)
- Council member: Activation of Dioxygen and Homogeneous Oxidation Catalysis (**ADHOC**)
- Guest Editor Virtual Issue of Inorganic Chemistry, J. Am. Chem. Soc. And ACS Catal. *The way forward in Molecular Electrocatalysis* **2016.**

Factors Deciding the Selectivity of O_2, NO, CO_2 and SO_2 Reduction.

Abhishek Dey

School of Chemical Sciences, Indian Association for the Cultivation of Science
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The talk will describe the intermediates involved in the multiple electron and multiple proton reduction of small molecules like O_2, NO (NO_2^-), CO_2 and SO_2. These intermediates are either observed in solution during stoichiometric reaction or in-operando using spectro-electrochemistry and characterized using a combination of spectroscopic techniques like EPR, Mossbauer, FTIR and resonance Raman spectroscopy. These transient intermediates are found to determine the selectivity of ne^-/nH^+ reduction of these small molecules which allows predictive design of catalysts for the purpose. While the reactions are very different, there seems to be certain commonalities in these reaction intermediates which can be taken advantage of when designing catalysts for selective reduction of these small molecules.

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1. P. Saha, Sk Amanulla and A. Dey, *Acc. Chem. Res.*, 2022, **55**, 134–144
2. S. Chatterjee, K. Sengupta, B. Mondal, S. Dey and A. Dey *Acc. Chem. Res.* 2017, **50**, 1744-1753.
3. P. Saha, S. Barman, Sk Amanulla and A. Dey *ACS Catalysis*, 2023, **13,** 13181-13194

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Flash Lectures

Bio-Sketch of Speaker

Dr. Thirupathi Barla
Assistant Professor

Department of Chemical Sciences
Indian Institutes of Science Education and Research Berhampur
Transit Campus, Industrial Training Institute (ITI)
Engineering School Road
760010, Ganjam District, Odisha
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Dr. Thirupathi Barla was born in Madavelli, Manchirial district, Telangana, India 1984. After completing his M.Sc. (Organic Chemistry) from Osmania University (2006-2008), he worked as a research chemist at Aragen Life Sciences, formerly known as GVK-Biosciences, Hyderabad (2008-2009). In early 2009, he joined as a Junior Research Fellow (JRF) at CSIR-Indian Institute of Chemical Technology, Hyderabad, with Dr. D. K. Mohapatra for doctoral studies (2009-2014). Afterwards, he worked as an associate research scientist in the process R&D division at Sai Life Sciences, Hyderabad (2014-2015). Then Dr. Barla moved to Harvard University as a postdoctoral fellow to work with Prof. E. J. Corey (2015-2018), where he was involved in the development of highly active fluorinated second-generation oxazaborolidine catalysts and their application in Diels-Alder reactions. In July 2018, he became an Assistant Professor of Chemistry at the Indian Institute of Science Education and Research Berhampur. Dr. Thirupathi's area of research includes the total synthesis of biologically active natural products or model compounds having potential bioactivities. Dr. Thirupathi's group is also working on developing novel carbon-corban bond formation reactions and their application towards natural product synthesis.

Awards:
Thieme Chemistry Journal award-**2023**
Received the Outstanding Reviewer award from Tetrahedron Letters in August **2018**.
Received a postdoctoral fellowship from Harvard University, USA, in **2015**.

Synthetic Approaches to Various Carbocyclic-, Heterocyclic Compounds Involving 1, 3-Indanediones.

Barla Thirupathi*

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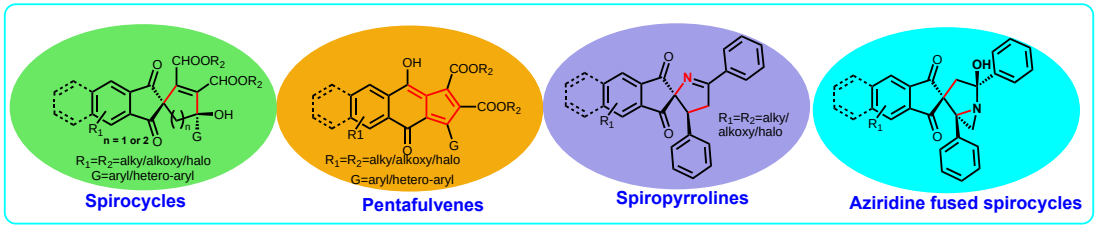
Abstract

2-keto-1,3-indandiones serve as an important precursor for the construction of various bicyclic, spiro cyclic systems with suitable partners. Accordingly, the reaction of arynes with 2-keto-1,3-indandiones provided dibenzobicyclo[3.2.1]octadienone core[1] and the reaction of dimethyl acetylene dicarboxylate (DMAD) with 2/3-keto-1,3-Indandiones afforded spiro[4.4]nonane, spiro[4.5]decane compounds in presence of a catalytic amount of DABCO.[2] Moreover, the spiro[4.4]nonanes were transformed into highly conjugated pentafulvene motifs via unprecedented C-C bond rearrangement in an acidic medium. Similarly, we have also developed a catalyst-free method to access various 1,3-indandione-containing spiropyrrolines.[3]



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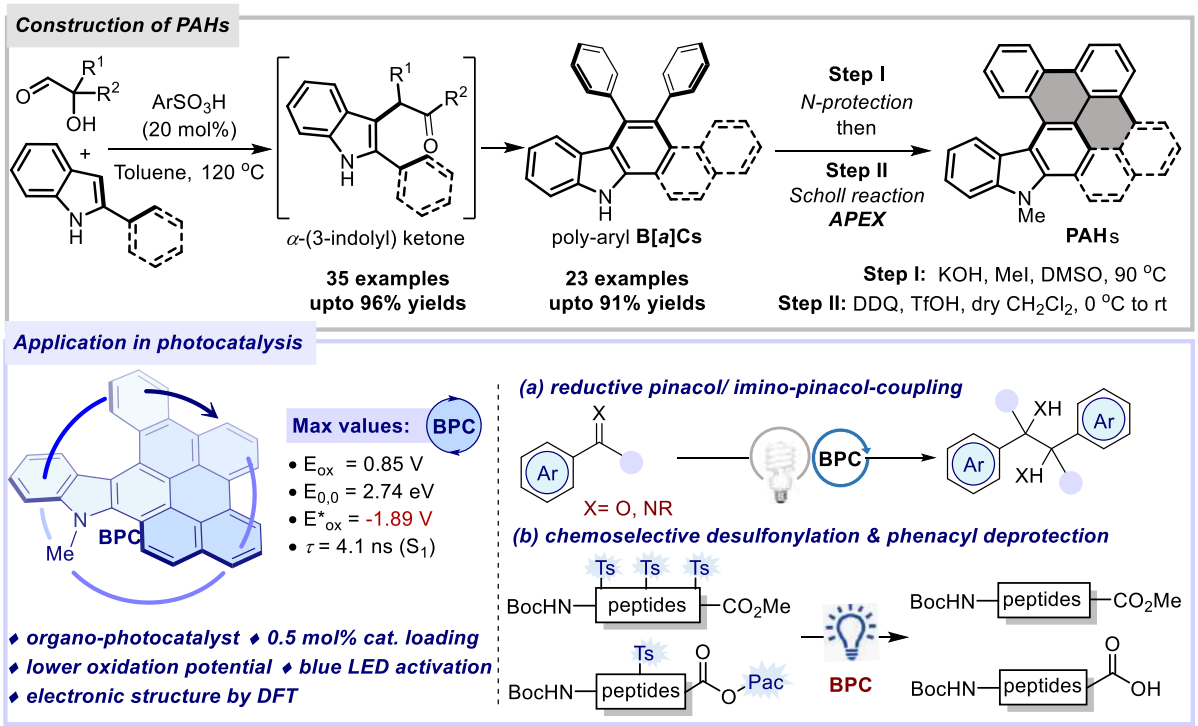
2. Mishra, G.; Sasmal, M.; Chakraborty, A. **Thirupathi, B**. *Chem. Eur. J.* **2023** *e202301976*.
3. Sahoo, K.; Patra, N.; Dandela, R.; **Thirupathi, B**. *J. Org. Chem.* **2024** (In revision)

Synthesis of π-Excessive Carbazole Based Polyaromatic Hydrocarbons and Their Applications in Photocatalysis

Samrat Kundu, Ankush Banerjee, and Modhu Sudan Maji*
Department of Chemistry, Indian Institute of Technology Kharagpur, Kharagpur-721302

Nitrogen containing polycyclic aromatic compounds (N-PACs) have potential applications in material chemistry and organo-photocatalysis.[1] The central objective of our work is to develop a synthetic strategy for constructing carbazole derivatives and its further utilization for synthesizing polycylic aromatic hydrocarbons (PAHs) which can potentially be used in photocatalysis to develop novel strategies in organic synthesis.[2] Keeping this in mind, we have developed the pinacol-type rearrangement strategy for the synthesis of α-(3-indolyl) ketones as an immediate precursor of carbazole derivatives.[3] The applicability was further endorsed in synthesis of poly-aryl substituted benzo[*a*]carbazoles through cascade benzannulation strategy followed by synthesis of structurally unique PAH analogues with extensive annulated π-conjugation.[4] Thorough investigation on photophysical properties of PAHs intrigue us to evaluate their potential applicability in photocatalysis. In connection with that, we introduce one of the synthesized PAH analogue, benzoperylenocarbazole (BPC) as potent organo-photo-reductant in pinacol and imino-pinacol coupling reactions for the synthesis of vicinal diols and diamines.[5] Furthermore, we also evaluate the potential capability of BPC in solution phase chemoselective late-stage desulfonylation from Trp, Tyr and His side chains in oligopeptides up to octamer and phenacyl deprotection from C-terminal in peptide backbone.[6]



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One pot Conversion of Phenols and Anilines to Aldehydes and Ketones Exploiting α-gem Boryl Carbanions

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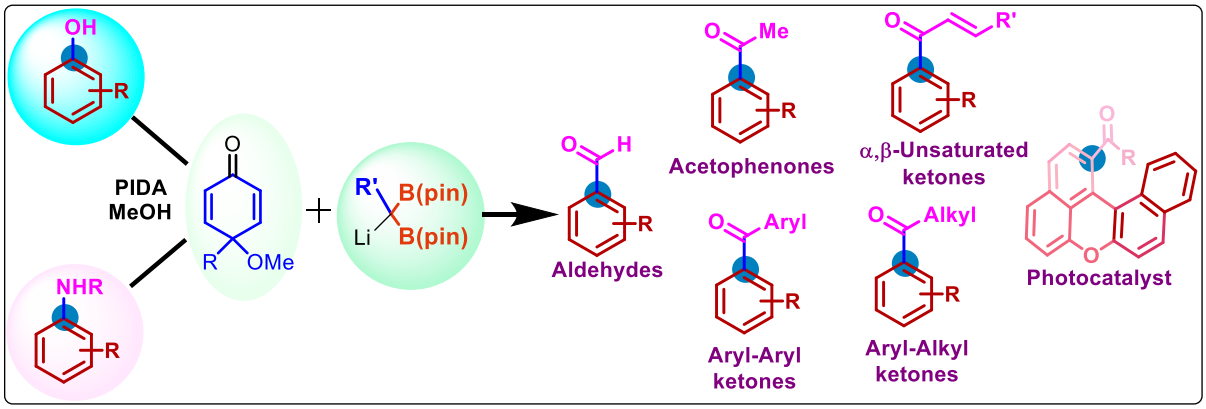
Senior Research Fellow, Department of Chemistry
Indian Institute of Technology Kharagpur, Kharagpur-721302, West Bengal
(E-mail: kanakiitmadras@gmail.com)

Functional group interconver sion is a beneficial synthetic transformation for everyday organic synthesis.[1] Phenols and anilines are naturally abundant and commercially available scaffolds whereas the acyl functionalities are the key components of various natural products, bioactive molecules, and phermaciticules.[2] Most of the current strategies rely on the conversion of phenols and anilines to the corresponding oxidative coupling partner and their subsequent transformations using carbon monoxide and Pd/Ni-based catalysts.[3] Herein we have developed a one-pot, transition metal-free pioneering strategy for the synthesis of a diverse range of aldehyde and ketones, starting from phenols and protected anilines via C-O and C-N bond cleavage.[4] A wide range of mono aryl, fused biaryl as well as substituted phenols and anilines have been successfully acylated resulting a variety of ketones, such as aryl-alkyl, aryl-aryl, acetophenone, and conjugated ketones etc. This method has an excellent selectivity towards the keto and 1,2-addition over the ester and 1,4-addition. The regioselective synthesis of acetophenones has been developed with 100% selectivity. Several bioactive molecules and pharmaceutically active intermediates have been synthesized within short steps from the reported procedure. We have designed a fused BINOL-based polycyclic compounds and further exploited as a photocatalyst under sunlight irradiation.



Scheme 1. α-Gem Boryl Carbanions for the one-pot synthesis of aldehydes and ketones

References: [1] A. Leslie, A. M. Joseph, M. Baumann, *Curr. Org. Chem.* **2021**, *25*, 2217. [2] M. M. Rahman, M. S. Rahaman, M. R. Islam, F. Rahman, F. M. Mithi, T. Alqahtani, M. A. Almikhlafi, S. Q. Alghamdi, A. S. Alruwaili, M. S. Hossain, *Molecules* **2022**, *27*, 233. [3] A. M. Echavarren, J. K. Stille, *J. Am. Chem. Soc*. **1988**, *110*, 1988. [4] K. K. Das, D. Aich, S. Dey, S. Panda, "One-pot Conversion of phenols and anilines to aldehydes and ketones using boron-Wittig reaction*."* (Manuscript Submitted).

Bio-Sketch of Speaker

Dr. Soumitra Maity
Associate Professor
Department of Chemistry & Chemical Biology
Indian Institute of Technology (ISM), Dhanbad
Jharkhand – 826004, India

Web site: https://ccb.iitism.ac.in/ccb_faculty_details

Professional Experience:

2022-	Associate Professor, IIT(ISM) Dhanbad
2015-2021	Assistant Professor, IIT(ISM) Dhanbad
2014-2015	Inspire Faculty, CSIR-CSMCRI, Bhavnagar, Gujarat 364002
2012-2013	Postdoctoral Fellow, University of California, Berkeley, USA with Professor T. Maimone
2010-2012	Postdoctoral Fellow, University of Arkansas, USA with Professor Nan Zheng

Education Qualification:

2005-2010	PhD. at the IACS, Kolkata, supervisor (Prof. Subrata Ghosh)
2002-2004	M.Sc. Chemistry at the University of Calcutta
1999-2002	B.Sc. Chemistry at Ramakrishna Mission Residential College, Narendrapur

Awards/ Honors/ Membership:

2018	Fellow, Indian Chemical Society
2013	INSPIRE Faculty Award, DST – New Delhi

Research Interest:

Methodology development based on light induced free radical generation and it's application in organic synthesis.

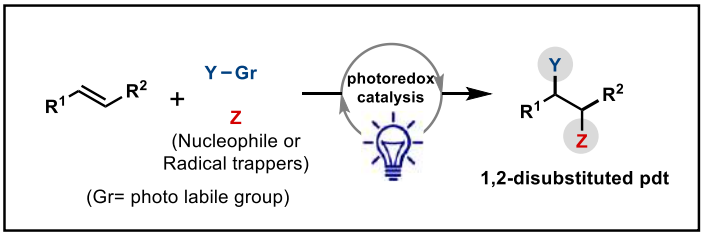
Radical Functionalization of Olefins by Photo-Redox Catalysis

*Dr. Soumitra Maity**

Department of Chemistry and Chemical Biology, Indian Institute of Technology Dhanbad, Dhanbad-826004

(E-mail: smaity@iitism.ac.in)

Visible light photoredox catalysis is one of the emerging fields in recent times, and much attention has been paid to exploring the activities of visible light in organic transformations from the aspect of pure science as well as sustainable chemistry. Visible light is clean, inexpensive, safe, and environmentally benign. So using sunlight as the reaction component in any transformation would be one of the most efficient approaches ever. Direct functionalization of alkenes is a valuable synthetic tool for the preparation of functionalized alkanes, which have high utility in organic synthesis. More recently, Radical initiated functionalization by visible-light-mediated single-electron transfer (SET) process has further matured this functionalization strategy under environmentally benign mild conditions. The synthetic potential of this radical photo-redox catalysis will be discussed through the assembly of various backbones (C-C and C-X) of organic molecules from alkenes.



Scheme 1. *Photocatalytic alkene functionalization*

References: *[a]* I. Ul Hoque, S. R. Chowdhury and S. Maity, *J. Org. Chem.,* **2019**, *84*, 3025. *[b]* S. R. Chowdhury, D. Singh, I. Ul Hoque and S. Maity, *J. Org. Chem.,* **2020**, *85*, 13939. *[c]* A. Samanta, S. Pramanik, S. Mondal and S. Maity, *Chem. Commun,* **2022**, *58*, 8400. *[d]* S. Pramanik, P. P. Mondal and S. Maity, *J. Org. Chem.,* **2023**, *88*, 15256.

Bio-Sketch of Speaker

Dr. S. Easwar
Associate Professor
Department of Chemistry
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e-Mail: easwar.srinivasan@curaj.ac.in

Academic background

M.Sc. Chemistry	:	University of Pune, ***2000***
Ph.D.	:	National Chemical Laboratory (NCL) Pune, ***2006*** *Mentor*: Dr. N. P. Argade
Post-Doctoral Fellow	:	University of Bologna, Italy, ***2006-'08*** *Mentor*: Prof. Claudio Trombini

Experience*:*

Research Scientist, SAI Life Science, Pune	:	2009-'11
Assistant Professor, Central University of Rajasthan, India	:	Aug '11 - May '19
Associate Professor, Central University of Rajasthan, India	:	*Jun '19 – till date*

Current Research Interests:

- Development of synthetic methodologies related to the Morita–Baylis–Hillman (MBH) reaction
- Design of bifunctional organocatalysts for asymmetric C-C bond forming transformations
- Stereoselective cascade reactions for the construction of fused and bridged heterocycles

Significant recent publications:

⇒ Mechanistic Investigations on the Interaction of Morita–Baylis–Hillman Ketones with 2-Aminothiophenol
R. Kumari, A. K. Jha, A. G. H. Khan and **S. Easwar***, *J. Org. Chem.* **2024**, *89, accepted*

⇒ Acyl Transfer-Driven Rauhut–Currier Dimerization of Morita–Baylis–Hillman Ketones
R. Kumari, A. K. Jha, S. Goyal, R. Maan, S. Rajagopala Reddy and **S. Easwar***, *J. Org. Chem.* **2023**, *88*, 2023

⇒ Synthesis of 2,2-Disubstituted Dihydro-1,4-benzothiazines from Morita–Baylis–Hillman Ketones by an Oxidative Cyclization
A. K. Jha, R. Kumari and **S. Easwar***, *J. Org. Chem.* **2022**, *87*, 5760

⇒ Diamine-Mediated Degradative Dimerisation of Morita-Baylis-Hillman Ketones
A. K. Jha, A. Kumari and **S. Easwar***, *Chem. Commun.* **2020**, *56*, 2949

⇒ A Hydrazine Insertion Route to N'-Alkyl Benzohydrazides by an Unexpected Carbon-Carbon Bond Cleavage
A. K. Jha, R. Kumari and **S. Easwar***, *Org. Lett.* **2019**, *21*, 8191

Awards: "Prof. D. K. Banerjee Memorial Lecture Award", IISc Bangalore, April 2023

Memberships: Life Member, CRSI

Website: http://www.curaj.ac.in/faculty/easwar-s

Intriguing Reactivity of Baylis-Hillman Ketones with Diamines

*Dr. S. Easwar**

Department of Chemistry, Central University of Rajasthan, Distt. Ajmer-305817

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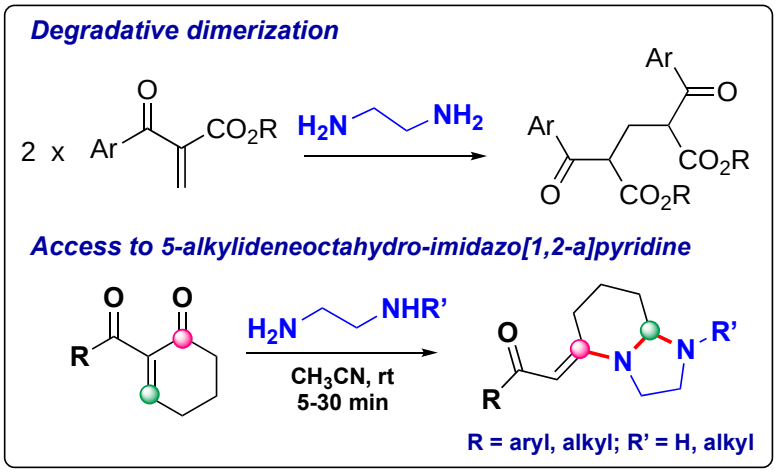
*Our recent studies on reactivity patterns of Morita-Baylis-Hillman (MBH) ketones have led to some interesting observations.[1] For instance, reaction with a vicinal diamine mediated a degradative dimerization, leading to the formation of methylene-bridged bis-1,3-dicarbonyl compounds. A retro-Mannich reaction was thought to be the key step of the pathway.[1b] The proposed mechanism was validated by using MBH adducts derived from a cyclic precursor, which eventually gave access to saturated imidazopyridines (**Scheme 1**).[2] Further results on the formation and reactivity of dienamines derived from MBH ketones will also be discussed.*



Scheme 1. *Diverse patterns in the reactivity of MBH ketones with diamines*

References: *[1] For examples, see: (a) Jha, A. K.; Kumari, R.; Easwar, S. Org. Lett. 2019, 21, 8191-8195; (b) Jha, A. K.; Kumari, A.; Easwar S. Chem. Commun. 2020, 56, 2949-2952; (c) Jha, A. K.; Kumari, R.; Easwar, S. J. Org. Chem. 2022, 87, 5760-5772. [2] Sharma, S.; Easwar, S. Manuscript communicated*

Bio-Sketch of Speaker

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Web page: http: http://www.bmajilab.com

1987: Born, Howrah, India
2007: B.Sc. University of Calcutta (Chemistry Hons.)
2009: M.Sc. Indian Institute of Technology Kanpur (Chemistry)
2012: PhD Ludwig Maximillan Universität Munich, Supervisor: Prof. Herbert Mayr
2013-2015: Postdoc: Chubu University, Mentor: Prof. Hisashi Yamamoto
2016: Alexander von Humboldt fellow: Westfälische Wilhelms-Universität Münster, Mentor: Prof. Frank Glorius
2016-2021: Assistant Professor, Indian Institute of Science Education and Research Kolkata
2021-: Associate Professor, Indian Institute of Science Education and Research Kolkata

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

Awards:
2021: "2021 Young Investigator Award ", Sponsored by Molecules
2021: Merck Young Scientist Award (runner-up) in Chemical Science
2021: INSA Medal for Young Scientists
2021: Associate of the Indian Academy of Sciences (IASc)
2020: NASI-Young Scientist Platinum Jubilee Award (2020) in Chemical Sciences
2019: Thieme Journal Award

Selected publication:

- A.Palai, P.Rai, **B. Maji**, *Chem. Sci.*, **2023**,*14*, 12004.
- A. Jati, S. Dam, S. Kumar, K. Kumar, **B. Maji**, *Chem. Sci.* **2023**, *14*, 8624.
- S. Waiba, K. Maji, M. Maiti, B. Maji, *Angew. Chem. Int. Ed.* **2023**, *Angew. Chem. Int. Ed.* **2023**, *62*, e202218329.
- P. Rai, K. Maji, S. K. Jana, B. Maji, *Chem. Sci.* **2022**, *13*, 12503-12510.
- K. Das, S. Waiba, A. Jana, B. Maji, *Chem. Soc. Rev.* **2022**, *51*, 4386-4464.
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Dearomative Cycloaddition Reactions via Visible Light Energy Transfer Catalysis

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Dearomative cycloaddition reaction is a blueprint for creating sp3-rich three-dimensional molecular topology from flat-aromatic compounds. However, the reaction involving the arene system is highly challenging because of the high chemical stability inherent due to aromaticity. Further, severe reactivity, selectivity, and reversibility issues make this process arduous. One such process to overcome these challenges is the photochemical approach that induces the loss of aromaticity. Herein, we describe visible-light-induced triplet-triplet energy-transfer catalysis for the dearomative meta- and para-cycloaddition reaction of feedstock naphthalene molecules with tethered alkenes and vinyl benzenes. We performed DFT studies, photoluminescence, electrochemical, UV-VIS, and triplet energy quenching studies to understand the mechanism of those cycloaddition reactions. The developed protocol can be accessed for the cycloaddition reaction of feedstock naphthalene molecules with tethered alkenes and vinyl benzenes where structurally diverse 2-acyl naphthalenes with various functional groups could easily be converted to a diverse range of scaffolds in high yields and selectivities. The reaction can be scaled up to a gram scale and is also amicable for late-stage modification of various complex bioactive molecules. Furthermore, milder reaction conditions and substantially higher triplet energy of the dearomatized product prevent the reverse reaction, resulting in higher product yields. The research shed insight into visible light energy transfer catalysis, which is in the early stages of chemical synthesis.

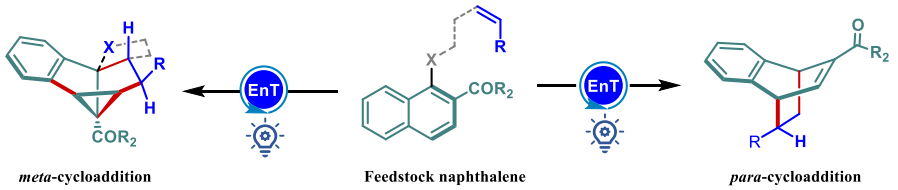

Figure 1. Visible light-induced triplet energy-transfer mediated *meta*- and *para*-cycloaddition of naphthalene derivatives.

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Research Interests

New synthetic and catalytic methodologies to design novel strategic approaches for the total synthesis of bio-active natural and unnatural molecules.

Professional Experiences

Since 2020 **Assistant Professor,** IIT Kanpur, India

2018-2020 **Post-Doc,** Rice University, Houston, Texas, USA
Advisor: Prof. K. C. Nicolaou

2017-2018 **Post-Doc**, University of Göttingen, Germany
Advisor: Prof. Lutz Ackermann

2015-2016 **Post-Doc**, ESPCI ParisTech, Paris, France
Advisor: Prof. Janine Cossy

Educational Details

2009-2015 **Ph. D. Chemistry**, Indian Institute of Technology Bombay, Mumbai, India
Advisor: Prof. Krishna P. Kaliappan

Thesis Title: Copper-Catalyzed Domino Reactions to Pharmaceutically Relevant Heterocycles

2004-2006 **M.Sc. Chemistry**, Madras Christian College University of Madras, Chennai, India

Selected Academic Honors/Awards

2016 *Eli Lilly and Company Asia Outstanding Thesis Award*

Robust Synthesis of Terpenoid Scaffolds under Mn(I)-Catalysis

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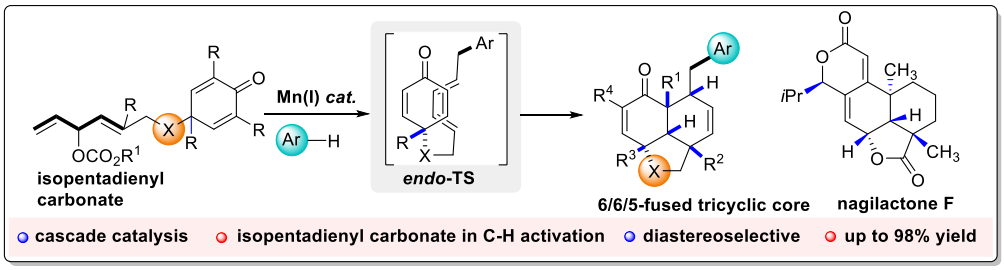
The 6/6/5-fused tricyclic scaffold is a central feature of structurally complex terpenoid natural products. A step economical cascade transformation that leads to a complex molecular skeleton is regarded as a sustainable methodology. We recently reported a cascade Mn(I)-catalyzed C(sp^2)−H chemoselective dienylation and diastereoselective intramolecular Diels−Alder reaction using *iso*-pentadienyl carbonate to access 6/6/5-fused tricyclic scaffolds. The broad substrate scope of this method demonstrates a wide range of functional group tolerances with a high-yielding synthesis of nagilactone-type and endiandric acid-type 6/6/5-fused tricyclic cores. Salient features of this method include (i) *iso*-pentadienyl carbonate as a reactant in C−H activation catalysis, (ii) regio-, stereo-, and chemo-selective arylomanganese(I) insertion on terminal olefin of tetra-olefin containing substrate to obtain 1,3-dienes, and (iii) final product, homo-aryl 6/6/5-fused tricyclic scaffold contains five contiguous chiral centers, including an epimerizable α-center at the ring junction. Further, extensive mechanistic studies, including isolation of catalytically active organo-manganese(I)complex, 1,3-dienyl-intermediates, and isotopic labeling experiments, have supported the proposed mechanisms. Moreover, the late-stage diversification of these products led to several valuable new transformations. This cascade transformation for the synthesis of 6/6/5-fused tricyclic terpenoid scaffolds will be discussed.



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Bio-Sketch of Speaker

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Academic Career:

2022 - till date: Associate Professor, Dept. of Chemistry, IISER-Tirupati, Tirupati.

2017 – 2022: Assistant Professor, Dept. of Chemistry, IISER-Tirupati, Tirupati.

Research Experience:

Dec 2013 – Feb 2017: **Postdoctoral fellow, Prof. Ronald Breslow group,** Department of Chemistry, Columbia University, New York, U.S.A

April 2011 – Nov 2013: **JSPS Postdoctoral Fellow. Prof. Masakatsu Shibasaki group,** Laboratory of Synthetic Organic Chemistry, Institute of Microbial Chemistry, Tokyo, Japan.

Education:

Aug 2005 – Feb 2011: **Ph.D in Organic Chemistry. Supervisor: Prof. S. Chandrasekaran**

Thesis title "**Synthesis of Novel Chalcogenides using Acyloxyphosphonium Intermediates and Doubly Activated Cyclopropanes**" Indian Institute of Science, Bangalore, India.

July 2003 – May 2005: **Master of Science in Organic Chemistry,** First class with distinction **(80%)** University of Madras, Chennai, India.

Academic Achievements and Awards:

- **ECRA (Early Career Research Award),** 2019
- **Ramanujan** Fellowship, 2017
- **JSPS** (Japan Society for the Promotion of Science) Postdoctoral fellowship.
- Prof. S. Swaminathan Endowment Lectureship and **Prize** for **outstanding student** in M.Sc Organic Chemistry at University of Madras.

Enhancing Radical Cascade Reactions for Accessing Functionalized Heterocycles by Shining Light

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Cascade reactions significantly improve the efficiency of a chemical process as multiple bonds are formed in a single transformation without isolation of any intermediates, increasing the atom economy, reducing the waste generated, etc. Recently, photomediated radical cascade reactions has received much attention in the literature for the synthesis of interesting heterocycles. In this direction, our group explored radical cascade addition-annulation of ortho alkenyl aryl ureas and 1,7 enyne systems with various radical precursors under photoredox conditions (Figure 1). Controlled chemoselective nitrogen vs oxygen cyclization of o-alkenyl aryl ureas for the synthesis of the desired heterocycles will be discussed. Similarly, a three-component reaction involving regioselective addition of radicals on 1,7 enynes followed by cyclization for accessing interesting heterocycles will be demonstrated.

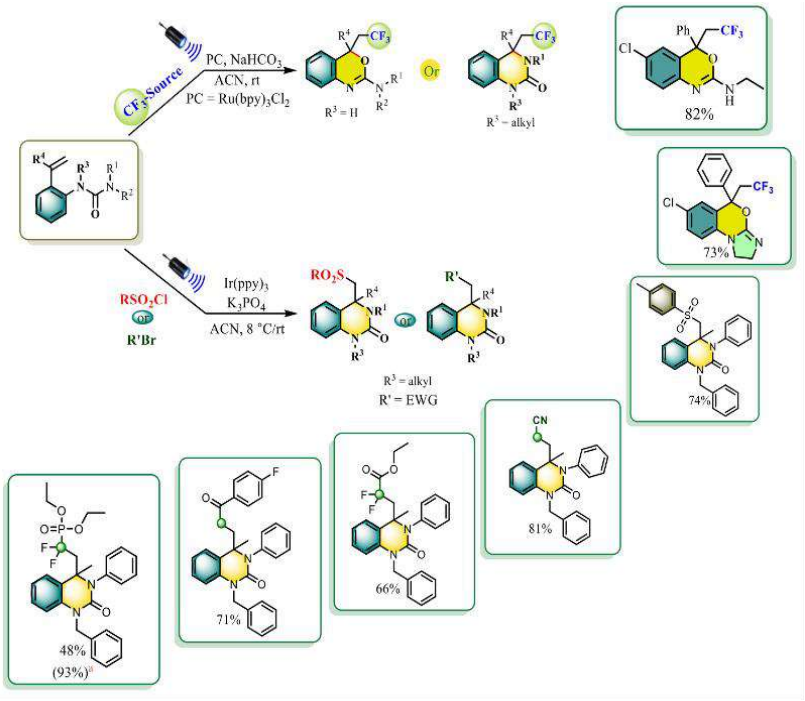

Figure 1: Diverse molecular frameworks synthesized using radical cascade approach.

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Stereodivergent Zweifel Olefination and its Mechanistic Dichotomy[1]

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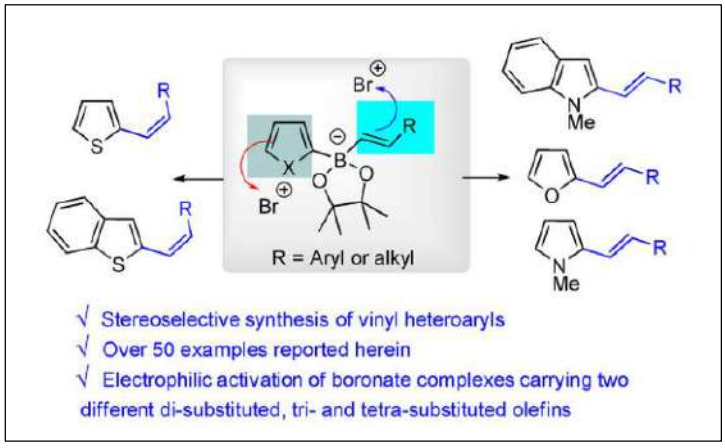
Zweifel olefination[2] is an important olefination reaction for the stereoselective synthesis of olefin from the corresponding vinyl organoboron compounds. The reaction is thought to proceed by activation of olefin by iodine, followed by 1,2-migration then base-induced anti-elimination. However, stereoselective Zweifel olefination using boronate complex carrying two different π-systems is challenging and remains unexplored. Our efforts have focused on stereoselective Zweifel olefination using boronate complex carrying two different reactive π-systems to synthesize the vinyl heteroarenes and conjugated 1,3-dienes in good yield and up to 100% stereoselectivity. Most importantly, we reported the stereoselective formation of *E* vs. *Z*-vinyl heteroarenes in the case of different heteroarenes after tedious optimization. Thorough DFT studies unveil the mechanistic dichotomy while activation of boronate complex in the presence of electrophilic halide source. Stereodivergent synthesis of *E* vs. *Z*-heteroarenes was observed using DDQ as an electrophile, which has not been shown before. Further, DFT studies for the DDQ reaction elucidate their underpinning mechanism. Surprisingly, Zweifel olefination using boronate complex carrying two different disubstituted olefins and their reaction optimization afforded conjugated 1,3-diene in 100% stereoselectivity, which was further expanded to tri- and tetra-substituted olefins.



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Carbonyl-Assisted Asymmetric Migratory Allylation of α-Keto-Imines: A Concise Pathway towards Hapalindole Alkaloids

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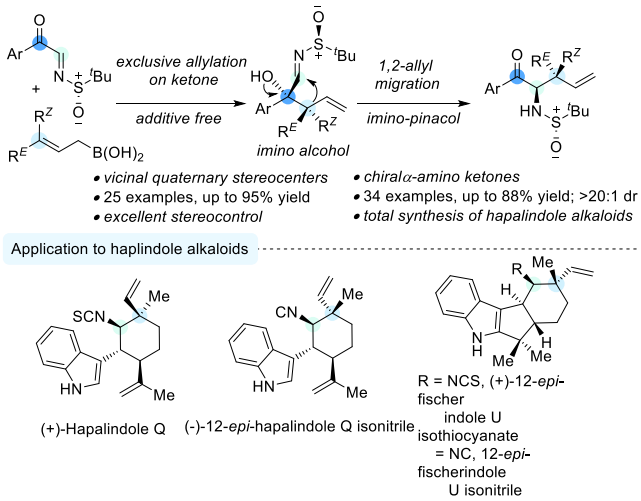
Carbonyl assisted a mild asymmetric migratory allylation of *α*-keto imines using allylboronic acids is reported for the generation of highly challenging vicinal quaternary carbon stereocenters, α-amino ketones, and amino-alcohols with excellent yields and diastereoselectivities. In a remarkable divergence, despite having higher steric hindrance, the reaction distinctly engages ketones for the allylation over imines in the first step, followed by a face-selective allyl transfer, highlighting an intriguing interplay between two distinct electrophilic trajectories. The methodology distinguishes itself through its adaptability to gram-scale synthesis, showcasing broad functional group tolerance, and stereodivergence. The DFT analysis elucidate a deeper understanding of its selectivity and mechanistic framework. Highlighting its transformative potential, the total synthesis of hapalindole alkaloids were adeptly achieved.



Scheme 1. 1,2-allyl migration strategy

References: [a] S. Sahu, G. Karan, L. Roy and M. S. Maji, *Chem. Sci.*, **2022**, *13*, 2355-2362 [b] G. Karan, S. Sahu, A. Metya, and M. S. Maji.(manuscript submitted)

Bio-Sketch of Speaker

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Objective:

Dedicated NIT Assistant Professor with over 10 years of experience in computational and inorganic chemistry. Proven track record of excellence in teaching, research, and mentorship. Seeking opportunities to contribute to the academic community and drive research innovations.

Education:

- Ph.D. in Inorganic & Computational Chemistry
- Indian Association for the Cultivation of Science (Jadavpur University), 2018
- Supervisor – Prof. Dipankar Datta & Prof. Abhishek dey
- M.Sc.
- IIT Kanpur, 2012

Professional Experience:

1) Assistant Professor
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Oct 2023 – Till date

2) Postdoctoral Fellow (Supervisor: Prof. Pratim K. Chattaraj)
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Oct 2021 – Sept 2023

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4) Postdoctoral Fellow (Supervisor: Prof. Dan Meyerstein)
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Ariel University
Ariel 40700, Israel
June 2018 – Nov 2020

Professional Memberships:

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- Member of the American Chemical Society (ACS).
- Member of the Chirantan Rasayan Sanstha, Paschim Medinipur, West Bengal.
- Served as reviewer for the Journal Inorganic Chemistry, American Chemical Society (ACS).
- Served as reviewer for the Journal ACS Omega, American Chemical Society (ACS).
- Served as reviewer for the Journal ChemCatChem, Wiley-VCH.
- Served as reviewer for the Journal Polyhedron, Elsevier.

Fischer and Schrock carbene complexes in the light of global and local electrophilicity based descriptors

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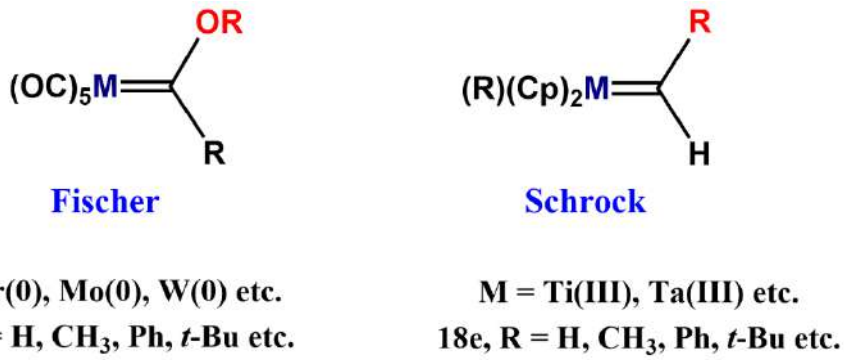
The carbon atom (carbene) of Fischer and Schrock complexes are electrophilic and nucleophilic respectively (Scheme 1). The reactivity index electrophilicity is a global reactivity parameter and can tell only about the total electrophilicity of the complexes. To differentiate between the reactivity patterns of these two carbenes the philicity and multiphilic descriptor are calculated. In Fischer complexes, it is found that the philicity of the nucleophilic attack (ω_C^+) is higher than that of philicity of the electrophilic attack (ω_C^-) implying the electrophilic nature. A reverse order is found in the Schrock complex pointing nucleophilic character. The multiphilic descriptor ($\Delta\omega_C = \omega_C^+ - \omega_C^-$) is found to be positive in Fischer but negative in Schrock leading to the same conclusion.[a] Fischer carbene complexes having general formula $(CO)_5Cr{=}CH\text{-}R$ (R = CH_3, Ph, C≡CH, $CH{=}CH_2$, OCH_3, OH, $NHCH_3$ and NH_2) the order of ω_C^+ and $\Delta\omega_C$ better describe the trend. The trend has been justified through energy decomposition in the purview natural orbital for chemical valence (EDA-NOCV) analysis owing to the π contribution from the R group. The change in the reactivity patterns along the intrinsic reaction coordinate of two representative reactions is plotted. This way of understanding the reactivity parameters would help experimental chemists to predict the catalytic application of carbene complexes of transition metal without the classification of Fischer and Schrock type.



Scheme 1. Pictorial representation of Fischer and Schrock carbene complexes.

References: [a] S. G. Patra, R. Jha, H. Mondal, P. K. Chattaraj, *J. Phys. Org. Chem.* **2023**, *36* (12).

Bio-Sketch of Speaker

Akshai Kumar hails from Mangalore. He obtained his B.Sc. in 2002 from Mangalore University. From the same university in 2004, he received his Master's degree in inorganic chemistry. He pursued his doctoral studies under the supervision of Prof. Ashoka G. Samuelson at the Indian Institute of Science, Bangalore, where he was awarded a Ph.D. degree in 2009. After a postdoctoral stint in the same laboratory, in October 2010, he joined the group of Prof. Andreas Terfort at Goethe University, Frankfurt, Germany, as a postdoctoral fellow. In 2012, he extended his postdoctoral activities and worked in the Goldman group at Rutgers, The State University of New Jersey, New Brunswick. In 2015, he was appointed as Assistant Professor in Chemistry at the Indian Institute of Technology Guwahati.

He utilizes his expertise in catalysis (heterogeneous and homogeneous), organometallics and organofluorine chemistry to bring about; (i) Upgradation of light hydrocarbons and their derivatives to fuel grade chemicals. (ii) Utilzation of petrochemicals and alkanes to generate aromatics. (iii) Biomass conversion and transformation of waste biomass to value –added fine chemicals (iv) Greenhouse gas to fuels and fine chemicals (v) Synthesis of heteroatom and fluorine doped π-conjugated molecules for material applications (vi) Asymmetric catalysis The targets are achieved via pincer−metal-catalyzed C−H and C−F activation reactions for the synthesis of fuel chemicals and heteroatom- doped π-conjugated organic materials.

Dr. Akshai Kumar has about 18 years of experience in the area of organometallic chemistry, homogeneous catalysis and heterogenization of molecular catalysts. He has 52 research articles in peer-reviewed journals, including one in Chemical Reviews (Impact Factor = 54. 301) apart from 6 book chapters and 4 US patents (granted), 1 INDIAN patent (granted), 6 International patents (filed) and 6 INDIAN patents (filed). He has vast experience in using these organometallic compounds for homogeneous and heterogeneous catalysis. Career highlights include the development of efficient catalyst for transformation of waste to fuel and value-added chemicals. This includes conversion of unproductive hydrocarbons to fuel-grade chemicals, generation of green hydrogen, transformation of inexpensive glycerol to high value lactic acid and upgrading low-energy density ethanol to high-energy density fuels.

He is a member of Indian Young Academy of Science, Member of Bureau of Indian Standards, and fellow of the Indian Chemical Society. In addition to Associate Professor at the Department of Chemistry, currently, he is the Head, Centre for Nanotechnology at IIT Guwahati.

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Base Metal Catalysis for Generation of Hydrogen, Fuel & Specialty Chemicals

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Department of Chemistry, Indian Institute of Technology Guwahati,
Centre for Nanotechnology, Indian Institute of Technology Guwahati,
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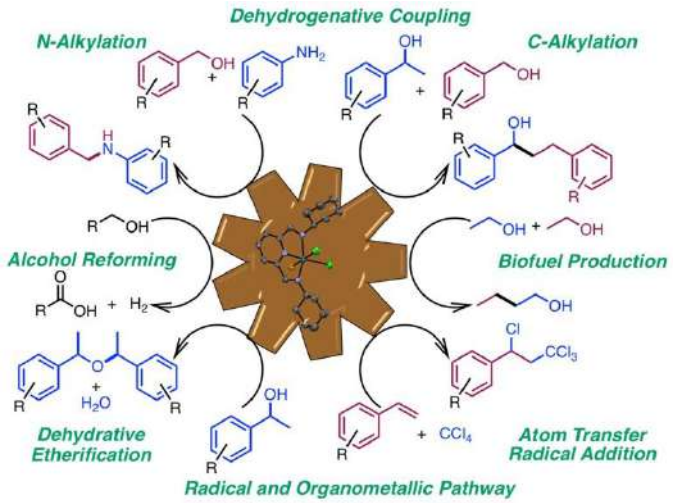
Organometallic complexes have enjoyed great success in catalyzing and/or mediating organic transformations which otherwise are not possible.[1] The ease of ligand synthesis along with the ability to tailor the functionalities and ligating atoms have led to a plethora of complexes with a wide variety of metals.[1] This has facilitated one, to pick complexes with desired steric and/or electronic parameters to suit their requirement. For efficient catalysis, it would be desirable to have a subtle balance between catalyst stability and reactivity.[1] In the past four decades, it has been more often found, that pincer-metal complexes perform exceedingly well in striking this balance.[2] Not surprisingly, pincer chemistry has grown in leaps and bounds ever-since the first report in 1976 by Moulton and Shaw,[3] and now pincer-metal complexes have been used in a myriad of applications promoting stoichiometric and catalytic transformations relevant to fuels, commodity chemicals and fine chemicals.[4] With a particular emphasis on base metals, the current flash talk would provide a glimpse on the pincer chemistry that is being investigated in our lab, while shedding light on their role in catalyzing C-H activation/functionalization of alcohols via radical/organometallic pathways that ultimately lead to synthesis of hydrogen, high value fuels and specialty chemicals starting from waste.[5]



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Bio-Sketch of Speaker

Dr. Indubhusan Deb
Principal Scientist, Associate Professor (AcSIR)

Organic and Medicinal Chemistry Division
CSIR-Indian Institute of Chemical Biology-Kolkata
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Contact Number: +91-9836297770
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Group webpage:
https://debchemgroup.wixsite.com/mysite/pi
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Dr. Indu Bhusan Deb obtained his M.Sc. in organic chemistry from Banaras Hindu University. He completed his Ph.D in 2008 at the Indian Institute of Technology Bombay (IITB) under the supervision of Professor I. N. N. Namboothiri. After that, he moved to Rutgers University, USA to conduct postdoctoral research with Professor Daniel Seidel, where he was involved in researching the synthesis of chiral heterocycles. After spending three years at Rutgers, he joined Professor Naohiko Yoshikai's group at Nanyang Technological University, Singapore, for his 2nd postdoctoral research. In April, 2013 He joined as a research investigator (Project leader) in the process chemistry division of Bristol-Myers Squibb Research center, Bangalore. Dr. Deb worked as a senior scientist in the Organic and Medicinal Chemistry division at CSIR-IICB, (Jan, 2014-2018). Dr. Deb is in the same division's Principal scientist and associate Professor (AcSIR). His research group is actively involved in asymmetric synthesis and designing synthetic methodology employing transition-metal–catalyzed C□H bond activation chemistry, metal-free reaction and Organo-electrosynthesis for the synthesis of potential bioactive small molecules.

Research Interests: (max 30 words)

Our research group has substantially contributed in the field of catalysis in the organic chemistry area (electrochemical synthesis/C-H bond activation/functionalization) to develop affordable, efficient, and innovative as well as industry-friendly synthetic processes for the synthesis of functionalized potential bio-active molecules such as Anthrone, Benoxazine, Benzosultam, Oxaziridine, acridine, as well as Benzofuranone, employing transition metal(free)-catalysis employing the concept of electrochemical synthesis and transition metal-catalyzed C–H/C–X bond activation and metal-free C–H/C–X bond functionalizations.

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

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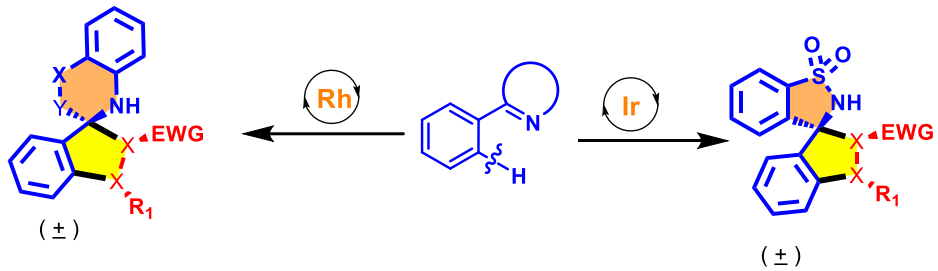
Abstract:

The ubiquitousness of dibenzoxazepines, benzazepines, benzoxazine, benzosultam, quinazolines, indoles and acridines in various natural products and pharmaceuticals make them immensely valuable heterocycles. Hence, the development of new and efficient methods for their synthesis and derivatization assumes high significance. Recently, we have developed several efficient and mild methodologies via direct and selective C-H functionalization employing the electrochemical, metal-catalyzed, and spiro-annulation reactions for synthesizing densely functionalized potential bioactive heterocycles. This fundamental research directed us to develop cost-effective processes for synthesizing commercially available drug molecules, which will be discussed during the presentation.



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[1] PATENT: 0163NF2021, 202111047806. PCT/IN2022/050940, 20 Oct, 2022.
[2] PATENT: 0211NF2020; 202111047809. PCT/IN2022/050931, 19 Oct, 2022.
[3] Deb, I. et al. *Chem. Commun*.2023, **59,**13899-13902
[4] Deb, I. et al. *Chem. Commun*.2023, **59,**9074-9077
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[6] Deb, I. et al. *Chem. Commun*.2022, **58**,2902-2905
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[8] Deb, I. et al. *Org. Lett.* 2020, 22, 1340-1344
[9] Deb, I. et al. *Org. Lett.* 2019, **21,** 2056-2059

Bio-Sketch of Speaker

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Dr. Debayan Sarkar is presently an Associate Professor of Chemistry at the Indian Institute of Technology Indore (IIT Indore). Before this he worked as an Associate Professor in the Department of Chemistry at National Institute of Technology, Rourkela, Odisha, India. He has completed his M.Sc with Organic Chemistry specialisation from University of North Bengal (NBU) in the year 2005 followed by a Ph.D in Organic Synthesis from Indian Association For The Cultivation of Science (IACS) in the year 2011, Jadavpur Kolkata under the supervision of Prof. R. V.Venkateswaran. After that he travelled to carry out his post-doctoral studies at Stanford University (USA) under the mentorship of Prof. Barry M Trost (2012-2013). He was recently deputed as a Visiting Senior Assistant Professor at Graduate School of Pharmaceutical Sciences, Tohoku University (Japan) under the mentorship of Prof. M. Yamaguchi (Dec 2015-March 2016). He was at the University of Leipzig Germany as a DAAD Research Professor with Prof. Christoph Schneider (2018-2019). He worked with Prof. Burkhard Koenig at University of Regensburg Germany as an ICMR International Fellow from Jan-Dec 2020. He has been recipient of prestigious awards like SERB TETRA Award, RC Tripathy Research Excellence Award by Orissa Chemical Society, DST Inspire faculty award (2013),BRNS-DAE Young Scientist Award (2014), Indo-US Research Award(2012), DAAD Visiting Professor (2018). Research interest includes Visible Light Catalysis, Asymmetric Dearomatisation reactions, Atom Economic couplings, Complex total synthesis of natural products. He has 60 research publications in International Journals of Repute, 2 Patents and guided 6 Ph.D students and 12 Ph.d students are presently undergoing their doctoral studies under his supervision. Presently, he is also heading the Centre for Rural Development and Technology (CRDT) at IIT indore.

Title: Solving Molecular Complexities with Visible Light Dearomatisation Reactions (VDRs)

Presenter(s) name:**Dr. Debayan Sarkar***
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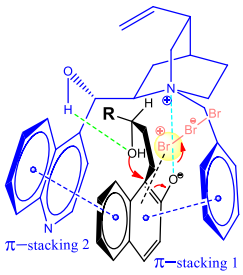
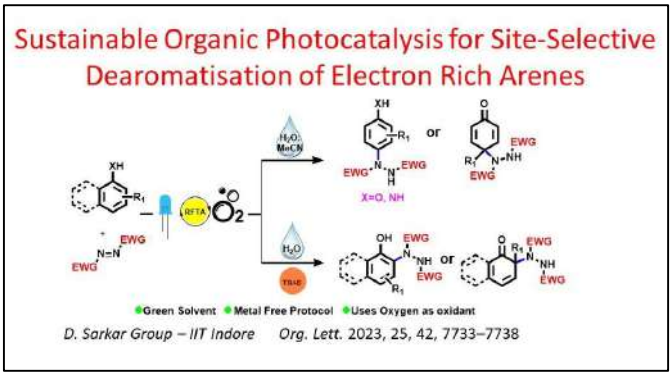
Abstract:

D earomative transformations has grasped immense attention of chemists and in this context, **Dearomatization** of arenols is considered to be the shortest and most powerful approach towards the construction of a range of molecular architectures from simple planar starting materials.We have been working on *intra*- or *inter*- Dearomative transformations. The talk will represent our journey from Tribromide based dearomatisations to visible light dearomatization of arenes from natural resources as a powerful strategy for the generation of three-dimensional molecular architectures.





References and Notes: D. Sarkar et. al.

Org. Lett 2023, 25, 7733; ChemSusChem 2024 (Just Accepted), J. Org. Chem 2023, 88, 13, 7977-7987; J. Org. Chem 2023, 88, 13, 7977-7987; *Chem Photo Chem 2023* 87, *(Accepted Article) doi/abs/10.1002/cptc.202200335*; *J. Org. Chem 2022*. 87, 21, 13529–13541; *J. Org. Chem 2022* 87, 15, 9729–9754; *J. Org. Chem* 2021, 86, 23, 16369-16395; *J. Org. Chem* 2022, 87, 15, 9729-9754; *J. Org. Chem* 2022, 87, 21, 13529-13541; *Asian Journal of Organic Chemistry* 2021, 10, 1786-1794; *Organic and Biomolecular Chemistry* 2020, *18*, 4619-4627; *European Journal of Organic Chemistry* 2020, 11, 1727-1731; *Tetrahedron Letters* ,2020 (cover page Article), 61, 151646; *European Journal of Organic Chemistry* 2020, 397-401; *European Journal of Organic Chemistry* 2020, 7, 891-896 ; *Organic Letters* 2019 21, 11, 4132-4136; *Advanced Synthesis and Catalysis* 2019, 361, 24, 5648-5653. (Most Downloaded Paper 2020)

Annulative π-Extension by Transition-Metal-Catalyzed Ketone-Directed *peri*-Annulation: En Route to Fused Arenes

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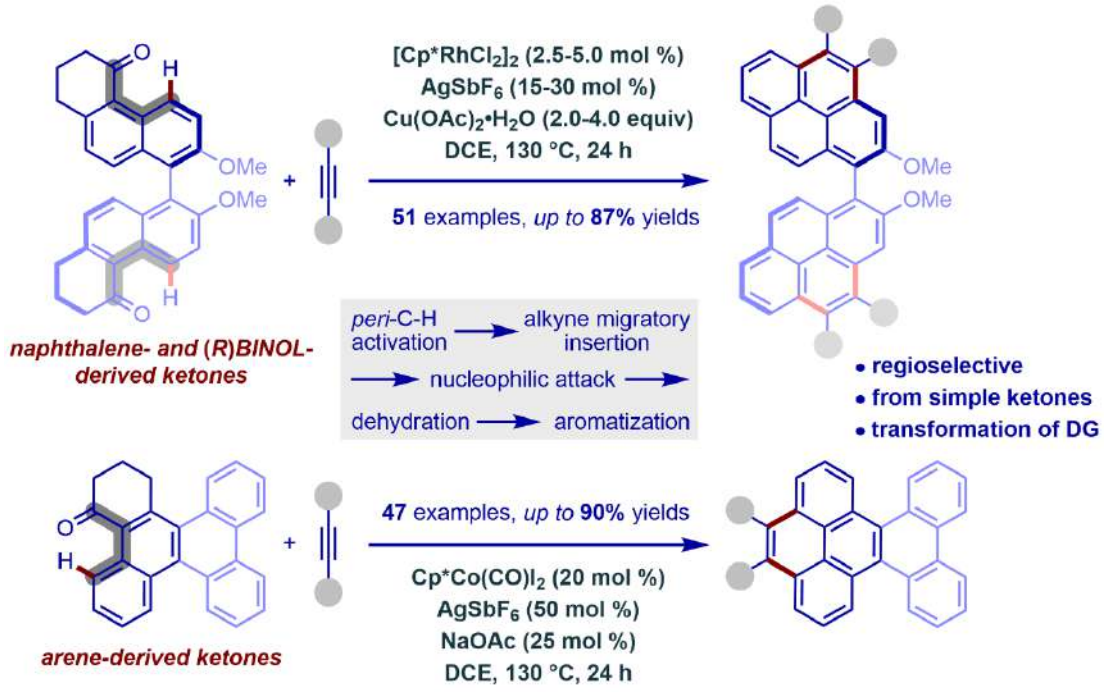
A proficient incognito bay-region selective transition-metal-catalyzed ketone-directed APEX reaction of arene-derived ketones is achieved to afford perplexing K-region functionalized benzo[*e*]pyrenes and pyrenes. This strategy comprises key steps like the formation of a six-membered metallacycle intermediate by *peri*-C-H activation, alkyne-1,2-migratory insertion, nucleophilic attack towards ketone, dehydration and aromatization. Furthermore, enantiopure axially-chiral naphthyl-pyrenes and 1,1′-bipyrenes are also accessed from the corresponding (*R*)-BINOL-derived ketones. Detailed DFT studies are incorporated to buttress the mechanistic pathway.



References: [a] H. Ito, K. Ozaki, and K. Itami. *Angew. Chem. Int. Ed*. **2017**, *56*, 11144. [b] M. R. Sk, A. Bhattacharyya, S. Saha, A. Brahma, and M. S. Maji. *Angew. Chem. Int. Ed*. **2023**, *62*, e202305258. [c] A. Bhattacharyya, M. R. Sk, S. Sen, S. Kundu, and M. S. Maji. *Org. Lett*. **2023**, *25*, 8622.

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Introduction: Dr. Bagdi is working as an Assistant Professor in the Department of Chemistry, University of Kalyani, India. His current research interest includes employment of visible light photocatalysis in synthesis and functionalization of bio-active heterocycles.

Academic Background:
B.Sc.: Visva-Bharati (2004-07) (First class with 3rd Rank)

M.Sc.: Visva-Bharati (2007-09) (First class)

Ph.D.: Visva-Bharati, (2009-2014); Supervisor- Dr. Alalkananda Hajra

Post-Doctoral Research: Okinawa Institute of Science and Technology, Okinawa, Japan

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Awards / Honors / Membership:
i. “2014 Eli Lilly & Company Asia Outstanding Thesis Award”.

ii. One year visiting researcher Contract from Okinawa Institute of Science and Technology, Okinawa, Japan (01/11/2017-31/10/2018).

iii. Post-doctoral Fellowship form Okinawa Institute of Science and Technology, Okinawa, Japan (2016-2017).

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Shinning Light on C-H Chalcogenation of Electron-Rich Heteroarenes

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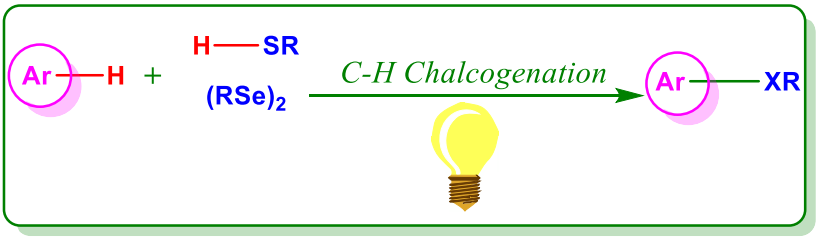
The development of new synthetic routes to heteraryl chalcogenides is a very important research area duo to their presence in a vast array of natural products and pharmaceuticals.[1] These derivatives have also wide applications in catalysis and material science. Among the various strategies for the synthesis of chalcogenated heterocycles, direct C-H chalcogenation is the most attractive one as it avoids the prefunctionalization step. It is a step-, time- and atom-efficient approach. As a consequence, efforts have been paid to synthesizing heteraryl chalcogenides via C-H chalcogenation and various catalytic systems like transition-metal catalysis, iodine catalysis, etc have been extensively employed for this purpose. Recently, visible-light-induced organic transformations have attracted the attention of chemists due to the use of renewable energy resources.[2] So, designing new protocols for the synthesis of chalcogenated heterocycles through C-H functionalization is highly desirable from the viewpoint of green chemistry.[3-4] We have successfully employed this strategy in chalcogenation of electron-rich heterocycles.[5-6] Some fascinating aspects observed during our efforts towards this light-promoted C-H functionalization will be discussed.



Scheme 1: Organophotocatalyzed C-H Chalcogenation.

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Dr. Koena Ghosh obtained her Ph.D. (2009, Prof. M. K Ghorai) from Indian Institute of Technology Kanpur, INDIA sponsored by a scholarship from Council of Scientific and Industrial Research, INDIA. After post doctoral research at Purdue University, USA (Prof. A. K Ghosh) and Indian Association for the Cultivation of Science, Kolkata, INDIA (Prof. A. Sarkar) she moved to Bangalore, INDIA with industrial position (team leader) at BMS Biocon R & D Centre at Syngene Intl. Ltd. Since 2013, she is Assistant Professor at the Department of Chemistry, Presidency University, Kolkata, INDIA. Her research interest includes development of new methods exploiting sustainable, catalytic chemistry, their mechanistic investigations and application in synthesis of bioactive pharmacophore.

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Synthesis and application of biologically relevant azoles and indoles

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Design and synthesis of new organic compounds suitable for application in technology or medicinal purpose is prime focus of modern organic chemistry research. In this domain, development of new molecules containing *N*-heretocyclic core is typically advantageous from application point of view. Often, they play crucial role in regulating various biological processes that are relevant for the maintenance of life. Among *N*-heterocycles, azoles and indoles are privileged substructures owing to their wide occurrence in a large number of natural products, bioactive compounds and materials of industrial relevance.[1-3] Consequently, design of new molecules incorporating appropriate functionalities to various *N*-heterocycles e.g. pyrazolines, pyrazoles, indoles, indolines etc. is advantageous from medicinal chemistry point of view[4].

Recently, we have synthesized a series new ferrocenyl-pyrazolines, pyrazoles, cyclopenta[*b*]indoles etc. following simple approach. Anticancer activity of various ferrecene-azole hybrid compounds are tested and compared with their aryl analogue against MB 231 breast cancer cell line.[5-7]

References:

[1] A. J. Kochanowska-Karamyan and M. T. Hamann, *Chem. Rev.*, **2010**, *110*, 4489.

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[7] K Ghosh, K. Singha; D. Mallick. (*submitted).*

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Dr. Chatterjee is working as an Associate Professor in the Department of Chemistry, National Institute of Technology Durgapur, India. His current research interest includes catalysis in homogeneous and heterogeneous media.

Academic Background:

B.Sc.: Ramakrishna Mission Vidyamandira (2000-03), under University of Calcutta

M.Sc.: University of Calcutta (2003-05)

Ph.D.: Indian Institute of Technology Kharagpur (2006-2012); Supervisor- Prof. Sujit Roy and Prof. Manish Bhattacharjee

Exploring the Lability of 2,4,6-Trimethoxyphenyl Moiety in Allylic/Benzylic Systems under Acidic Conditions

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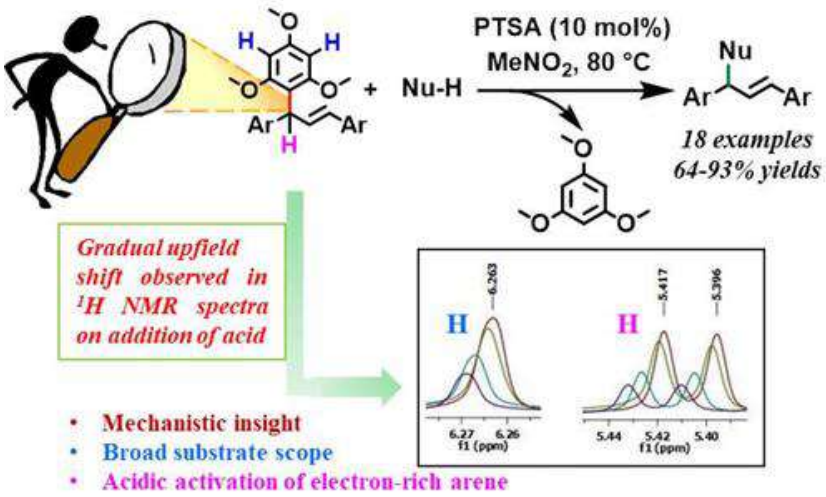
An investigation of the readily cleavable C_{sp3}–C_{sp2} bond connecting 2,4,6-trimethoxyphenyl group and an allylic moiety is carried out. We observed that the catalytic presence of either Lewis or Brønsted acid can render such 2,4,6-trimethoxyphenyl group labile. Several nucleophiles were found to substitute the labile C–C bond in mild reaction conditions resulting in very good yields of the allylated product. Even in the absence of a nucleophile, intramolecular cyclization of the parent substrate under acidic activation caused the labile C–C bond to cleave. A major motivation of this study is to understand the activation of electron-rich arene in acidic medium, employing 1,3,5-trimethoxybenzene as a case study. A plausible mechanism is proposed after carrying out several control reactions as well as UV-vis and ^{1}H NMR spectroscopic studies. This work provides an insight into the activation of electron-rich arenes in acidic medium while also adding a conceptually novel C–C bond breaking approach to the vast literature of allylation of arenes.



Scheme 1. C–C bond cleavage in acidic condition

References: [a] D. Paul, P. N. Chatterjee*, *Eur. J. Org. Chem.* **2020**, *2020* (30), 4705-4712.

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

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

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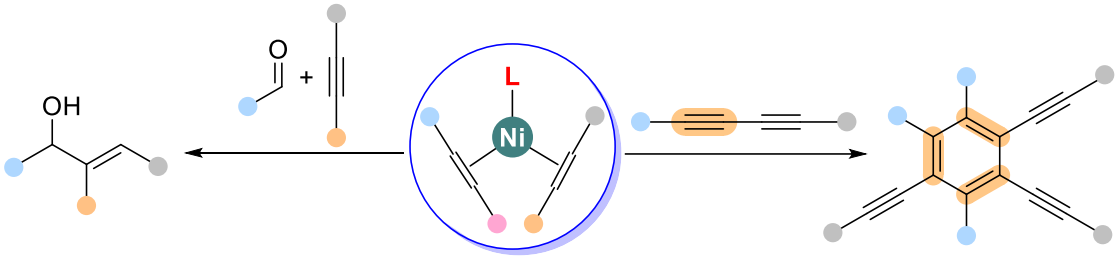
Nickel (0) complexes have been traditionally stored and used under highly controlled environments. Our research focuses on bringing sensitive nickel chemistry to the benchtop. We have demonstrated the potential of Schrauzer's Ni(COD)(Duroquinone),[1] an air-, and moisture-stable Ni0 complex as a catalyst for the reductive coupling of aldehydes and alkynes.[2] Control experiments revealed the exceptional bench stability of Ni(COD)(DQ) under ambient conditions for >200 days. The infrastructural cost associated with a glove box for storing and handling $Ni(COD)_2$ is avoided. A wide range of aromatic and aliphatic aldehydes/alkynes furnished the desired silyl allyl ethers in excellent yields and regioselectivities. Further, we demonstrated a regioselective [2 + 2 + 2] cyclotrimerization of 1,3-diynes catalyzed by Ni0 to provide hexasubstituted benzenes (HSBs). HSBs have significant applications as functional materials and pharmaceuticals. The present protocol exhibited remarkable versatility, transforming 1,3-diynes with diverse alkyl, aryl, and heterocyclic groups to the corresponding HSBs. With the help of control experiments and density functional theory (DFT), the mechanism of the reaction and the origin of regioselectivity were elucidated.



Chem. Commun. **2023**, 11141 *Org. Lett.* **2024**, 792

References:

[1] Schrauzer, G. N.; Thyret, H. *Naturforsch.* **1962**, *17*, 73-76.
[2] Tran, V. T.; Li, Z.-Q.; Apolinar, O.; Derosa, J.; Joannou, M. V.; Wisniewski, S. R.; Eastgate, M. D.; Engle, K. M. *Angew. Chem. Int. Ed.* **2020**, *59*, 7409-7413.
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Dr. Basudev Sahoo completed his BSc in chemistry from the Ramakrishna Mission Residential College, affiliated to the University of Calcutta in 2009 and MSc in Chemistry from the Indian Institute of Technology (IIT) Kanpur in 2011. Then, he moved to Germany to pursue his PhD under the supervision of Prof. Frank Glorius at the University of Muenster. After completing his PhD in 2015, he moved to the group of Prof. Matthias Beller at the Leibniz Institute for Catalysis (LIKAT), Rostock, Germany as a Leibniz Postdoctoral Fellow. In 2018, he received Marie Curie (MSCA) postdoctoral fellowship and joined the group of Prof. Ruben Martin at the Institute of Chemical Research of Catalonia (ICIQ), Tarragona, Spain. Since March 2020, he is holding a position of assistant professor in the school of chemistry, IISER Thiruvananthapuram. He was one of the recipients of Thieme Chemistry Journals Award 2022 from the Thieme Verlag, Germany. He is a member of the Chemical Research Society of India (CRSI), India. His group is pursuing research on organic synthesis and catalysis enabled by transition metal catalysis and visible photocatalysis.

Alkylboration of Benzylidenecyclopropanes: Access to Csp^3-Enriched Cyclopropyl Boronic Esters

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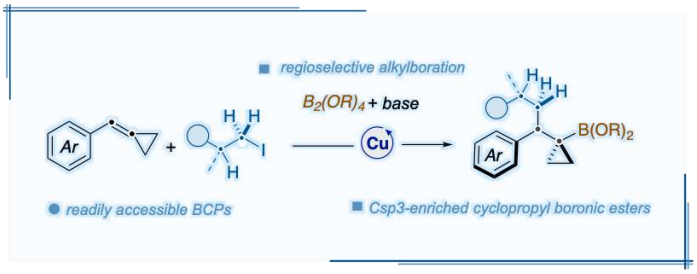
Organoboron compounds have received vast prominence as carbon nucleophile and radical progenitor in C-C/C-X bond forming transformations, hinging upon their innate reactivity, stability, and easy handling.[1] Catalytic alkylboration of alkenes represents a modular and efficient technique to construct organoboron building block, elaborating core carbon-skeleton through Csp^3-Csp^3/sp^2 linkage, alongside the decoration of boron functionality *via* B-Csp^3 bond formation.[2] A regioselective 1,2-alkylboration of versatile (hetero)benzylidenecyclopropanes with □-H containing alkyl iodides and bis(pinacolato)diboron, enabled by copper catalysis.[3] This three-component method allows for consecutive B-Csp^3 and Csp^3-Csp^3 bond formation to access Csp^3-enriched diverse tertiary cyclopropyl boronic esters with broad functionality tolerance and so-formed C-B bond is amenable to further structural diversification. Experimental studies and DFT calculation suggest for a polar mechanism rather than radical manifold, and nucleophilic substitution-type C-C bond formation was found to be rate-limiting step, instead of migratory alkene insertion.



Scheme 1. Alkylboration of BCPs with alkyl iodides enabled by copper catalysis

References:

[1] (a) J. W. B. Fyfe, A. J. B. Watson, *Chem* **2017**, *3*, 31-55; (b) J. Hu, M. Ferger, Z. Shi, T. B. Marder, *Chem. Soc. Rev.* **2021**, *50*, 13129; (c) S. Mondal, K. K. Das, S. Panda, *Chem. Asian J.* **2022**, *17*, e202200836. (d)

[2] (a) D. Hemming, R. Fritzemeier, S. A. Westcott, W. L. Santos, P. G. Steel, *Chem. Soc. Rev.* **2018**, *47*, 7477; (b) Z. Liu, Y. Gao, T. Zeng, K. M. Engle, *Isr. J. Chem.* **2020**, *60*, 219. (c) A. Whyte, A. Torelli, B. Mirabi, A. Zhang, M. Lautens, *ACS Catal.* **2020**, *10*, 11578. (d) E. Rivera-Chao, L. Fra, M. Fañanás-Mastral, *Synthesis* **2018**, *50*, 3825.

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

Selected Publications:

1. M. Baidya, J. Dutta, **S. De Sarkar***, *Org. Lett.* **2023**, *25*, 3812.
2. K. Mahanty, S. K. Saha, A. Halder, **S. De Sarkar***, *Chem. Commun.* **2023**, *59*, 4467.
3. M. Baidya, D. Maiti, L. Roy*, **S. De Sarkar***, *Angew. Chem., Int. Ed.* **2022**, *61*, e202111679. **(Hot Paper)**
4. M. Baidya, S. Mallick, **S. De Sarkar***, *Org. Lett.* **2022**, *24*, 1274.
5. S. K. Parida, T. Mandal, S. Das, S. K. Hota, **S. De Sarkar*** and S. Murarka* *ACS Catal.* **2021**, *11*, 1640.
6. **S. De Sarkar***, *Angew. Chem., Int. Ed.* **2016**, *55*, 10558.

Awards/Achievements:

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

Electric Shock to Enamines: Facts and Findings

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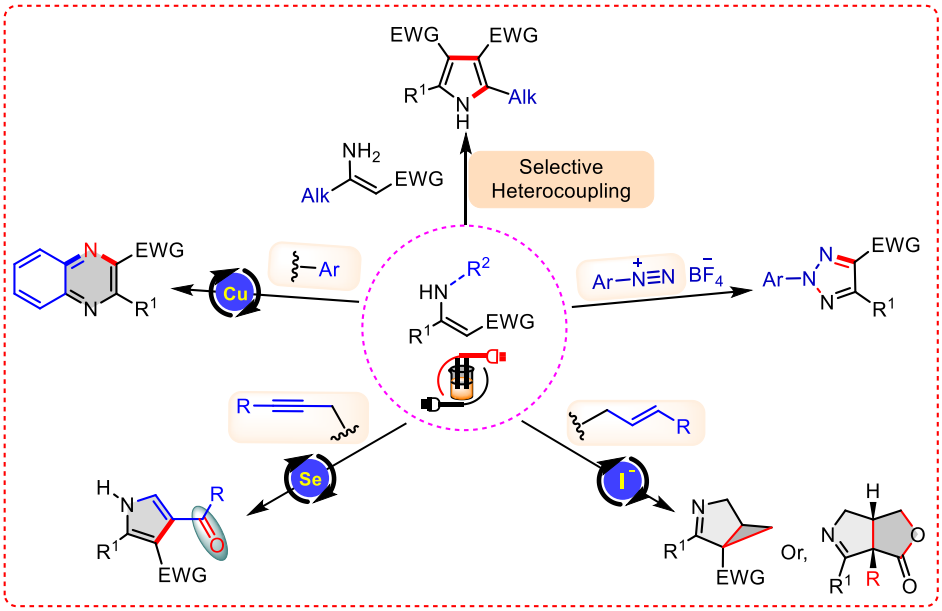
Enamines, with their nucleophilic and electrophilic properties, play a crucial role as synthons in synthesizing a diverse range of heterocycles.[1] Electrolysis of such versatile functionality unfolds further opportunities in synthesizing valuable scaffolds. The introduction reveals an electrochemical strategy tailored for efficiently synthesizing NH-pyrroles with unsymmetrical substitutions. This involves a proficient heterocoupling of aryl- and alkyl-substituted enamines.[2] The second part delves into the construction of N^2-aryl 1,2,3-triazoles through sequential C–N bond formation and electro-oxidative N–N coupling.[3] The final segment highlights the effectiveness of electrocatalysis in azidation or alkyne/alkene activation, enabling access to structurally significant heterocycles or azabicyclic scaffolds.[4]



Scheme 1. *Electrosynthetic derivatizations of enamines.*

References:

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12. *a) Baidya, M.; Dutta, J.; De Sarkar, S. Org. Lett.* ***2022****, 20, 3812. b) Baidya, M.; De Sarkar, S. Org. Lett.* ***2022****, 20, 3812. c) Baidya, M.; De Sarkar, S. - Unpublished.*

Bio-Sketch of Speaker

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Academic and professional career:

(2022-2023):	SERB-visiting faculty with Prof. F.P Gabbai at Texas A&M University, USA
2017-till date:	Assistant Professor, Jadavpur University.
(2015-2017):	DST-Inspire Faculty, NIT Rourkela.
(2014-2015):	Senior Research Associates (IISER-Kolkata, India).
(2012-2014):	Postdoctoral Research Fellow (TU Dresden, Germany).
(2007-2012):	Ph.D (Indian Institute of Technology Madras, India).
(2006-2007):	Assistant Research Scientist, Advinus Therapeutics Pvt. Ltd.; A TATA Enterprise, Bangalore, India.
(2004-2006):	M.Sc.; University of Calcutta, India
(2001-2004):	B.Sc.; (Ramakrishna Mission Vidyamandira, Belur, University of Calcutta).

Research interest

- Fabrication and development of dithienylethene (DTE) based organic materials and their applications in security technologies, catalysis, and controlled singlet oxygen generation.

- Our principal aim is to develop strategies for synthetically important organic transformations like C-C, C-X (X = O, S, N, etc.) bond formation by C-H activation using earth-abundant and cheap transition metals (mostly Cu and Co) as homogenous catalysts.

Cu(II) promoted C(sp^3)-H activation in unactivated cycloalkanes: Oxo-alkylation of styrenes to synthesize □-disubstituted ketones

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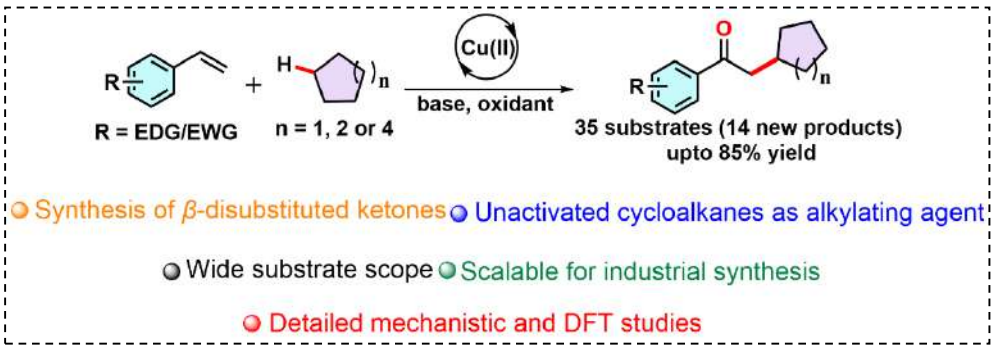
□-disubstituted ketones form a class of synthetically important building blocks, which are widely used as industrial solvents, and in the construction of pharmaceuticals. They are known to be synthesized by using either expensive and presynthesized Ru/Ir complexes, or low-cost metal complexes (*e.g.*, Fe, Mn) with activated species like aldehyde, acid, alcohol, or phthalimide derivatives as the alkylating agent, however, use of unactivated cycloalkanes directly as the alkylating agent *via* functionalization of electron-rich C(sp^3)-H bond remains challenging. We present here the Cu(II) catalyzed synthesis of □-disubstituted ketones from styrene *via* oxo-alkylation with unactivated cycloalkanes as the alkylating agent for the first time in presence of *tert*-butylhydroperoxide (TBHP) and 1-methylimidazole as oxidant and base respectively. The reduction potential of Cu(II)/Cu(I) couple (0.15 V vs SCE) greatly assists in the generation of peroxide radical from TBHP, which advances the mechanism of oxo-alkylation, followed by the action of base to give the final product *via* two sequential hydrogen atom transfer (HAT) mechanisms. A wide range of aliphatic C−H substrates as well as various olefinic arenes and heteroarene (35 substrates including 14 new substrates) are well-tolerated in this method. Hammett analysis shed more light on the substitution effect in the olefinic part on the overall mechanism. Furthermore, the controlled experiments, kinetic isotope effect study, and theoretical calculations (DFT) enable us to gain deeper insight of mechanistic intricacies of this new simple and atom-economic methodology.



Scheme 1. Oxoalkylation of styrenes with cycloalkanes to give □-disubstituted ketones.

References: [a] K. M. Das, A. Pal, L. Surya T, L. Roy, A. Thakur, *Chem. Eur. J.* **2024**, *30*, e202303776. [b] K. M. Das, A. Pal, N. N. Adarsh, A. Thakur, *Org. Biomol. Chem.* **2022**, *20*, 3540-3549. [c] S. Thiyagarajan, R. V. Sankar, C. Gunanathan, *Org. Lett.* **2020**, *22*, 7879−7884. [d] D. Bhattacharyya, B. K. Sarmah, S. Nandi, H. K. Srivastava, A. Das, *Org. Lett.* **2021**, *23*, 869−875. [e] C. -S. Wu, Rong Li, Q. -Q. Wang, L. Yang, *Green Chem.* **2019**, *21*, 269-274.

Bio-Sketch of Speaker

Ranjan Jana

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Research Interest

Synthetic Organic Chemistry, Green Chemistry, Catalysis, Medicinal Chemistry and Chemical Biology

Academic Qualifications and Professional Training

(i) B. Sc.; Midnapore College; **2000**; Chemistry (H).

(ii) M.Sc.; Vidyasagar University; **2002**, Organic Chemistry.

(iii) Ph.D.; Indian Association for the Cultivation of Science (IACS); **2007**; Green Chemistry with Prof. B. C. Ranu.

(iv) Postdoctoral Research I; Bar-Ilan University, Israel, **2007-2008** with Prof. S. Braverman; Organoselenium Chemistry.

(v) Postdoctoral Research II; Kansas University, USA, **2008-2010** with Prof. J. A. Tunge; Decarboxylative coupling, hydroformylations in CXL.

(vi) Postdoctoral Research III; University of Utah, USA, **2010-2012** with Prof. M. S. Sigman; Alkene difunctionalization, breast cancer research.

Awards and Fellowships

(i) Fellow of the West Bengal Academy of Science and Technology (WAST), 2020

(ii) Ramanujan fellowship; award no. SR/S2/RJN-97/2012; SERB, India, 2013-2019

Member of Learned Societies

(i) Member of the West Bengal Academy of Science and Technology (WAST).
(ii) Member of American Chemical Society (ACS).
(iii) Member of Chemical Research Society of India (CRSI).

Molecular Diversity via Switchable 1,2-Shift in C-H Activation Cascade

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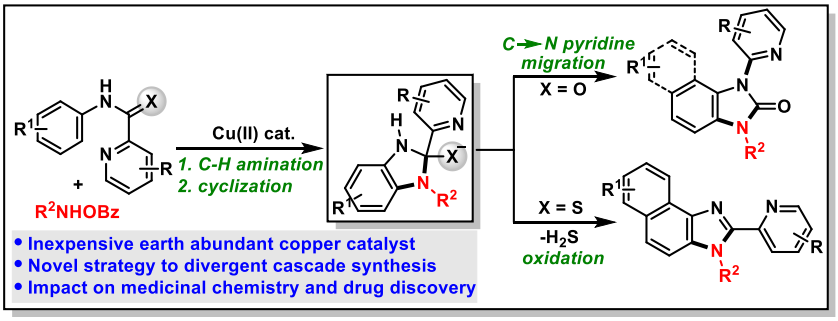
Despite a plethora of organic reactions that are available in the synthetic arena, a hand-picked number of reactions are used in the medicinal chemistry. The Suzuki reaction for carbon-carbon bond formation and the Buchwald-Hartwig reaction for carbon-nitrogen bond formation are among the top five organic transformations practiced in the pharmaceutical industry. However, both of these reactions are catalysed by highly expensive and depleting palladium catalyst which is not only economically unviable but also residual metal contamination brings toxicity to the finished product. Hence, at the threshold of an era of automated organic synthesis, artificial intelligence and environmental concern, we are geared to streamline the chemical synthesis in a semi-automated cascade manner integrated with green chemistry concepts. We have created a niche area of cascade C-H activation for the synthesis of bioactive natural products and late-stage functionalization where multiple C-H bond activation take place simultaneously in a single operation. This concept has tremendous potential to achieve molecular complexity; chemical methodology and library development (CMLD) for the structure activity relationship (SAR) studies in drug discovery. We have accomplished practical syntheses of indole, indoline, carbazole, fused-2-quinazolones, imizazole moieties and commercial drug candidates such as mefenamic acid, omeprazole a block buster proton pump inhibitor etc. Interestingly, we have developed synthetic methodology for the late-stage modification of amino acids via C-H activation to generate unnatural amino acids. We have developed a controllable 1,2-shift strategy as a switch for the divergent synthesis of molecular structure. This concept will translate into the process development of Boscalid and Glufosinate off-patent agrochemicals for the agricultural sector in India. The present talk is focused on the journey from metal to metal-free switchable divergent and cascade synthesis of privileged medicinal scaffolds.



1. Begam, H. M.; Nandi, S.; Jana, R.* *Chem, Sci*. **2022**, 13, 5726-5733.
2. Nandi, S.; Mondal, S.; Jana, R.* *iScience,* **2022**, *25*, 104341.
3. Begam, H. M.; Chowdhury, R.; Behera, A.; Jana, R. *Org. Lett.* **2019**, 21, 4651-4656.
4. Manna, K.; Ganguly, T.; Baitalik, S.*; Jana, R.* *Org. Lett.* **2021**, *23,* 8634–8639.

Bio-Sketch of Participant

Dr. Kiran Kumar Pulukuri

Assistant Professor
Department of Chemistry
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Dr. Kiran is working as an Assistant Professor in the Department of Chemistry, IISER-Tirupati, India. His current research interest includes Total Synthesis of Natural Products, Synthetic Methodology, Asymmetric Catalysis, Electro Organic Synthesis and Natural Product based Drug Discovery.

Academic Background:

B.Sc.: Osmania University (2002-05) (First class)

M.Sc.: Pondicherry University (2007-09) (First class)

Ph.D.: CDRI-Lucknow (2007-2013); Supervisor- Prof. Tushar Kanti Chakraborty.

Post-Doctoral Research: Rice University, Houston, USA

(2013–2019) With Prof. K. C. Nicolaou

CSIR-HRDG NET: CSIR (Dec, 2007)

GATE: AIR-96 (2007)

Awards / Honors / Membership:

1. “2014 Eli Lilly & Company Asia Outstanding Thesis Award”.

2. Early Career Advisory Board member, ChemMedChem

Website:
https://www.iisertirupati.ac.in/oldwebsite/faculty/kiran/kiran_lab_website/home.html

Total Synthesis of Eudesmane Sesquiterpenes through Site-selective Olefine Functionalization Strategy

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

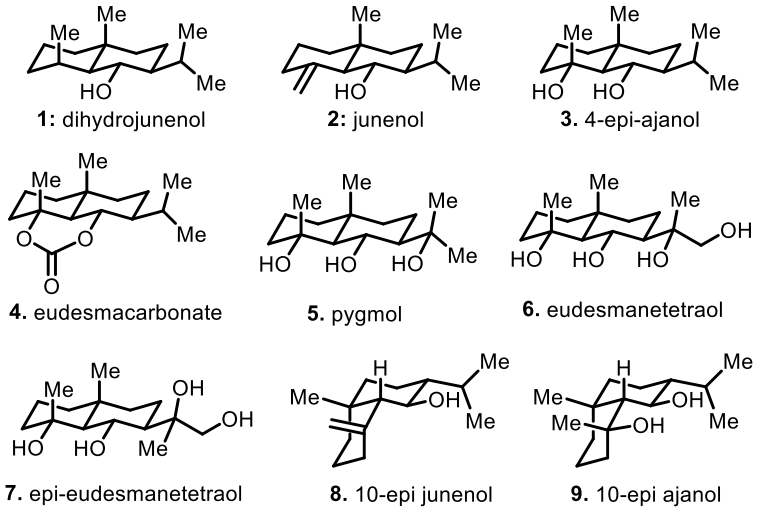

Fig. 1: Chemical Structures of Eudesmane sesquiterpens **1**-**9**.

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

Poster Presentation

Poster Presentation (PP-01)
International Conference on Emerging Trends in Catalysis & Synthesis (IC-ETCS 2024)

Catalytic Generation of Remote C–N Axial Chirality through Atroposelective *de novo* Arene Construction

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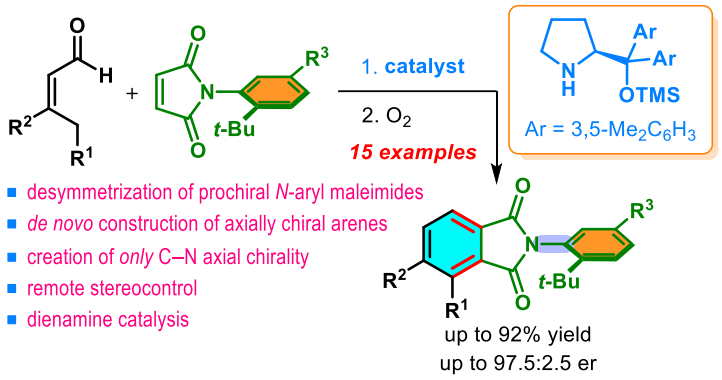
(Email: sm@iisc.ac.in)

Abstract: Axial chirality arising out of restricted rotation around the C–N has witnessed renewed interests in the past few decades due to application of these compounds in areas chemistry and biology.[1] A *de novo* arene construction technique is used to create the first atroposelective desymmetrization of prochiral *N*-aryl maleimides by its conversion to axially chiral phthalimides.[2] A [4+2]-cycloaddition[3] of prochiral *N*-aryl maleimides with unsaturated aldehydes, followed by a DABCO promoted aromatization under oxygen atmosphere, makes up the operationally straightforward technique. Catalyzed by bis(3,5-dimethylphenyl)prolinol TMS-ether, this reaction proceeds via dienamine intermediate[4] to generate a chiral C–N axis remote from the reaction sites with good yields (up to 92%) and excellent enantioselectivity (up to 97.5:2.5 er).



References

1) (a) Perreault, S.; Chandrasekhar, J.; Patel, L., *Acc. Chem. Res.* **2022**, *55*, 2581. (b) Mei, G.-J.; Koay, W. L.; Guan, C.-Y.; Lu, Y., *Chem* **2022**, *8*, 1855.

2) Mondal, S.; Mukherjee, S., *Org. Lett.* **2022**, *24*, 8300

3) Jeon, B.-s.; Wang, S.-A.; Ruszczycky, M. W.; Liu, H.-w., *Chem. Rev.* **2017**, *117*, 5367.

4) Ramachary, D. B.; Reddy, Y. V., *Eur. J. Org. Chem.* **2012**, *2012*, 865. (b) Jensen, K. L.; Dickmeiss, G.; Jiang, H.; Albrecht, Ł.; Jørgensen, K. A., *Acc. Chem. Res.* **2012**, *45*, 248.

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Poster Presentation (PP-02)
International Conference on Emerging Trends in Catalysis & Synthesis (IC-ETCS 2024)

Novel Bifunctional NHC Catalyzed Asymmetric Intramolecular Conjugate Addition via Non-covalent Interaction

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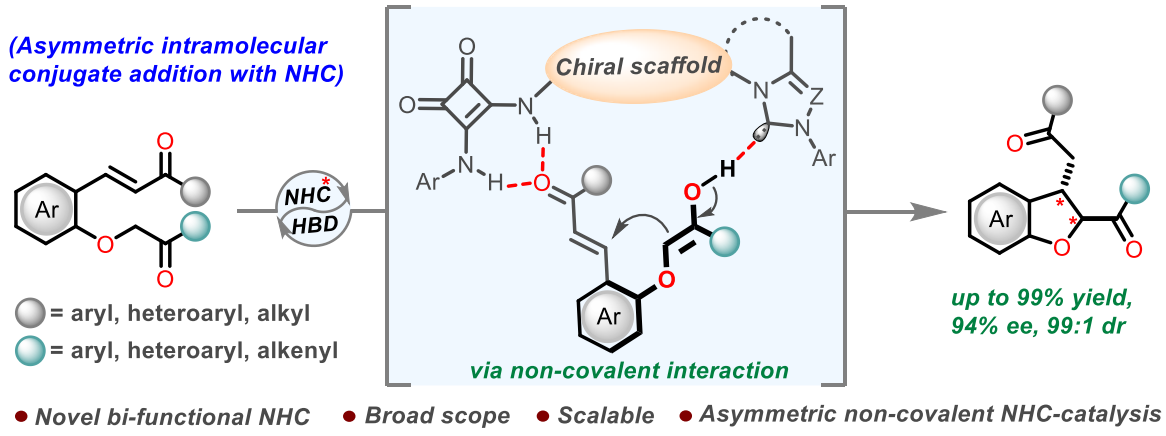
NHCs are well-appreciated in organic synthesis as a versatile organocatalyst.[1] Although, asymmetric NHC catalysis is largely dominated by substrate/NHC covalent interaction, the interest in developing new asymmetric transformations utilizing the non-covalent mode of NHC-catalysis is constantly rising. There are few reports on asymmetric intermolecular polar conjugate additions with non-covalent NHC-catalysis.[2] However, the utilization of non-covalent NHC catalysis in developing asymmetric intramolecular conjugate addition that provides rapid access to enantioenriched carbo(hetero)cyclic compounds remains a challenge. Recently, we have developed a novel chiral bifunctional NHC that catalyzes an intramolecular conjugate addition reaction with a high level of enantioinduction through the concurrent activation of substrate possessing both nucleophile and electrophile via non-covalent interaction. Using the newly designed squaramide containing bifunctional NHC as a catalyst, the reaction proceeds through a well-organized transition state thereby affording various functionalized dihydrobenzofurans with good ees and drs.[3] In the poster presentation, studies of reaction development, substrate scope evaluation and reaction mechanism will be discussed in detail.



References:

[1] D. M. Flanigan, F. Romanov-Michailidis, N. A. White, T. Rovis, *Chem. Rev.* **2015**, *115*, 9307-9387.
[2] a) J. Chen, Y. Huang, *Sci. China Chem.* **2016**, *59*, 251-254; b) U. Maji, B. D. Mondal, J. Guin, *Org. Lett.* **2023**, *25*, 2323-2327; c) B. D. Mondal, S. Gorai, R. Nath, A. Paul, J. Guin, *Chem. – A Eur. J.*, *n/a*, e202303115.
[3] *Manuscript submitted for publication.*

Poster Presentation (PP-03)
International Conference on Emerging Trends in Catalysis & Synthesis (IC-ETCS 2024)

Phosphonium Ion Tethered Secondary Amines for Chemospecific 5-*Enolexo* Aldol Condensations of 6-Ketoaldehydes

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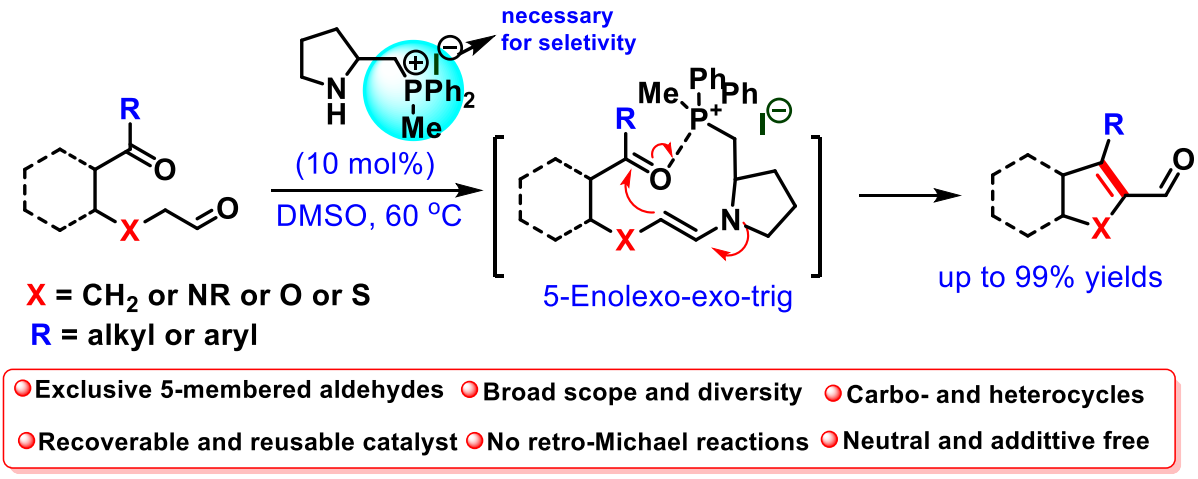
A novel and highly selective 5-enolexo-exo-trig aldol condensation of 6-ketoaldehydes is presented using a prolinebased alkylphosphonium ion catalyst. Bulky and oxophilic phosphonium ion plays a vital role in facilitating kinetic aldenamine formation and activating keto groups for aldol addition. This innovative approach exclusively targets five-membered carbo- and heterocyclic aldehydes, involving unusual aldehydes as donors and ketones as acceptors. Especially, enolizable aryl keto aldehydes and heteroatom-embedded ketoaldehydes exclusively produced cyclized products with our new catalyst, while other catalysts provided predominantly self-aldol or decomposed products. The scope and diversity of the method demonstrated by synthesizing different carboxaldehydes, including cyclopentene, indene, dihydrofuran, benzofuran, dihydropyrrole, indole, thiofuran, dihydrothiofuran, and benzothiofurans.



Scheme 1. Synthetic scheme of cyclopentene aldehydes.

References:

[a] Wolinsky, J.; Slabaugh, M. R.; Gibson, T. *J. Org. Chem.* **1964**, *29*, 3740-3742.

[b] Akash,S.; Aparna, V. M.; Rajendar, G*, *J. Org. Chem.* **2023**, *88*, 17472-17478.

A Toolbox Approach on Developing Carbazole-Cored Organo-Photocatalysts to Unveil Reductive Synthetic Transformations

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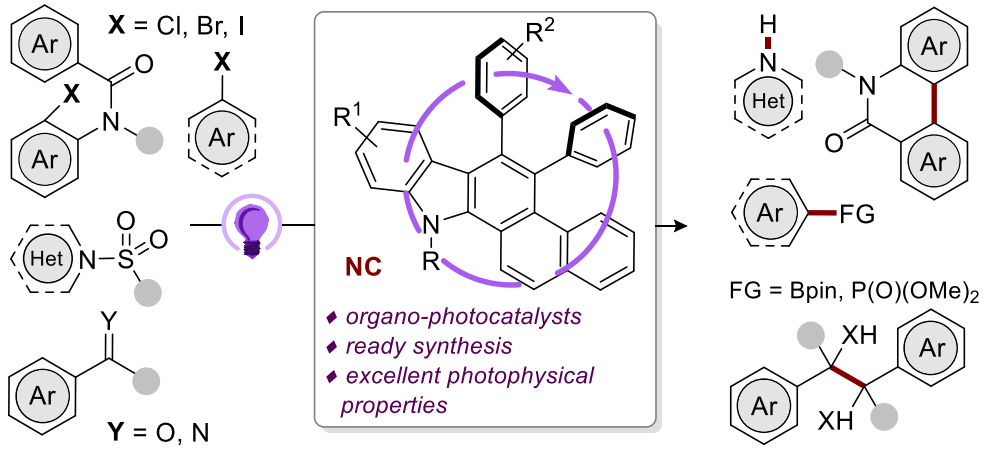
Recent advancement in photoredox catalysis offer to reshape synthetic transformations in a general catalytic platform by activating inert substrates comprising of strong covalent bonds and low reduction potentials under mild reaction conditions.[1] Concerning on availability of versatile organic photocatalysts, choice of specific one with strong reducing properties has been evolved as continuous interest to rationalize challenging catalytic transformations.[2] Herein, readily accessible naphthocarbazole derivatives (NCs)[3] have been reported as unique series carbazole-based organo-photocatalysts in reductive synthetic transformations. Judicial structural variants with detailed photophysical characterizations (E^*_{ox} = -1.75 V to -2.14 V vs SCE , τ = 5.6 to 7.1 ns) modulate their success as strong photoreductant upon excitation with visible light (390 nm) and able to show as sustainable replacement of precious metal photocatalysts by unlocking photocatalytic organic transformations. The NCs have been evaluated in potentially challenging and mechanistically distinct benchmark reactions such as, reductive dehalogenations, borylations, phosphorylations with a high functional group tolerance. Efficient reductive coupling in eminent pinacol and imino-pinacol[4a] type reactions as well as base-assisted chemoselective reductive desulfonylation[4b] from heteroaromatics also demonstrate their potential utility. Furthermore, reasonable excited state potentials trigger to utilize NCs in photocatalytic intramolecular dehydrohalide reductive coupling for C-C bond formation reactions and outperform their potential applicability towards new mechanistic manifolds in the field of photocatalysis.



References:
[1] C. K. Prier, D. A. Rankic, D. W. C. MacMillan *Chem. Rev*. **2013**, *113*, 5322−5363.
[2] N A Romero, D A. Nicewicz *Chem. Rev*. **2016**, *116*, 10075−10166.
[3] S. Kundu, A. Banerjee, S. C. Pal, M. Ghosh, M.S. Maji *Chem. Commun.*, **2021**, *57*, 5762.
[4] (a) S. Kundu, L. Roy, M. S. Maji *Org. Lett*., **2022**, *24*, 9001-9006, (b) S. Kundu, M. S. Maji **2023** (*manuscript submitted*)

Triplet Excited Nitroarene Converts Linear Alkynes to Bent Ketones by Deleting a Carbon Atom

Anirudh Dixit,# Sayan K. Jana#, Ayan Jati#, Animesh Das#, Pramod Kumar#, **Purusattam Dey**#, Netai Aditya, Koushik Sarkar, and.Biplab Maji*

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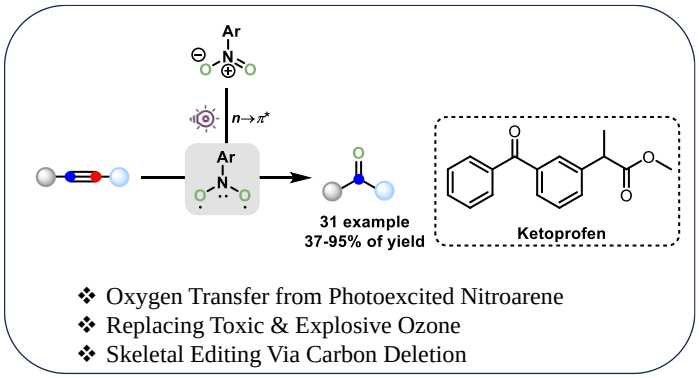
Alkynes are infrequently changed by molecular editing methods with visible light catalysis. In this work, we converted bent ketone fragments from linear alkyne topology using triplet excited nitroarenes. Concurrently, an oxygen atom is inserted and a carbon atom is deleted during the process. This approach is effective and broadly applicable based on its successful application to a variety of substrates (31 examples), compatibility with different functionalities and the modification of bioactive molecules, scalability in large-scale synthesis in continuous flow, and synthesis of drug molecules that are commercially available. Studies using UV-vis spectroscopy revealed how visible light stimulates nitroarene in its triplet form. Using a variety of kinetic and control tests, preliminary mechanistic investigations were able to identify ketene and nitrosoarene as important intermediates. The deleted carbon is released as CO and CO_2 gases.



Scheme 1. xx

References: [a] A. Dixit, S. K. Jana, A. Jati, A. Das, P. Kumar, P. Dey, N. Aditya, K. Sarkar, B. Maji* ChemRxiv. 2023; doi:10.26434/chemrxiv-2023-t1cvq. [b] A. Ruffoni, C. Hampton, M. Simonetti* and D. Leonori* *Nature* **2022**, *610*, 81.

Poster Presentation (PP-06)
International Conference on Emerging Trends in Catalysis & Synthesis (IC-ETCS 2024)

Organocatalysed one-pot three component synthesis of 3,3′-disubstituted oxindoles featuring an all-carbon quaternary center and spiro[2Hpyran-3,4′-indoline]

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Chemical Engineering and Process Development Division, CSIR-National Chemical Laboratory, Pune, India-410 008.
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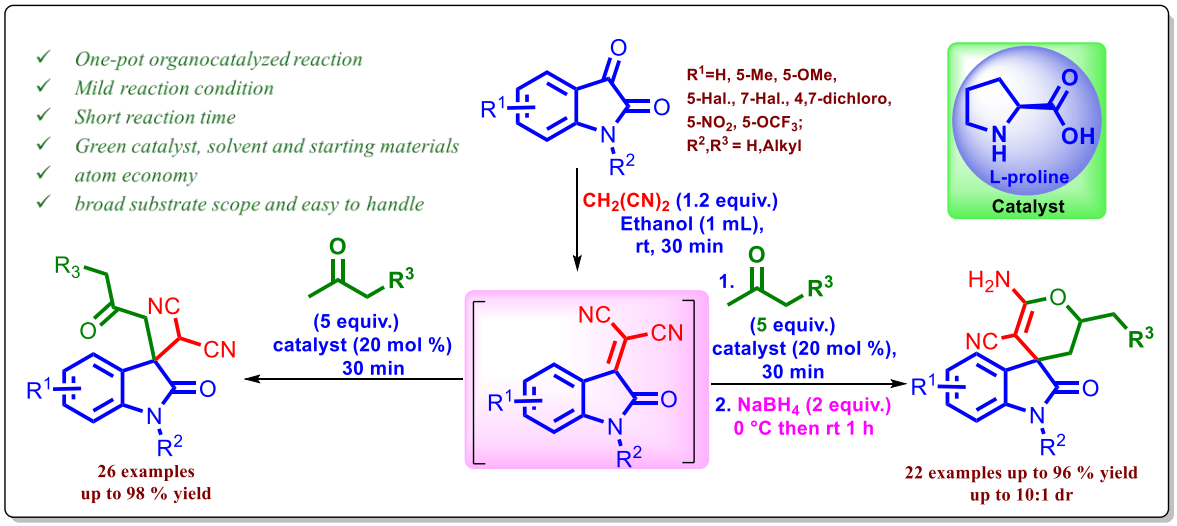
A simple and efficient methodology for the one-pot synthesis of 3,3′-disubstituted oxindoles featuring an all-carbon quaternary center has been demonstrated through L-proline catalysed three-component reaction based on sequential Knoevenagel condensation/Michael addition and also one-pot synthesis of spiro[2H-pyran-3,4′-indoline] through consecutive Knoevenagel condensation/Michael addition/reduction/cyclization reactions from readily available isatin derivatives, malononitrile, and ketones. The present methodology presents several advantages, including simple reaction set-up, short reaction times, and easy to work-up. Also, this strategy offers broad substrate scope with excellent yields and high atom economy, under mild reaction conditions.



References: [a] Patil B.R, Nichinde C.B, Chaudhari S.S, A. Mali B.P, Gonnade R.G, Kinage A.K* *RSC Adv.*, 2023, **13**, 13206-13212. https://doi.org/10.1039/D3RA00510K . [b] B. List, *Acc. Chem. Res*., 2004, **37**, 548. [c] A. Kumar and S. S. Chimni, *Beilstein J. Org. Chem.*, 2014, **10**, 929. [d] H. Zhao, Y. B. Lan, Z. M. Liu, Y. Wang, X. W. Wang and J. C. Tao, *Eur. J. Org. Chem.*, 2012, **2012,** 1935.

Poster Presentation (PP-07)
International Conference on Emerging Trends in Catalysis & Synthesis (IC-ETCS 2024)

Lewis acid mediated hydroamination/[1,3]-sulfonyl migration on *N*-homopropargyl hydroxylamine for the Stereoselective Synthesis of sulfonyl-containing cyclic nitrone

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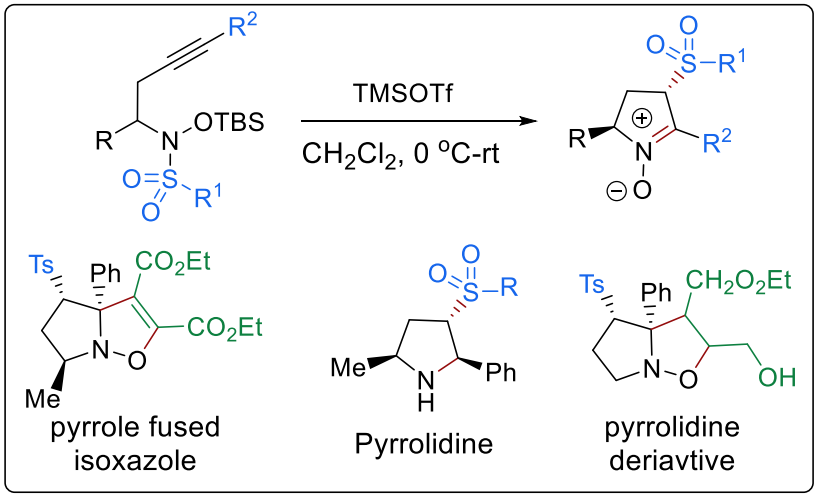
Nitrones are versatile synthetic intermediates used for the synthesis of nitrogen-containing heterocycles and fused isoxazolidine, which are widespread in natural products and biologically active molecules.[1] They show anti-senescent activity. Cyclic nitrones are known radical scavengers; this property has led to their investigation as potential agents for neuroprotection and treatment of stroke. The presence of sulfonyl moiety augments their binding feature with the biological targets, thus enhancing drugs potency. Various, transition metal-catalyzed intramolecular hydroamination on alkynyl amine followed by 1,3-sulfonyl migration from N- to C has been explored for the synthesis of sulfone-containing indole and pyrrole derivatives.[3] Surprisingly, intramolecular hydroamination on N-alkynyl hydroxylamine followed by 1,3-sulfonyl migration for the synthesis of sulfonyl-containing cyclic nitrone is largely unexplored. Herein we disclose the Lewis acid mediated hydroamination followed by 1,3-sulfonyl migration for the stereoselective synthesis of cyclic nitrones. The methodology could be utilized for the synthesis of trisubstituted tetrahydropyrrole derivatives in a stereoselective manner.



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[1] Lisnyak, V. G.; Colameta-Lynch, T.; Snyder, S. A. *Angew. Chem. Inte.Ed.* **2018**, *57*, 15162-15166.(b) Sandmeier, T.; Carreira, E. M. *Angew. Chem. Int. Ed.*. **2021**, *60*, 9913-9918.(c) Hiraika, S.; Matsumoto, T.; Matsuzaka, K.; Sato, T.; Chida, N. *Angew. Chem. Inte.Ed.* **2019,** *58*, 4381-4385.
[2] Murahashi, S.-I.; Imada, Y. *Chem Rev*. **2019**, *119*, 4684-4716.
[3](a) Nakamura, I.; Yamagishi, U.; Song, D.; Konta, S.; Yamamoto, Y. *Angew. Chem. Int. Ed.* **2007**, *46*, 2284-2287.(b).Clarke, A. K.; Ho, H. E.; Aossi-Ashton, J. A.; Taylor, R. J. K.; Unsworth, W. P. *Chem. Asian.* **2019**, *14*, 1900-1911.(c).Jiang, P.; Liu, R.; Meng, X.; Zheng, B.; Zheng, Y.; Huang, S. *Synthesis*, **2023**, *55*, 2959-2968.

Poster Presentation (PP-08)
International Conference on Emerging Trends in Catalysis & Synthesis (IC-ETCS 2024)

Carbazoquinocin Analogues as Small Molecule Biomimetic Organocatalysts in Dehydrogenative Coupling of Amines

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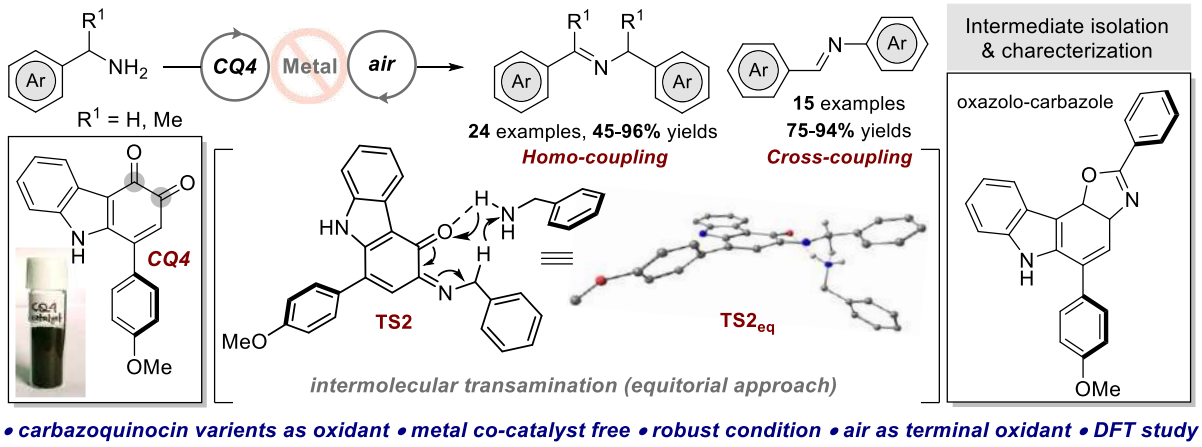
The use of metalloenzymes has been a guiding principle for designing easily accessible small molecule catalysts to execute biomimetic aerobic oxidations toward postsynthetic modifications.[1] A new series of carbazole-cored biomimetic *ortho*-quinone catalysts, structurally resembling to carbazoquinocin alkaloids have been introduced to promote tunable, metal co-catalyst free organocatalytic dehydrogenative amine oxidation under aerobic conditions. Differently substituted benzyl amines were tolerated under optimized conditions providing imines in excellent yields. Further efficacy of the catalyst was demonstrated by synthesizing cross-coupled imines efficiently. Control experiment and in-depth DFT studies disclosed covalent transamination pathway as plausible mechanism for this newly developed catalytic system.[2]



Scheme 1. Organocatalytic dehydrogenative amine oxidation.

References: [1] (a) Janes, S. M.; Mu, D.; Wemmer, D.; Smith, A. J.; Kaur, S.; Maltby, D.; Burlingame, A. L.; Klinman, J. P. *Science*, **1990**, *248*, 981–987. (b) Largeron, M.; Neudorffer, A.; Fleury, M.–B. *Angew. Chem., Int. Ed.* **2003**, *42*, 1026–1029. (c) Wendlandt, A. E.; Stahl, S. S. *J. Am. Chem. Soc.* **2014**, *136*, 506−512. [2]. Kundu, S.; Ghosh, C.; Metya, A.; Benerjee, A.; Maji, M. S. *Org. Lett.* **2024**, (https://doi.org/10.1021/acs.orglett.4c00229)

Poster Presentation (PP-09)
International Conference on Emerging Trends in Catalysis & Synthesis (IC-ETCS 2024)

Organo-Photocatalytic C-N Bond Formation

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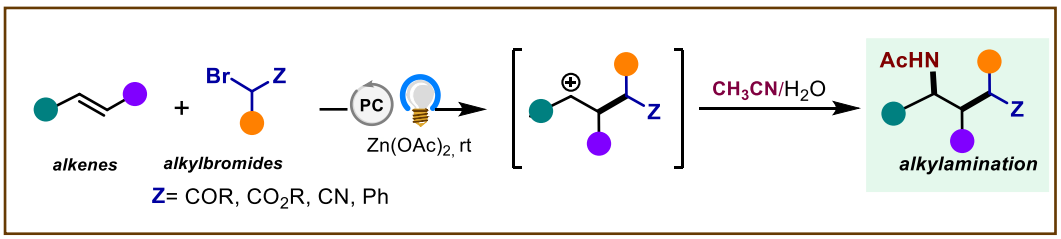
Molecules containing C-N bonds are found in many building blocks and are important precursors to other functional groups. Meanwhile, C-N bond formation via the addition of the C=C double bond is gaining prominence. In the last few years, the photo-redox process via single-electron transfer (SET) has received substantial attention for the synthesis of targeted organic compounds due to its environmental friendliness and sustainability. Of late visible-light-mediated difunctionalization of alkenes has gained much attention because of its step economy, which allows the consecutive installation of two functional groups across the C=C bond in a single operation. Herein, we are interested to report organo-photoredox catalysed C-N bond formation introducing Ritter type amination reaction.



Scheme 1. Organo-photoedox catalysed Ritter type caboamination of alkene.

References: [a] A. Samanta, S. Pramanik, S. Mondal and S. Maity, *Chem. Commun*., 2022, ***58***, 8400-8403.

Poster Presentation (PP-10)
International Conference on Emerging Trends in Catalysis & Synthesis (IC-ETCS 2024)

Photocatalysed C-N cross-coupling for synthesis of Hydrazones *via* C(sp2)-H/C(sp3)-H functionalization

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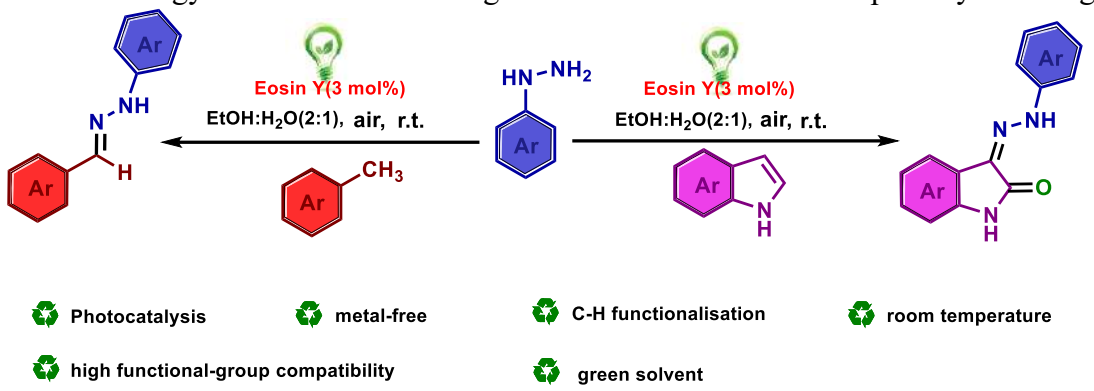
* *Department of Chemistry, Indian Institute of Technology (BHU), Varanasi – 221 005, U.P., India*

An efficient C–N cross-coupling approach for the synthesis of hydrazones was developed through C(sp2)–H and C(sp3)–H functionalization of indole and methylarene under visible light irradiation using photocatalyst eosin Y, ethanol:water as a green solvent and atmospheric air as an oxidant. With the aid of eosin Y, the C–H bonds of indole and methylarenes were activated followed by coupling with arylhydrazines. The procedure was applied to a wide variety of substrates with good functional group compatibility, offering a creative way to make hydrazones from inexpensive and easily accessible raw materials. The absence of metals, low cost, environmental friendliness, green solvent, non-toxicity, ease of handling, and utilization of renewable energy sources like visible light are some of this method's primary advantages.



Poster Presentation (PP-11)
International Conference on Emerging Trends in Catalysis & Synthesis (IC-ETCS 2024)

Synthesis of 3-Sulfenylindole derivatives from 4-hydroxy-2*H*-chromene-2-thione and indole using oxidative cross-dehydrogenative coupling reaction and antiproliferative activity study of some of their sulfone

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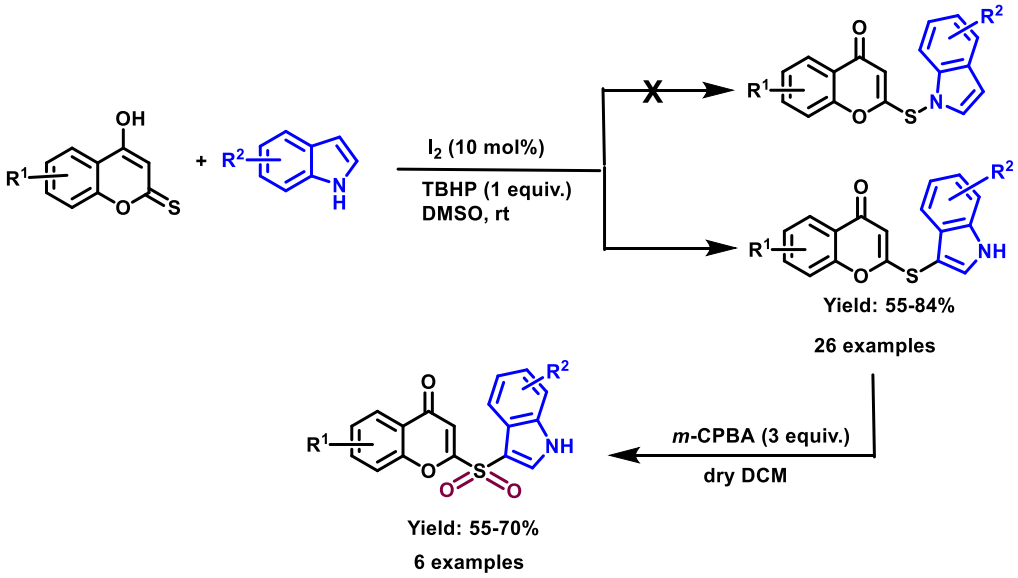
The synthesis of hitherto unreported 3-sulfenylindole derivatives is achieved from 4-hydroxy-2*H*-chromene-2-thione and indole by employing an oxidative cross-dehydrogenative coupling reaction. Then, some of the 3-sulfenylindole derivatives were converted into their corresponding sulfone derivatives because of lead likeness properties. Subsequently, a target prediction and docking study of six sulfone derivatives was performed, and four sulfones, were selected for further *in-vitro* studies. The four sulfones were found to exhibit prominent anti-proliferative activity on breast cancer (MCF7) cell lines. In addition, this reaction was exergonic through quantum chemical analysis of the mechanistic steps. The salient features of this reaction are mild reaction conditions, good yields, and broad substrate scope.



Scheme 1. Synthesis of 3-sulfenylindole and some of the sulfone derivatives

References: [a] A. Xalxo, U. J. Goswami, S. Sarkar, T. Kandasamy, K. Mehta, S. S. Ghosh, P. V. Bharatam, and A. T. Khan*, *Bioorg. Chem.* **2023**, 141, 106900. [b] R. T. Ruhee, L. A. Roberts, S. Ma, K. Suzuki, *Front. Nutr.* **2020**, 7, 64.

Palladium-Catalyzed Aerobic Oxidative Spirocyclization of Alkyl Amides with Maleimides *via* β-C(sp^3)-H Activation

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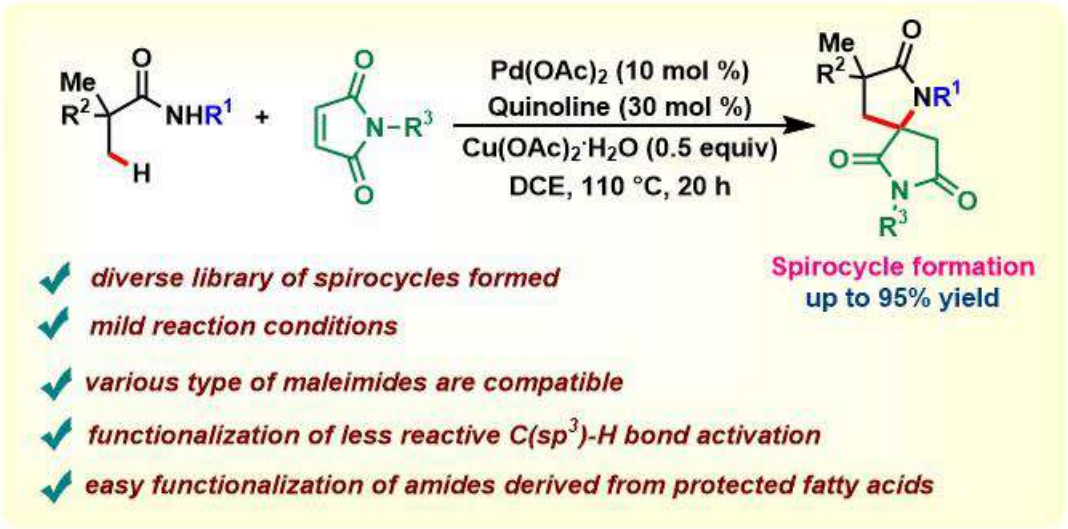
Spirocyclic scaffolds are a diverse set of compounds that are extracted from many biological sources, ranging from plants to marine life. These compounds have gained significant importance throughout many years due to their vast application in drug discovery and chiral ligand development.[1] Among various categories of spiro motifs present, nitrogen-based heterocycles generally referred to as spirodiamine scaffolds have been widely isolated from many biologically active compounds and also exhibit antiviral, antipsychotic and antitumor activities. Owing to the importance of such scaffolds, there has been many synthetic approaches to spirodiamine molecules but strategies involving transition metal catalyzed C(sp^3)-H bond activation followed by functionalization are hardly explored.[2]

Therefore, an efficient method for the synthesis of bicyclic spirodiamine molecules *via* *β*-C(sp^3)-H bond activation of aliphatic amides followed by cyclization with maleimides has been developed. The methodology is found to be highly compatible with a wide variety of maleimides. In this work, a palladacycle is also synthesized and is found to be the active intermediate for this reaction. A plausible reaction mechanism has also been proposed to account for this spirocyclization.



Scheme 1. Pd-Catalyzed Spirocycle Formation *via* C(sp^3)□H Bond Activation

References: 1. [a] L. Li, S. Wang, P. Luo, R. Wang, Z. Wang, X. Li, Y. Deng, F. Peng, Z. Shao*, *Nat. Commun.* **2021**, *12*, 5667. [b] L. K. Smith, I. R. Baxendale, *Org. Biomol. Chem.* **2015**, *13*, 9907-9903. 2. [a] B. Ramesh, M. Tamizmani, M. Jeganmohan*, *J. Org. Chem.* **2019**, *84*, 4058-4071. [b] S. Laru, S. Bhattacharjee, M. Singsardar, S. Samanta, A. Hajra*, *J. Org. Chem.* **2021**, *86*, 2784–2795. [c] S. Dutta, T. Bhattacharya, F. J. Geffers, M. Bürger, D. Maiti*, D. B. Werz*, *Chem. Sci.* **2022**, *13*, 2551-2573.

Poster Presentation (PP-13)
International Conference on Emerging Trends in Catalysis & Synthesis (IC-ETCS 2024)

Organocatalytic Asymmetric Synthesis of Carbo- and Oxa-Cyclic Seven-Membered Bridged-Biaryls *via* Nucleophile-Dependent Switchable Domino Processes

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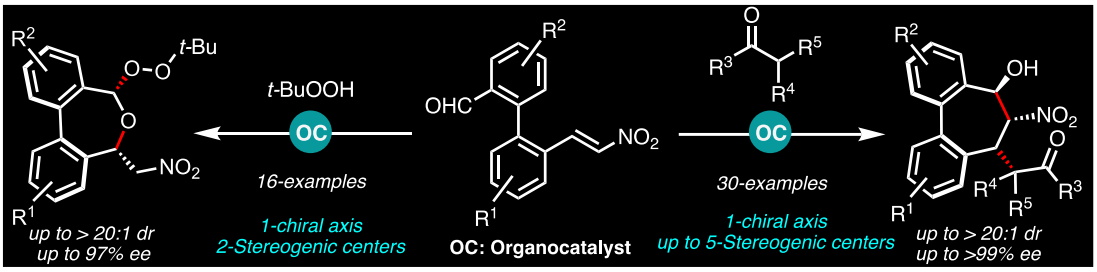
Despite the ubiquitous occurrence of biaryl-bridged seven-membered scaffolds in valuable natural products, bioactive compounds, chiral catalysts, and molecular motors, their asymmetric synthesis remained underdeveloped.[1] The seven-membered bridged-biaryl framework possesses more configurational stability than the related smaller ring structures and, therefore, could be resolved as atropisomers. To the best of our knowledge, there has been only one earlier report for the catalytic asymmetric synthesis of dibenzocycloheptanes *via* chiral phosphine-catalyzed Morita-Baylis-Hillman reaction of the enone-aldehyde to generate only one chiral center in low-yield, moderate ee and dr-values for a few examples.[2] On the other side, no direct catalytic enantioselective methods have been intended for procuring the 5,7-dihydrodibenzo[c,e]oxepines. Acquainted with the importance of developing asymmetric methods for acquiring the biaryl-bridged seven-membered skeletons, we have disclosed a nucleophile-controlled switchable reactivity for the asymmetric synthesis of dibenzocycloheptanes and 5,7-dihydrodibenzo[c,e]oxepines. To achieve our objective a new class of substrate bearing two different acceptor sites at the two *ortho*-positions of the biaryl rings has been developed and found that with a correct choice of the nucleophile and activation *via* bifunctional hydrogen-bonding organocatalyst, a switchable reactivity can be achieved, affording the seven-membered carbo- or oxa-cyclic biaryl bridged compounds bearing multiple chiral centers and a chiral axis in highly stereoselective manner.[3] The findings of our research in this endeavour will be presented in detail.



References:

1. **Kotwal, N.**; Tamanna.; Chauhan, P.; *Chem. Commun.*, **2022**, *58*, 11031-11044.
2. Mondal, A.; Shivangi; Tung, P.; Wagulde, S. V.; Ramasastry, S. S. V.; *Chem. Commun.;* **2021**, *57*, 9260 - 9263.
3. **Kotwal, N.**; Tamanna.; Chauhan, P.; *Org. Lett.*, **2023**, *25*, 7523−7528.

Poster Presentation (PP-14)
International Conference on Emerging Trends in Catalysis & Synthesis (IC-ETCS 2024)

Collective Total Synthesis of Pyrrolidine and Piperidine Alkaloids *via* Reductive Hydrofunctionalization of Enynes and Application of D-A Cyclopropane in the Total Synthesis of Pyrrolizidine Alkaloid

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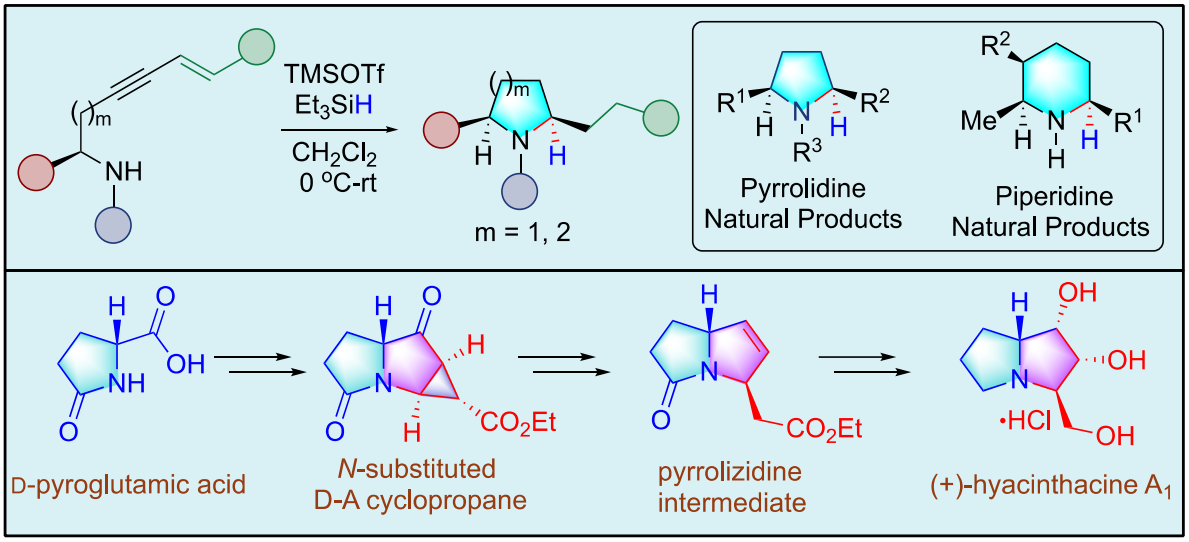
The pyrrolidine, piperidine and pyrrolizidine structural motifs are present in many bioactive alkaloid natural products.[1-2] The development of synthetic methods that enable expedient access to disubstituted pyrrolidine, piperidine, and pyrrolizidine derivatives is an important objective in organic synthesis. Herein, we report transition metal-free Lewis acid mediated 5/6-*endo-dig* reductive hydroamination cascade of enynyl amines, which gave expedient access to cyclic amines with long aliphatic chains. The brevity of the developed strategy allowed for the collective stereoselective total synthesis of various alkaloids, including (±)-pyrrolidine *cis*-225H, (±)-*epi*-197B, (±)-*epi*-225C, and (+)-solenopsins, (+)-isosolenopsins family, as well as the formal synthesis of (±)-bgugaine and (+)-azimic acid.[3] A concise and efficient enantiospecific total synthesis of (–)-hyacinthacine A_1 and (+)-hyacinthacine A_1 was achieved from commercially available starting material L-pyroglutamic acid and D-glutamic acid, respectively.[4]



References:
[1] Vitaku, E.; Smith, D. T.; Njardarson, J. T. *J. Med. Chem.* **2014**, *57*, 10257.
[2] Ilardi, E. A.; Vitaku, E.; Njardarson, J. T. *J. Med. Chem.* **2014**, *57*, 2832.
[3] Gharpure, S. J.; Patel, R. K.; Gupta, K. S. *Org. Lett.* **2023**, *25*, 5850.
[4] Gharpure, S. J.; Patel, R. K. *Eur. J. Org. Chem.* **2023**, e202300818.

Poster Presentation (PP-15)
International Conference on Emerging Trends in Catalysis & Synthesis (IC-ETCS 2024)

Palladium-Catalyzed [3+2] Annulation of *ortho*-Substituted Iodoarenes with Maleimides *via* Consecutive Double Heck-type Strategy

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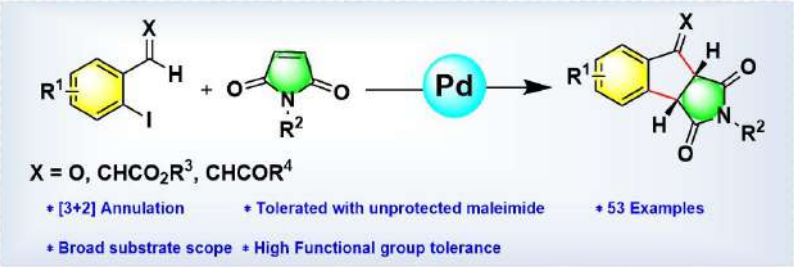
Herein, we report an efficient [3+2] annulation of *ortho*-substituted iodoarenes with maleimide *via* palladium-catalyzed consecutive double Heck-type strategy, leading to fused tricyclic frameworks of pharmaceutical relevance. The protocol ensued through consecutive inter- and intra-molecular Heck couplings effectively and compatible with a large variety of substrates and functional groups; remarkably, tolerated with unprotected maleimide.[1]



Scheme 1. Palladium catalyzed [3+2] annulation of *ortho*-Substituted Iodoarenes with Maleimides.

References: [1] Naveen, J.; Satyanarayana, G. *J. Org. Chem.* **2023**, *88* (23), 16229–16247.

Stereoselective Synthesis of Silylated Vinylboronates by a Boron-Wittig Reaction and Their Application to Tetrasubstituted Olefins

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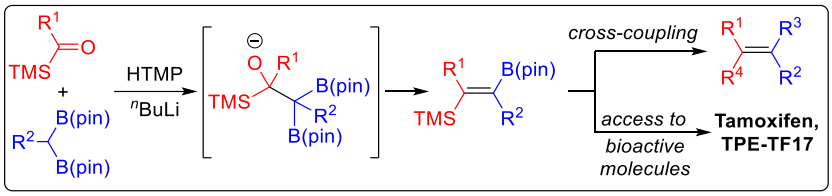
Highly stereoselective synthesis of a series of tetrasubstituted mono- as well as disilylated vinylboronates were reported using the boron-Wittig approach. The condensation between acylsilanes and gem-diborylalkanes gave the desired tetrasubstituted olefins in good to excellent yield and high stereoselectivity. Also, a series of trisubstituted silylated vinyl MIDA-boronates were synthesized using the boron-Wittig followed by a transesterification reaction. This methodology allows direct incorporation of B(pin) and TMS group in the anti-position of the olefin in a highly stereoselective manner. Further, sequential Suzuki coupling reaction with the silylated vinyl boronic esters generated all-carbon tetrasubstituted alkenes, which have been applied in the total synthesis of the anticancer drug Tamoxifen and aggregation-induced luminogen agent TPE-TF17.



References: S. Hazra, S. Panda, *Chem. Eur. J.* 2023, e202303056.
https://doi.org/10.1002/chem.202303056

Poster Presentation (PP-17)
International Conference on Emerging Trends in Catalysis & Synthesis (IC-ETCS 2024)

Design and Synthesis of Out-Out, Out-In, and In-In Epoxides in Cage Polycyclic frameworks

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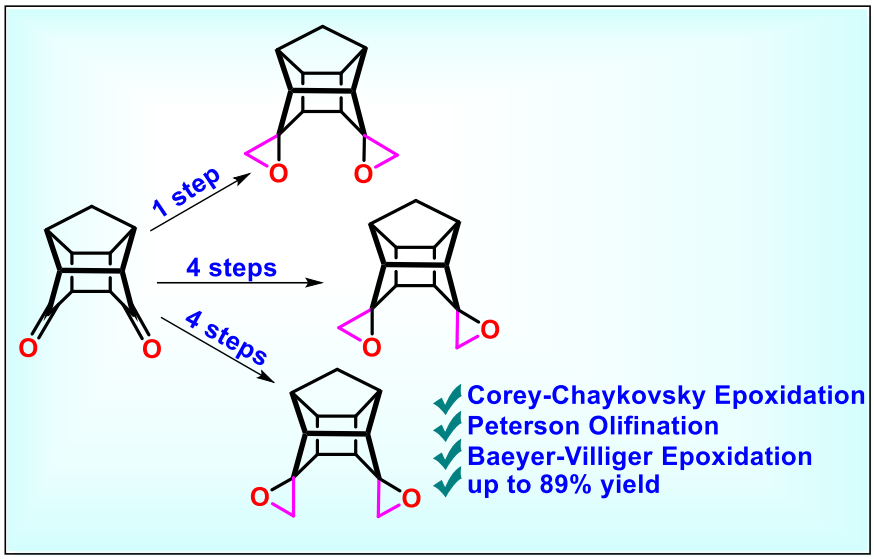
(E-mail: salman101d@gmail.com)

We defined a new synthetic approach to inner and outer epoxides using Corey-Chaykovsky reaction and Peterson olefination reaction. In this regard, a variety of pentacycloundecane (PCUD) based cage compounds containing oxiranes ring were synthesized via a simple synthetic method starting with cage diones. Eight PCUDs were used for epoxidation. These cage diones were prepared starting with easily accessible starting materials such as 2,3-dimethylhydroquinone, 1,4-dihydroxybenzene, and cyclopentadiene. Here, we have used Diels-Alder (DA) reaction, [2+2] photocycloaddition, Corey-Chaykovsky reaction, Peterson Olefination reaction, and Baeyer-Villiger Epoxidation as key steps.

Graphical Abstract



References:

1. A. P. Marchand and R. Kaya, *J. Org. Chem.* **1983**, *48*, 5392-5395.

Poster Presentation (PP-18)
International Conference on Emerging Trends in Catalysis & Synthesis (IC-ETCS 2024)

Electrochemical *N*-aroylation of sulfoximine using benzoyl hydrazine with H_2 generation

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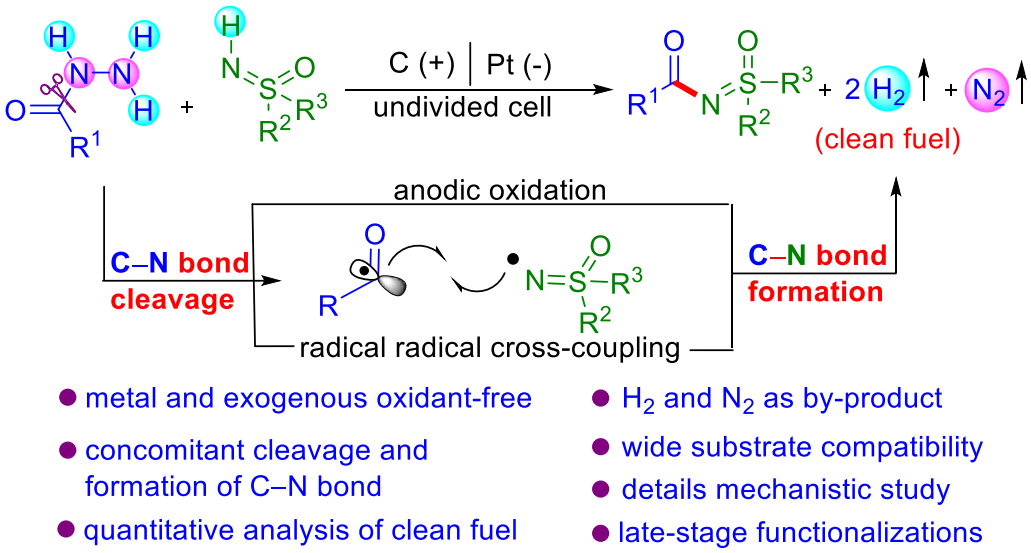
(E-mail: patel@iitg.ac.in; Web: https://bkpateliitg.wixsite.com/bkpatel)

Developed here is a robust electrochemical cross-coupling between aroyl hydrazine and *NH*-sulfoximine via concomitant cleavage and formation of C(sp^2)-N bond with the evolution of H_2 and N_2 as innocuous by-products. This sustainable protocol avoids the use of toxic reagents and occurs at room temperature. The reaction proceeds via the generation of an aroyl and a sulfoximidoyl radical via anodic oxidation under constant current electrolysis (CCE), affording *N*-aroylated sulfoximine. The strategy is applied to late-stage sulfoximidation of L-menthol, (-)-borneol, D-glucose, vitamin-E derivatives, and marketed drugs such as probenecid, ibuprofen, flurbiprofen, ciprofibrate, and sulindac. In addition, the present methodology is mild, high functional group tolerance with broad substrate scope and scalable



Scheme 1. Electrochemical strategies for *N*-aroylation of sulfoximines

References: [a] T. Alam, B. K. Patel*, *Chem. Eur. J.*. **2023**, *e202303444*.

A New Route for Electrochemical Green Ammonia Synthesis

Ashadul Adalder[†+] and Uttam Kumar Ghorai[†*]
[†]*Department of Industrial & Applied Chemistry, Ramakrishna Mission Vidyamandira, Belur Math, Howrah-711202, India*
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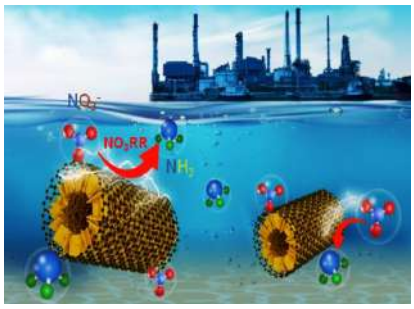
Ammonia serves as a vital raw material with extensive applications spanning various industries, such as agriculture, paints, explosives, and medicine. The prevalent method for ammonia production, the century-old Haber Bosch process, relies on high-pressure (~200 atm) and high-temperature (~450 ºC) reactions between nitrogen and hydrogen. However, this approach is notorious for its elevated energy consumption and significant cost, contributing to a global annual carbon dioxide emissions rate of 2%. Consequently, there is an urgent ecological imperative to devise more energy-efficient and environmentally friendly ammonia production methods. A promising alternative is the eight-electron nitrate reduction (NO_3RR) process, which presents an economically viable and eco-friendly approach for both ammonia production and wastewater remediation. This study introduces an innovative strategy that combines a two-dimensional graphene sheet with one-dimensional manganese (II) phthalocyanine to facilitate the electrochemical conversion of nitrate to ammonia. Making a pyrrolic-N coordinated electron-deficient manganese centers plays a crucial role in generating key intermediates for the NO_3RR process. Notably, this catalyst system achieves an impressive ammonia yield rate of 20,316 μg h^{-1} mg^{-1}_{cat}, a Faradaic efficiency (FE) of 98.3%, and electrocatalytic stability lasting for 50 hours. This comprehensive study offers novel insights into the active sites and the catalytic activity origin of MnPc:RGO concerning its NO_3RR application.

Keywords: metal phthalocyanine, nitrate reduction, green ammonia, Haber-Bosch process



References: A. Adalder, S. Paul, N. Barman, A. Bera, S. Sarkar, N. Mukherjee, R. Thapa, **U. K. Ghorai***, ACS Catal. **2023**, 13, 20, 13516–13527.

Poster Presentation (PP-20)
International Conference on Emerging Trends in Catalysis & Synthesis (IC-ETCS 2024)

Nickel-catalyzed Intramolecular Alkene-Aldehyde Reductive Coupling Strategies for *syn*-Selective Chromanol Skeletons

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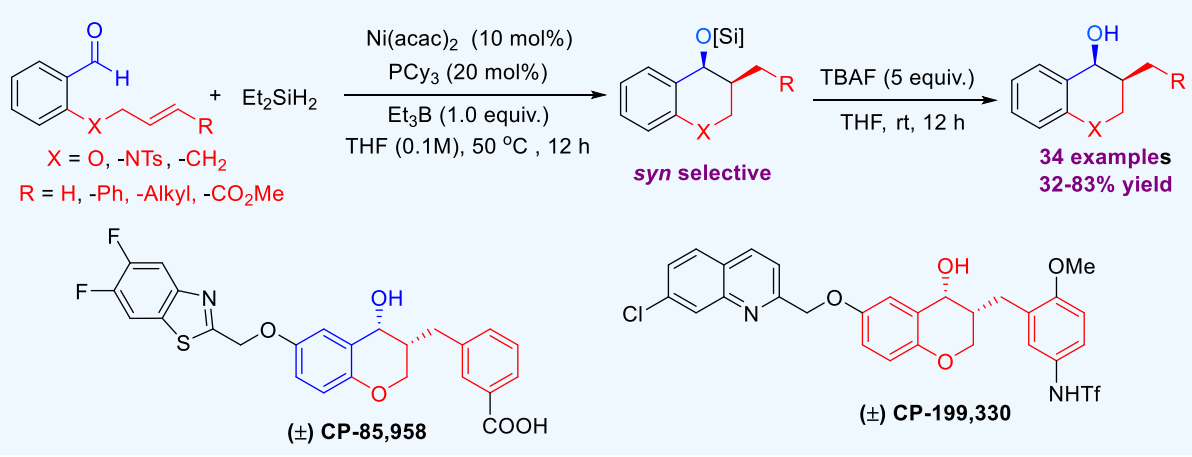
Abstract:

Syn-chromanol motif is a fundamental structural feature in various bioactive natural products, pharmaceuticals and drug molecules.[1] We have demonstrated an intramolecular reductive coupling of *O*-allylsalicylaldehyde using a bench-stable Ni^0-precatalyst to afford chromanol compound with exclusive *syn* selectivity.[2] We have successfully addressed two major challenges of this reaction: (a) Tsuji-Trost type deallylation of *o*-homoallyloxy benzaldehyde to give salicylaldehyde back (b) competing hydrosilylation of aldehyde moiety in presence of silane.[3] This methodology is applicable for both terminal and internal alkenes. A wide range of electron-rich/electron-deficient allylsalicylaldehyde provided the desire *syn*-chromanol derivatives in good to excellent yields. Our methodology is also tolerated with *o*-allyl/*o*-homoallyl benzaldehyde and N-allylanthranilalehyde. Control experiments and mechanistic studies revealed that the reaction is proceed through *in-situ* Ni^0 formation. Using this methodology, we have shown the formal synthesis of drug molecules like **CP-85.958**, **CP-199,330**.



- Fully Catalytic Version
- Hetero-atom Inclusive
- Applicable for Terminal and Internal Alkene
- In-situ Ni^0 Formation
- Inexpensive Catalyst
- Glove Box Free Condition
- Natural Products Core

4. **References:** [a] Li, W.; Yang, T.; Song, N.; Li, R.; Long, J.; He, L.; Zhang, X.; Lv, H.; *Chem. Sci*., 2022, *13*., 1808-1814. [b] Hoshimoto, Y.; Hayashi, Y.; Suzuki, H.; Ohashi, M.; Ogoshi, S; *Angew. Chem., Int. Ed*, **2012**, *51*., 10812-10815. [c] Ho, C.-Y; *Chem. Commun.*, **2010**, *46*., 466-468

Ligand Controlled Regioselective Hydrothiocarbonylation of Alkenes with Bench-Stable Thioester Surrogate Enabled by metallaphotoredox catalysis.

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Thioester represents a prominent functionality, prevalent in complex natural products, therapeutics, polymers, and foods.[1] It is ubiquitously engaged as high energy intermediate in various biochemical process, such as the regulation of cellular functions and biosynthesis processes, like metabolism or fatty acids, esters, polyketide synthesis in living systems and native chemical ligation (NCL) for protein and peptide synthesis.[2] Over the last decade, the progress of modern synthetic approaches for hydrothiocarbonylation is majorly relied on transition metal catalysis using 'CO' gas, 'CO' surrogates.[3] Most of these reaction are performed at high CO pressure, elevated temperature and using a Parr reactor or special H-type reaction setup. In this poster we will discuss about a ligand controlled regioselective hydrothiocarbonylation of alkenes under a metallaphotoredox condition to access a large library of different thioester products, showcasing the applicability for late stage thioesterification on various natural products/ alkaloids/ APIs/ Amino acid candidates.[4]

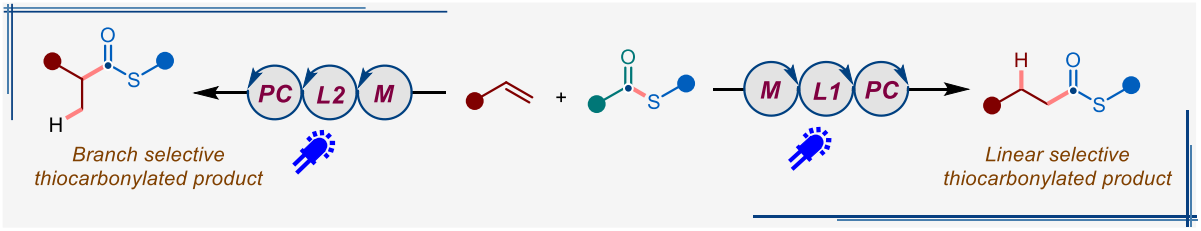

Figure 1: Ligand controlled regioselective hydrothiocarbonylation of alkenes.

References:

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2. a) Franke, J.; Hertweck, C. *Cell Chem. Biol.* **2016**, *23*, 1179–1192; b) Chandru, K.; Gilbert, K.; Butch, C.; Aono, M.; Cleaves, H. J. *Sci. Rep.* **2016**, *6*, 29883. c) Dawson, P. E.; Muir, T. W.; Clark-Lewis, I.; Kent, S. B. H. *Science* **1994**, *42*, 1330–1332; d) Kent, S. B. H. *Chem. Soc. Rev.* **2008**, *38*, 338–351.e) Pal, A.; Mondal, P. P.; Niloofar, F.; Sahoo, B. *Eur. J. Org. Chem.* **2022**, *2022*, e20220115.
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One pot telescopic approach to synthesize substituted triazolo-benzimidazole in green solvent

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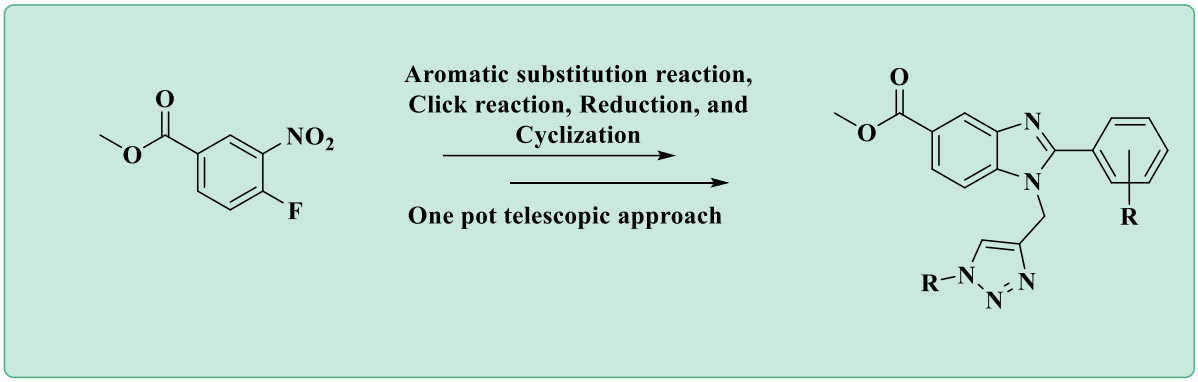
Heterocyclic compounds, which are essential to life, can be found across the natural environment. Heterocyclic compounds serve a crucial purpose in the metabolic processes of all known organisms. As a pharmacophore, heterocyclics make up about one-third of all marketed medications. Among which benzimidazoles and triazoles are of major importance as building blocks for the development of compounds possessing pharmacological activity. Herein, we have carried out a one-pot telescopic approach to synthesize triazolo-benzimidazole derivatives in green solvent medium to study a new class of biheterocycle moiety. In this method we have started with methyl 4-fluoro-3-nitrobenzoate, followed by aromatic substitution reaction, Click reaction, reduction, and cyclization which were performed in water: IPA medium, gave the best performance among other solvent in room temperature. The synthetic procedure we developed represents a cleaner route toward triazolo-benzimidazole as compared to traditional methodologies.



Scheme 1.:- One pot telescopic approach to substituted triazolo-benzimidazole.

References: [a] X. Zhu, F. Zhang, D. Kuang, G. Deng, Y. Yang, J. Yu and Y. Liang*, *Org. Lett.*, **2020**, 22, 3789–3793. [b] F. Himo, T. Lovell, R. Hilgraf, V. V Rostovtsev, L. Noodleman, K. B. Sharpless* and V. V Fokin*, *J. Am. Chem. Soc.*, **2005**, 127, 210–216.

Short, Divergent, and Diastereoselective Total Synthesis of Euolutchuols and Isolophanthins

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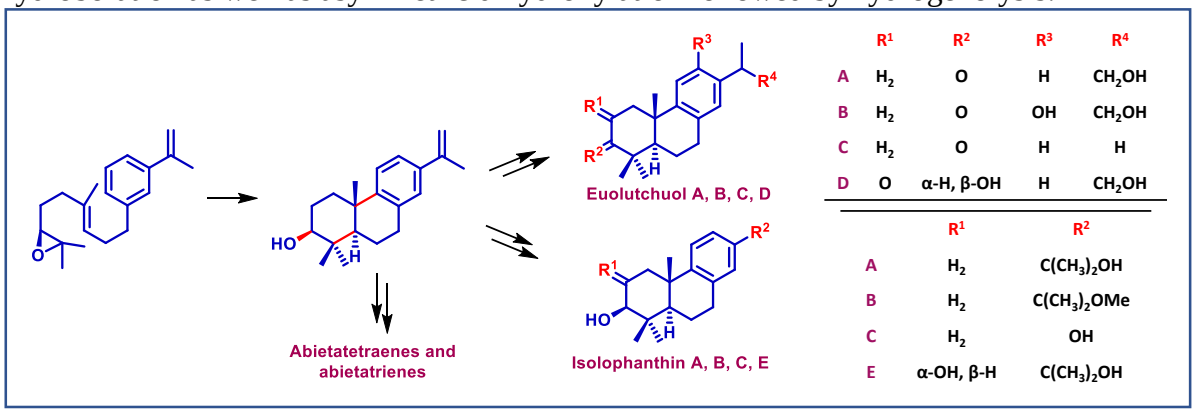
Aromatic abietane diterpenoids are of great interest in pharmacology due to their diverse biological activities. Euolutchuols and Isolophanthins are two different groups of aromatic diterpenoids that are isolated from Euonymus lutchuensis and Isodon lophanthoides respectively. Here we present a short diastereoselective total synthesis of Euolutchuols, Isolophanthines, and different abietatetraenes and abietatrienes through a divergent synthetic route. Tuning the electronic nature of the substituents on the intermediate tricyclic styrene derivative allowed access to divergent products. Key features of this synthesis are a Sharpless asymmetric dihydroxylation, a Grignard coupling and a Lewis acid catalyzed cationic polyenecyclization where styrene is used a nucleophilic terminating group for the first time. The absolute structure of Euolutchuol A and B was established using single crystal X-ray crystallography. The C15 stereogenic centre of the same was installed using asymmetric hydroboration as well as asymmetric dihydroxylation followed by hydrogenolysis.



References: [a] Y. Inaba, T. Hasuda, Y. Hitotsuyanagi, Y. Aoyagi, N. Fujikawa, A. Onozaki, A. Watanabe, T. Kinoshita, K. Takeya, *J. Nat. Prod*. **2013**, *76*, 1085-1090. [b] L Yang, L Li, S Huang, J Pu, Y Zhao, Y Ma, J Chen, C Leng, Z Tao, H Sun, *Chem. Pharm. Bull*. **2011**, *59*, 1102-1105. [c] K. Guo, YC. Liu, Y. Liu, SH. Luo, WY. Li, XN. Li, SH. Li, *Phytochemistry*, **2019**, *157*, 43-52 [d] R RS, S Surendran, G James, G Rajendar, *Eur. J. Org. Chem*. **2023**, *26*, e202300748.

Transition Metal Catalysed Straightforward Synthesis of Heterobiaryl Scaffolds using 1-Diazonaphthoquinones

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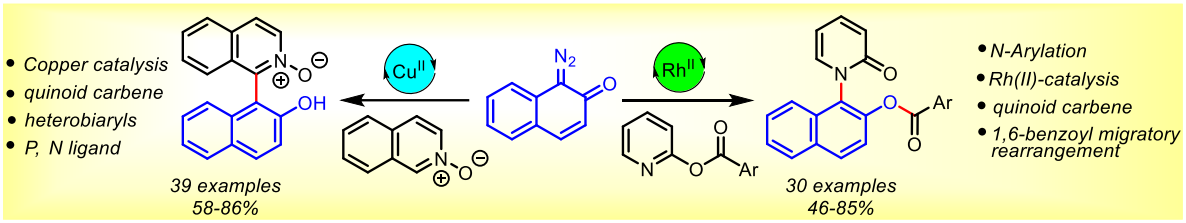
Heterobiaryl motifs are widely present in natural products and pharmaceuticals.[3,4] They have also been widely employed as preferred ligands in asymmetric catalysis.[5] Despite their useful properties, there is a lack of general straightforward methods for the synthesis of heterobiaryls. We have developed transition metal catalysed site-selective C-H arylation of isoquinoline *N*-oxide and dearomative *N*-arylation of 2-pyridone for step-economic construction of corresponding heterobiaryls.[1,2]



References: [a] Biswas, A.; Pan, S.; Samanta, R. *Org. Lett.* **2022**, *24*, 1631. [b] Pan, S.; Kundu, S.; Samanta, R. *Org. Lett.* **2023**, *25*, 2873. [c] Abulkhair, H. S.; El Gamal, K. M..; El Adl. K.; Fadl, M. F. *Med. Chem*. **2016**, *6*, 593. [d] Fu. W.; Tang. W. *ACS Catal*., **2016**, *6*, 4814. [e] Carroll, M. P.; Guiry. P. J.; *Chem. Soc. Rev*. **2014**, *43*, 819

Poster Presentation (PP-25)
International Conference on Emerging Trends in Catalysis & Synthesis (IC-ETCS 2024)

TMSCl Promoted Direct Conversion of Cyclic Anhydrides to (Un)Symmetric-Diesters/Amide Esters

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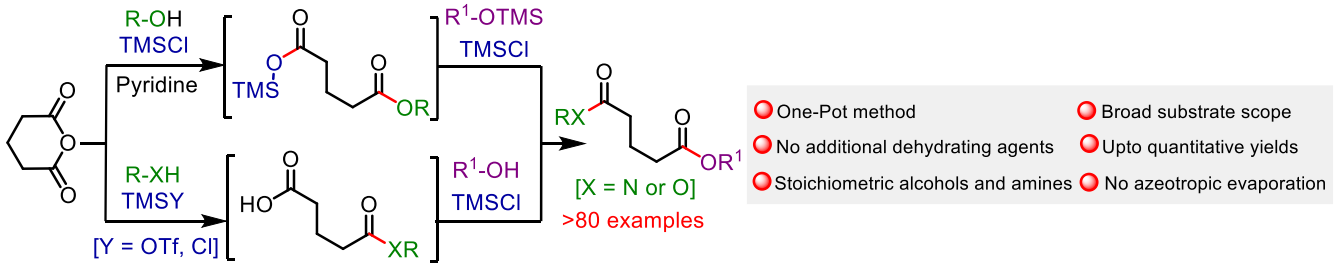
We present a mild, efficient, and one-pot method for the silyl-promoted transformation of cyclic anhydrides into homo- and hetero-dicarboxylic acid diesters and amide esters. This versatile reaction operates under ambient conditions, on a gram scale, and accommodates a wide range of alcohols, amines, and cyclic anhydrides. The one-pot process involves a two-step sequence, starting with the nucleophilic opening of anhydride by an amine or alcohol, followed by esterification. TMSCl serves a dual role, acting as a sacrificial reagent to remove *in situ* water and as a Lewis acid to promote the anhydride opening. The reaction proceeds successfully in the absence and presence of a base, as confirmed by NMR and crossover experiments, which validated the formation of dicarboxylic acid monoester and alkyl silyl mixed diester respectively. Controlled experiments have shown that the one-pot process yields higher efficiencies when compared to the same reaction conducted using a two-step process. This is the first comprehensive study demonstrating a broad substrate scope for the conversion of cyclic anhydride into diesters and amide esters. The method finds application in the synthesis of various commercial plasticizers.



Scheme 1. xxxxx

References: 1. M. Worzakowska, *J. Therm. Ana.l Calorim.* **2014**, *118*, 299-309.

2. M. G. A. Vieira, M. A. Silva, L. O. Santos, M. M. Beppu, *Eur. Polym. J.* **2011**, *47*, 254-26.

3. X. W. Kong, Y. H. Zhang, T. Wang, Y. S. Lai, S. X. Peng, *Chem. Biodivers.* **2008**, *5*, 1743-1752.

Poster Presentation (PP-26)
International Conference on Emerging Trends in Catalysis & Synthesis (IC-ETCS 2024)

Total Synthesis of Antibacterial Macrolide Sorangiolide A

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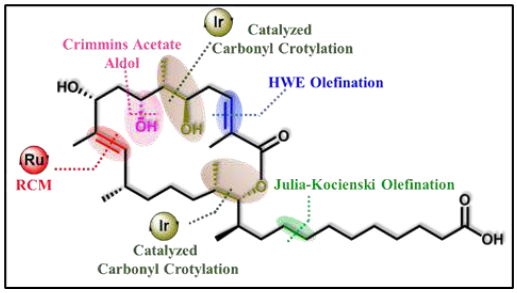
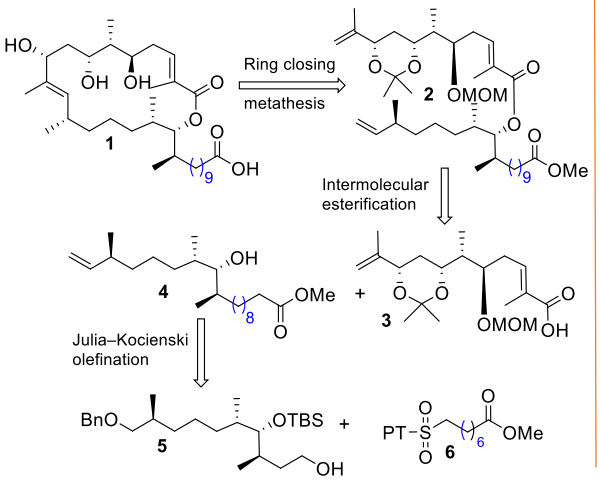
School of Chemical Sciences, Indian Association for the Cultivation of Science, Jadavpur, Kolkata-700032, India
(E-mail: ocrkg@iacs.res.in;)

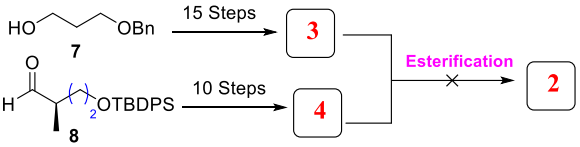
A convergent strategy for the first asymmetric total synthesis of antibacterial macrolide sorangiolide A has been developed. The salient feature of this synthesis comprise Krische Iridium catalyzed anti-diastereoselective carbonyl crotylation, Crimmins acetate aldol, Yamaguchi esterification, Julia-Kocienski olefination, HWE olefination, and ring closing metathesis. The origin of low intensity of some $^{13}C\{^{1}H\}$ NMR signals of the molecule have been investigated which clearly indicates exchange between the monomeric and dimeric forms of the natural product.



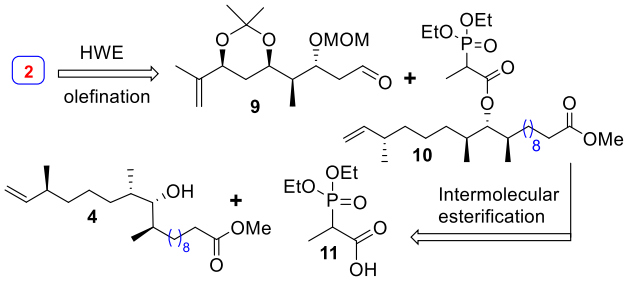
Scheme 1: Retrosynthetic analysis of Sorangiolide A(**1**)



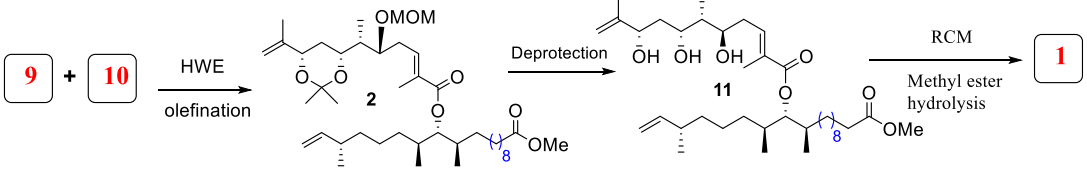
Scheme 2: Initial Efforts toward the Synthesis of RCM Precursor **2**



Scheme 3: Alternative Plan for RCM Precursor **2**



Scheme 4: Completion of Total Synthesis of Sorangiolide A (**1**)



References: [a] Irschik, H.; Jansen, R.; Gerth, K.; Höfle, G.; Reichenbach, H. Sorangiolid A, a new antibiotic isolated from the myxobacterium Sorangium cellulosum So ce 12. *J Antibiot.* **1995,** *48*, 886-887. [b] Sahana, M. H.; Paul, D.; Sharma, H.; Goswami, R. K. Total Synthesis of Antibacterial Macrolide Sorangiolide A. *Org. Lett.* **2023,** *25*, 7827–7831.

Copper-Catalyzed *N*, *N*-Alkyl Formylation of Sulfonamides

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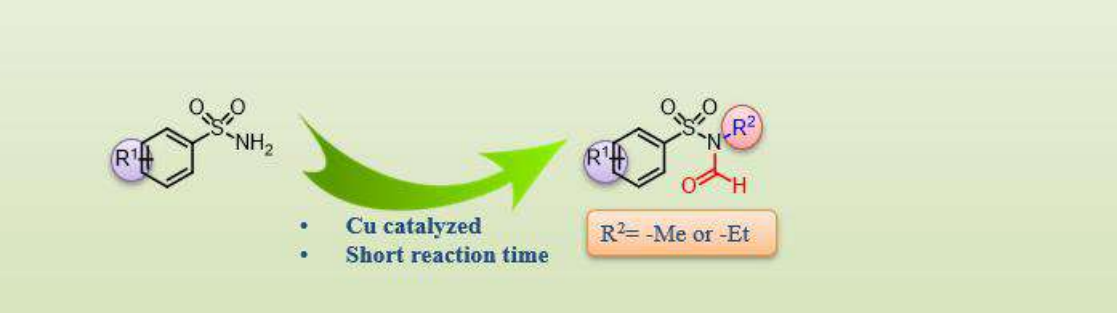
(E-mail: t.naveen@chem.svnit.ac.in)

We have developed a novel copper-catalyzed intermolecular alkyl formylation reaction of arene sulfonamides. This method represents a significant advancement in the field, as it does not require the use of any exogenous acid, base, or oxidant, and the reaction can be completed within two hours. A variety of *N*, *N*-alkyl formylated sulfonamides were synthesized in moderate to good yields. Hitherto, no reports have been found in the literature for the *N*-formylation of sulfonamides, making this reaction an important breakthrough in synthetic organic chemistry.



Scheme 1. Copper-catalyzed *N*, *N*-alkyl formylation of sulfonamides

References: [a] A. Ramani, R. S. Patil, H. Bhukya, T. Naveen*, *Asian J. Org. Chem.*, **2023**, *12*, e202300336.

Direct C(3)5-H Polyfluoroarylation of 2-Amino/alkoxy Pyridines Enabled by a Transient and Electron-deficient Palladium Intermediate

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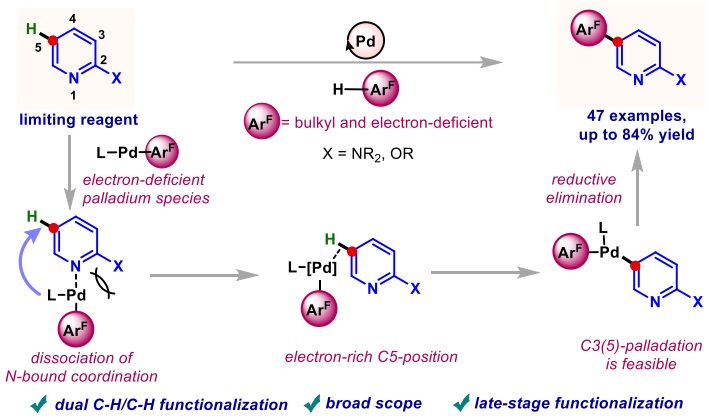
(E-mail: bm@iiserkol.ac.in; Web: https://www.iiserkol.ac.in/~bm/)

An unprecedented azine-limited C5−H polyfluoroarylation of 2-amino/alkoxy pyridines enabled by a transient and electron-deficient palladium species via C−H/C−H coupling is presented. The preliminary mechanistic investigations revealed that the synergistic combination of the bulky yet electrophilic polyfluoroaryl-Pd species and the partial nucleophilicity of the C5-position of 2-amino/alkoxy-pyridines is the origin of reactivity and selectivity. Importantly, the first experimental evidence for the role of diisopropyl sulfide (*i*-Pr_2S) in promoting C-H polyfluoroarylation is provided. Furthermore, the late-stage C−H functionalization of drugs, drug derivatives, and natural product derivatives demonstrated the method's utility.



Scheme 1. Palladium-catalyzed C5-H functionalization of 2-amino/alkoxy pyridine

References: [a] Das, A., Maji, B., Chem. Eur. J. 2023, 29, e202301436.

Construction of C2-Indolyl-Quaternary Centers by Branch-Selective Allylation: Enabling Concise Total Synthesis of the (±)-Mersicarpine Alkaloid

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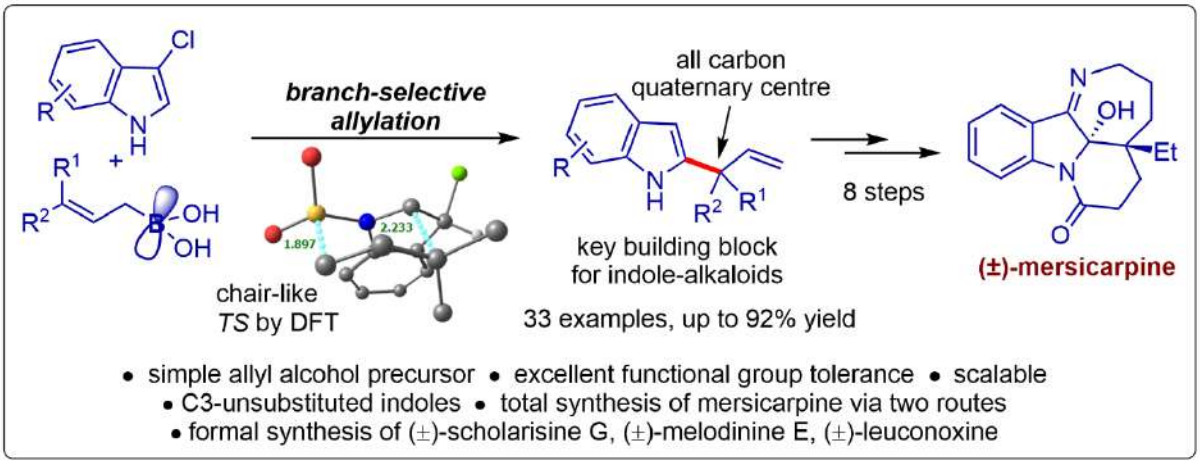
A branch-selective allylation strategy for accessing C2-indolyl-all-carbon quaternary centers using *γ,γ*-disubstituted allylboronic acids and 3-chloroindoles is achieved. Wide functional group tolerance, scalability and easily accessible allyl alcohol precursors are the key features of this method. Importantly, the C3-position of the indole remains free, offering a handle for further synthetic refinement. The reaction proceeds through indolenine intermediate, followed by allylboration through six-membered chair-like TS which was further supported by DFT calculations. Then, the total synthesis of (±)-mersicarpine alkaloid is accomplished by employing our protocol via two routes.



Scheme. Branch-selective allylation using allylboronic acids and application toward the total synthesis of mersicarpine alkaloid

References: [a] S. Sahu, G. Karan, L. Roy, M. S. Maji*, *Chem. Sci.* **2022**, *13*, 2355. [b] M. Ghosh, S. Sahu, S. Saha, M. S. Maji*, *Chem. Sci.* **2024**, DOI: 10.1039/d3sc04732f.

Synthesis of Quinolines and Their Derivatives by Nonphosphine Manganese (I) Complex

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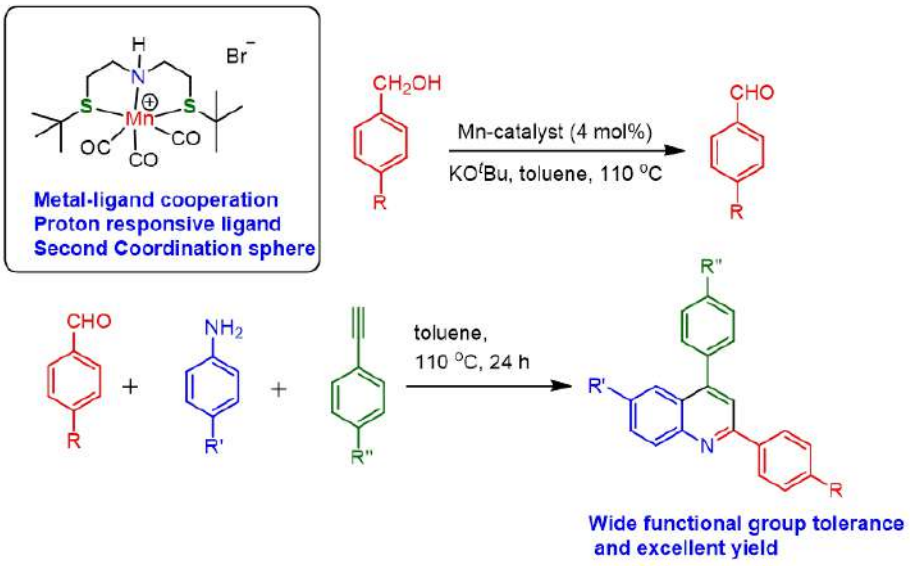
Quinolines and their derivatives have attracted a lot of interest due to their important biological and pharmacological properties. As a result, there is an increasing interest in developing sustainable methods for the synthesis of diverse functionalized quinolines derivatives in one step. Acceptorless dehydrogenative coupling[1] is a valuable method for the synthesis of *N*-containing heterocycles in a sustainable manner. This method does not require hydrogen acceptors or oxidants and does not pre-functionalize substrates. However, these reactions mainly rely on a precious metal-based catalyst supported by phosphine ligands. Therefore, to develop a cost-effective process, the replacement of precious metal catalysts with earth-abundant metal-based efficient catalysts (Fe and Mn) supported by simple, robust ligands is paramount important.[2] In this study, we developed a novel Mn(I) complex supported by simple S and N-donor ligand, which function as an efficient catalyst for alcohol dehydrogenation. Thus, in turn, this leads to a broad range of quinolone derivatives through three-component coupling/hydroarylation/dehydrogenation of aldehydes, alkynes, and amines. The synthetic strategy is flexible and would allow synthesis with different quinolines with different substitution patterns.



Scheme 1. Manganese catalyzed synthesis of quinolone derivatives

References: [a] C. S. Yeung, V. M. Dong*, *Chem. Lett.* **2011**, *111*, 1215. [b] A. Dubey, L. Nencini, R. R. Fayzullin, C. Nervi, J. R. Khusnutdinova*, *ACS Catal.* **2017**, *7*, 3864.

Organocatalyzed Enantioselective 1,6-Addition Reaction: A Key Step In The Desymmetrization Of Coumarin Tethered 2,5-Cyclohexadienones Involving A Domino Sequence

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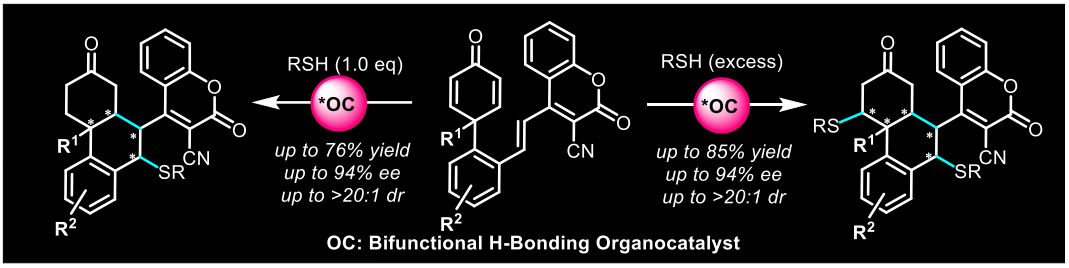
The applications of organocatalysis have widely been explored for more common 1,2- or 1,4-addition reactions and related domino reactions, where the enantiocontrol on the creation of stereogenic centers is more feasible as the reactive site of the substrates reside in proximity of the chiral environment of the organocatalyst. The development of 1,6-additions to an acceptor with prolonged conjugation are important but challenging task as the δ-position is less electropositive than the β-position due to the poor transmission of the charge density to the remote δ-position.[a-b] While exploring such remote functionalization reactions in a stereoselective manner, another difficulty could be envisioned as the reactive site of the acceptor gets stretched far from the chiral environment of the catalyst. We have demonstrated the design and application of coumarin bearing 2,5-cyclohexadienones as substrates for the organocatalysed enantio- and diastereoselective synthesis of polycyclic cyclohexadienones *via* domino 1,6-/1,4 addition desymmetrization sequence.[c] In this developed strategy, thiols have been used as nucleophiles to achieve the domino 1,6-/-1,4 and 1,6-/-1,4/-1,4 addition reactions resulting in the simultaneous formation of mono-and bi- thio substituted products in excellent level of enantio- and diastereoselectivities. The results of our finding will be presented in the poster.



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[c] **V. Sodhi,** D. Sharma, M. Sharma, P. Chauhan, *Under preparation*.

Co(III)-Catalyzed Three-Component Assembling of *N*-(2-pyrimidyl) Indoles with Dienes and Formaldehyde through C□H Bond Activation

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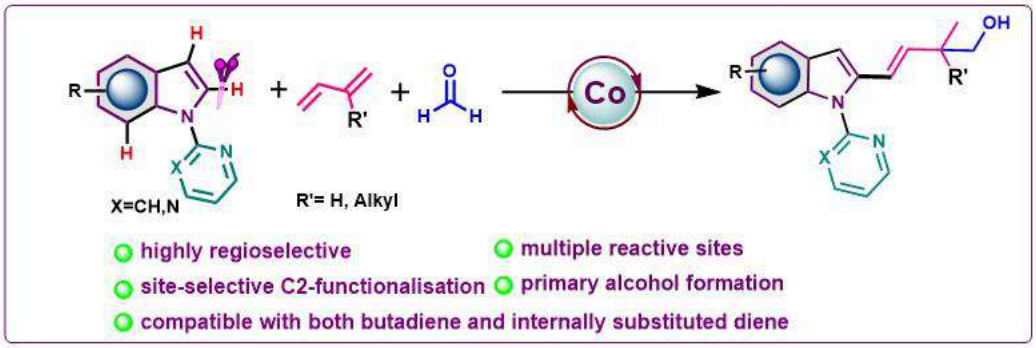
Multicomponent reactions (MCRs) have been proven as a powerful approach for the rapid and modular generation of molecular complexity *via* a step and atom economic manner and this strategy includes simple chemical inputs with mild reaction conditions. Over the past few decades, transition–metal–catalysed C–H bond functionalisation has garnered a great deal of attention in the field of synthetic organic chemistry.[a,b] In recent years, sequential three-component C–H bond addition across π-bond isosteres followed by coupling with different functionalities has been evolved as a prominent field of research.[c] Further the ubiquitous indole framework has been proven to be the most privileged class of heterocyclic compounds due to its widespread presence in a broad variety of natural, pharmaceutical, and biologically active molecules. Hence, the direct and selective C–H functionalization of indoles has received ample attention in medicinal and organic chemistry research areas. [d] In this regard, we have developed a highly regio- and chemo-selective three-component assembling of *N*-pyrimidyl indoles with dienes and formaldehyde in the presence of a Co(III) catalyst. The scope of the reaction was investigated with a variety of indole derivatives to synthesize substituted homoallylic alcohols. Both butadiene and isoprene units were compatible with the reaction and provided the desired products containing a stereogenic centre and an acyclic quaternary centre respectively. The easily available formaldehyde is used which acts as a crucial C1 building block and can be modified into different functional groups. [e]



Scheme 1. C2-Selective sequential C-H bond functionalization of *N*-pyrimidyl indoles

References: [a] T. Gensch, M. N. Hopkinson, F. Glorius, J. Wencel-Delord, *Chem. Soc. Rev.* **2016**, *45*, 2900. [b] G. Song, F. Wang, X. Li, *Chem. Soc. Rev.* **2012**, *41*, 3651. [c] D. S. Brandes, J. A. Ellman, *Chem. Soc. Rev.* **2022**, *51*, 6738. [d] P. Prusty, M. Jeganmohan, *Org. Lett.* **2022**, *24*, 1121. [e] P. Prusty, M. Jeganmohan, *Chem. Commun.* **2023**, *59*, 7216.

Complementary approaches for the synthesis of polyarylated N-naphthyl 2-pyridones via oxidative annulation

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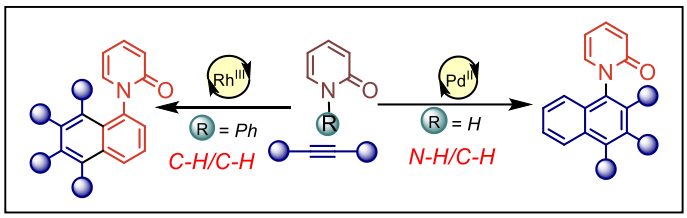
Abstract: Two distinct methodologies for the synthesis of polyarylated N-naphthyl 2-pyridones were described under transition-metal catalysis using twofold internal alkynes as coupling partner. The first involved Rh(III)-catalyzed oxidative annulation of N-aryl 2-pyridone derivatives via C-H/C-H bond activation. This formed a naphthyl ring containing a 2-pyridone-linked unsubstituted phenyl ring fused with an adjacent polyarylated phenyl ring. The second method detailed a Pd(II)-catalyzed oxidative naphthylation of unmasked 2-pyridone derivatives via N-H/C-H bond activation. This resulted in a polyarylated 2-pyridone-attached phenyl ring and adjacent unsubstituted phenyl ring. The photophysical properties of the obtained polyarylated N-naphthyl 2-pyridones were investigated



Scheme 1. Transition-metal catalyzed 2-pyridone directed oxidative annulation using Diarylacetylene

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Poster Presentation (PP-34)
International Conference on Emerging Trends in Catalysis & Synthesis (IC-ETCS 2024)

Regio- and Stereo-Controlled Hydrohalogenation of Ynamides with *N*-halosuccinimides (NXS) as Halogen Source: Synthesis of (*E*)-*α*-Haloenamides

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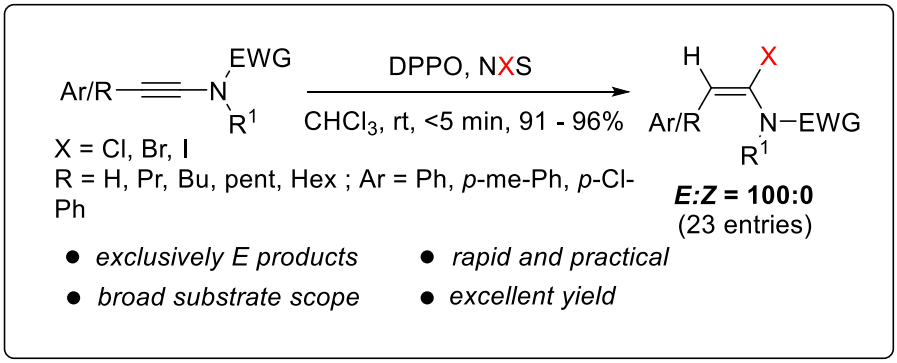
A facile stereoselective construction of synthetically versatile chiral and achiral (*E*)-*α*-haloenamides under mild conditions has been developed by utilizing *N*-halosuccinimides and diphenylphosphine oxide (DPPO).[1] This reaction is metal-free, mild, efficient, very rapid, practical and highlights the synthetic versatility of ynamides. The reaction has a broad substrate scope-both chiral and achiral ynamides have been transformed into the corresponding (*E*)-*α*-haloenamides within a very short period of time without compromising selectivity and complexity. This methodology has been successfully demonstrated on terminal alkynes which resulted in 2-halo alkenes stereospecifically with excellent yield. Furthermore, the synthetic utility has been demonstrated by performing Suzuki-Miyaura and Sonogashira coupling reactions on (*E*)-*α*-haloenamides. Details about the scope, mechanism and synthetic utility and versatility will be discussed in the poster.



Scheme 1. Stereo- and regio controlled hydrohalogenation of ynamides

References:

Pati, S. S.;[‡] Mishra, A.;[‡] Das, J. P. Regio- and Stereo-Controlled Hydrohalogenation of Ynamides with *N*-halosuccinimides (NXS) as Halogen Source: Synthesis of (*E*)-*α*-Haloenamides. Just accepted in the *J. Org. Chem*

Cu(II)-IL Mediated Synthesis of Quinazolinones from 2-Nitrobenzaldehyde: A Sustainable approach

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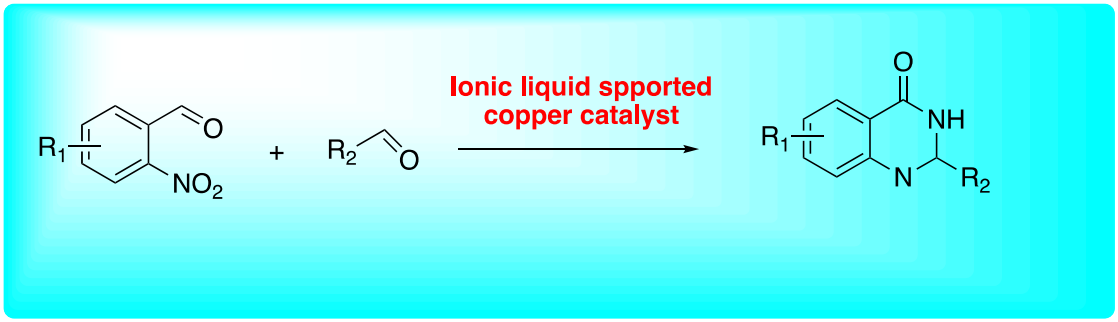
Quinazolines, a crucial class of heterocycles exhibit a broad range of biological properties, making them highly significant in the medicinal chemistry field. We have developed an one pot telescopic approach to synthesis quinazolinone moiety by using an ionic liquid supported copper actalyst. The copper catalyst, supported by an ionic liquid, enabled the effective extraction of quinazolinone products of high purity through simple organic solvent extraction. The catalyst could be reused for three cycles providing a cleaner and sustainable methodology in the synthesis of quinazolinone motifs with a vast substrate scope. However, the intermediates are isolated and charecterrized to establish the proposed reaction mecahnnism. Furthermore, this protocol was utilized in the production of natural products in gram scale. As far as we are aware, this type of ionic liquid suppoerted copper catalyzed approach have never not been reported previously for the synthesis of quinazolinone motifs.



Scheme 1. Synthesis of quinazolinone by using a copper catalyst, supported by ionic liquid

References: [a] S. sahoo, S. pal, *J. Org. Chem.*, 2021, **86**, 18067–18080.

[b] P. Arachchige, Y. Chae, *Org. Lett.*, 2019, **21**, 3337-3341.

Poster Presentation (PP-36)
International Conference on Emerging Trends in Catalysis & Synthesis (IC-ETCS 2024)

Carbonyl Group Directed Synthesis of 3-Boryl-3-Substituted Vinyl Oxindoles and Tetrasubstituted β-Borylenones

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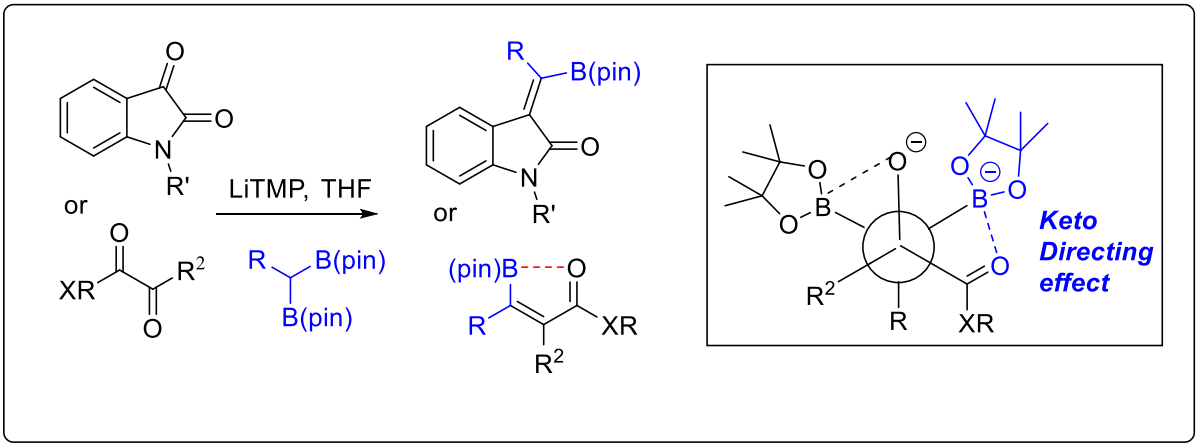
The synthesis of 3,3-substituted vinyl oxindole boronates and tetrasubstituted β-borylester and β-borylamide were achieved via transition metal-free carbonyl directed Boron-Wittig reaction of α-bis(boryl)carbanions and corresponding isatins, α-keto ester/amides, which are difficult to achieve via other known methods.



Scheme: Carbonyl Directed boron-wittig reaction.

References: D. Ghorai, K.K. Das, S. Panda, *Chem. Commun.*, 2023,**59**, 14447.

Photocatalytic Application of Free Base Corrole under Visible Light and Sunlight

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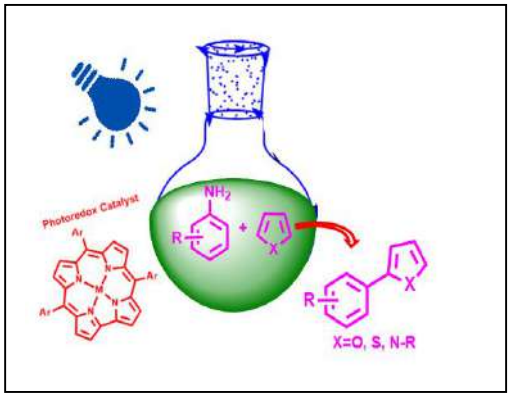
Corroles are tetrapyrrolic macrocycle that owes their name to the corrin ring found in Vitamin B_{12}.[1] Compared to porphyrin, it has one less methine bridge and is a tridentate ligand. Corrole exhibits attractive photophysical and electrochemical properties compared to porphyrin and thus should be an excellent photocatalyst.[2] Eosin Y, being cheap and readily available, has been used for various photocatalytic reactions. However, it is pH sensitive and thus limits the scope. Heavy metal compleses such as Ru and Ir polypyridyl complex are excellent alternatives, but they are costly and due to heavy metal they are toxic to the environment. Metallo-corroles found application in water splitting, CO_2 reduction, synthesis of novel solar cells and various organic transformations such as epoxidation, cyclopropanation and sulfoxidation.[3] However, photocatalytic applications of corrole is still underexplored as compared to porphyrin.

Our group at IIT Gandhinagar is working on synthesizing novel photosensitizers and exploring their application in photocatalysis and anti-cancer therapy.[4,5] In this poster, we will present the synthesis and photocatalytic application of meso aryl substituted corroles. X-ray structure and DFT studies will also be presented to shed some light on the reaction mechanism of organic transformation.

Keywords: Corrole; DFT-studies; Photo-catalyst.



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4 V. Pandey, A. Janaagal, A. Jain, S. Mori and I. Gupta, *Dyes Pigm.*, 2023, **209**, 110861.
5 A. Janaagal, N. Sanyam, A. Mondal and I. Gupta, *J. Org. Chem.*, 2023, **88**, 9424–9431.

Isoxazole group directed Rh(III)-catalyzed di-alkynylation using hypervalent iodine reagents (TIPS-EBX)

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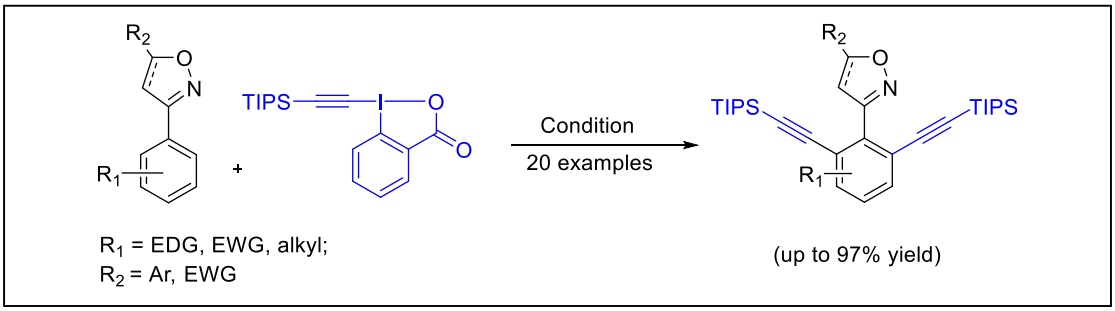
Functionalized isoxazoles operate as fundamental synthetic building blocks for a variety of organic transformation processes and are found as essential structural scaffolds in a wide range of natural products.[a-c] In addition, there are several benefits of alkynylation into organic compounds in drug development and pharmaceutical industry.[d] It has a wide range of functional group compatibility, and by changing the structure and characteristics of a pharmaceutical molecule containing an alkynyl group, it can provide better therapeutic candidates with stronger pharmacological qualities.



Scheme 1. C-H activation of aromatic/heteroaromatic isoxazoles using TIPS-EBX.

Herein, we report a successful catalytic system that uses the isoxazole as a directing group to catalyze the C-H activation process that results in the dialkynylation of aromatic and heteroaromatic isoxazoles via Rh(III) catalysis (Scheme 1). A variety of substrates were used to study the reaction's breadth, indicating its wide application. The scale-up synthesis and functional group transformations, as well as the possibility for other applications in organic synthesis and medicinal chemistry, will be reported in due course.

References: [a] X. Wang, Q. Hu, H. Tang, X. Pan, *Pharmaceuticals* **2023**, *16*, 228. [b] J. Zhu, J. Mo, H. -Z. Lin, Y. Chen, H. -P. Sun, *Bioorg. Med. Chem.* **2018**, *26*, 3065-3075. [c] N. Agarwal, P. Mishra, *Med Chem Res.* **2018**, *27*, 1309-1344. [d] F. Diederich, P. Stang, R. R. Tykwinski, *Acetylene Chemistry*; Wiley-VCH, **2005**, pp 508.

Asymmetric Synthesis of Quaternary Pyrazolone Derivatives Under Organocatalytic Conditions

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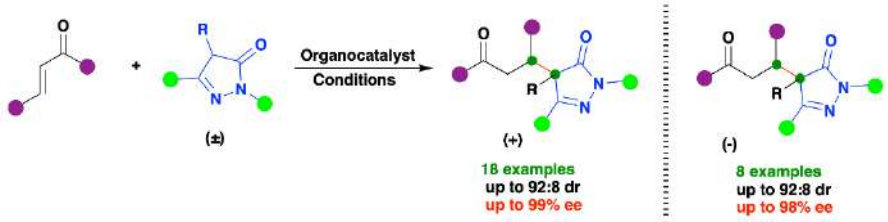
Pyrazolones and its derivatives with an in-ring all carbon quaternary stereocentre are commonly found in a wide range of biological active compounds.[1] Their biological importance and synthetic challenges have inspired to the synthetic organic chemistry community to synthesize novel pyrazolone derivatives with all carbon quaternary stereocentre.[2] However, construction of all carbon quaternary stereocentre in a catalytic enantioselective fashion is still possess challenges.[3] Recently, we have successful developed organocatalytic protocol for the synthesis of various pyrazolone derivatives with vicinal all carbon quaternary and tertiary stereocenters (Scheme 1) under mild reaction conditions. The desired pyrazolones were obtained in moderate to good diastereoselectivities and good to excellent enantiomeric excess (Scheme 1).



Scheme 1. Stereocontolled synthesis of pyrazolone derivatives.

References: (1) [a] E. Amata, N. D. Bland, R. K. Campbell, M. P. Pollastri, *Tetrahedron Lett*. **2015**, *56*, 2832. [b] Y. Zhang, C. Wang, W. Huang, P. Haruehanroengra, C. Peng, J. Sheng, B. Han, G. He, *Org*. *Chem*. *Front*. **2018**, *5*, 2229.
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(3) [a] B. M. Trost, C. Jiang, *Synthesis* **2006**, 369. [b] I. Marek, Y. Minko, M. Pasco, T. Mejuch, N. Gilboa, H. Chechik, J. P. Das, *J*. *Am*. *Chem*. *Soc*. **2014**, *136*, 2682. [c] G. Eppe, D. Didier, I. Marek, *Chem*. *Rev*. **2015**, *115*, 9175.

Poster Presentation (PP-40)
International Conference on Emerging Trends in Catalysis & Synthesis (IC-ETCS 2024)

Effect of electrostatic and hydrogen-bonding interaction of a meso-substituted porphyrin on CO_2 reduction

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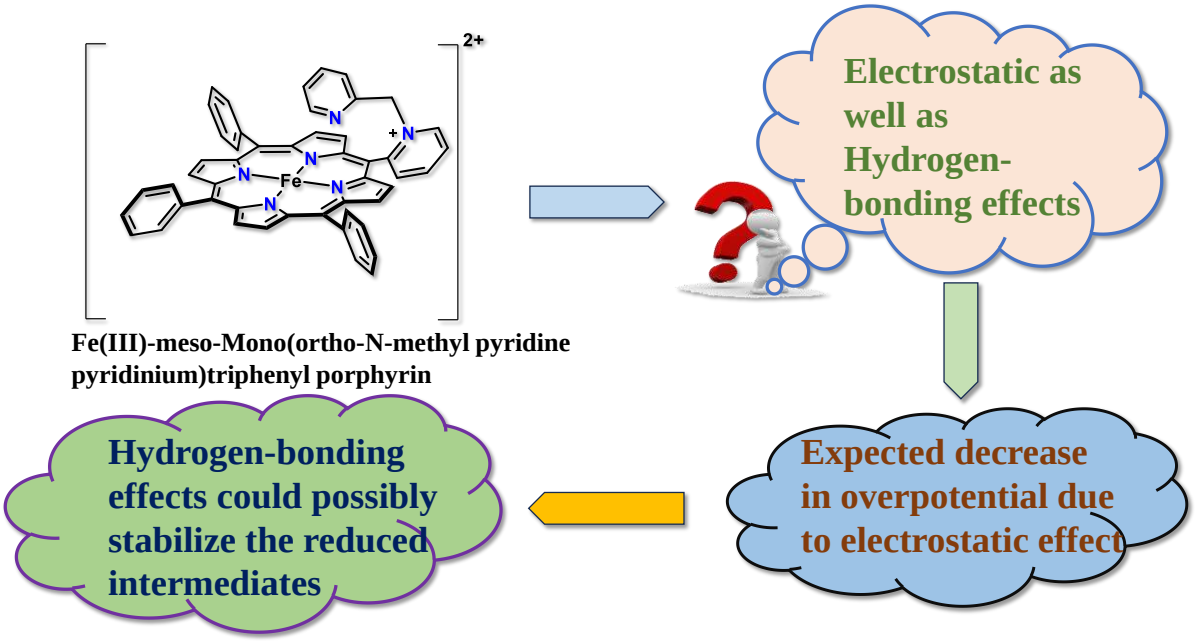
Reduction of CO_2 to value added chemicals is now of global interest to achieve sustainable and clean energy. This work focuses on synthesis, characterization and reactivity studies of a meso-substituted porphyrin having both electrostatic and hydrogen-bonding interactions. Characterization of this porphyrin has been done using NMR spectroscopy, mass spectrometry, UV-Visible spectroscopy and single crystal XRD. Both electrostatic and hydrogen-bonding effects cumulatively decreases the overpotential and determines the product selectivity upon CO_2 reduction. Electrochemical studies followed by GC-TCD and Ion-exchange chromatography reveals that CO_2 can be reduced to C1 and C2 products at a lower overpotential using H_2O as the proton source. Also, the ratio of the products changes with variation of the amount of H_2O used during the electrochemical studies.



Fe(III)-meso-Mono(ortho-N-methyl pyridine pyridinium)triphenyl porphyrin

Palladium-Catalyzed Synthesis of Diaryl Ketones and Amides from Aldehydes *via* Directed C−H Bond Activation

Dinesh Thakur and Subhash Chandra Ghosh*

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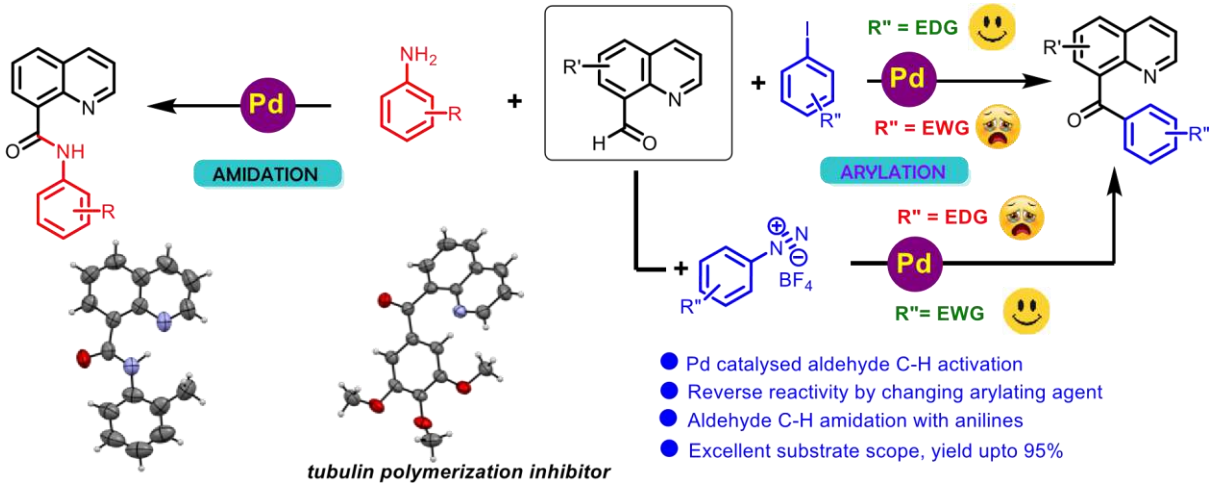
During the past decades, transition metal-catalyzed unactivated C–H bond transformations have been widely developed because of their promising features, such as step and atom economy. Directed C–H functionalization has been the key tool for synthetic organic chemists for the site-selective construction of C–C and C–Heteroatom bonds. Enormous progress has been made in chelation-assisted arene C–H activation, as compared to aldehyde C–H bond activation, which is mostly worked using expensive Rh catalysts.

Herein, we report Pd-catalyzed aldehyde C−H bond activation for the synthesis of dirayl ketone and amide with pseudo aryl halides and anilines respectively. Direct coupling of quinoline-8-carbaldehydes with two types of arylating agent, aryl iodide and aryl diazonium salts, to afford a variety of aryl quinolinyl ketones from readily available chemicals. Interestingly, aryl iodide substituted with an electron-donating group works well, whereas aryl diazonium salts containing electron-withdrawing groups are found to be superior; this phenomenon opens the scope to synthesize a range of aryl quinolinyl ketones in good to excellent yields with diverse electronic effects. On the other hand, Pd catalyzed aldehyde C−H amination with simple anilines and aliphatic amines to afford a variety of N−aryl/alkyl-quinoline-8-carboxamide was developed. It is important to note that aniline is a challenging substrate for amidation with aldehyde. Our methodology was successfully applied to synthesize highly potent tubulin polymerization inhibitors and an analog of known DNA intercalating agent and both the reactions can be easily scaled up to a gram scale.



References: [a] Thakur, D. G.; Sahoo, T.; Sen, C.; Rathod, N.; Ghosh, S. C. *J. Org. Chem*. **2022**, *87*, 16343–16350. [b] Thakur, D. G.; Rathod, N.; Patel, Patel, D; Patel, R; Sonawane, M; Ghosh, S. C. *J. Org. Chem*. **2023**, Accepted.

Enantioselective Synthesis of Chiral Amines via the Rhodium-Catalyzed Hydrogenation and Lewis Acid-Catalyzed Cyclization of Enamines

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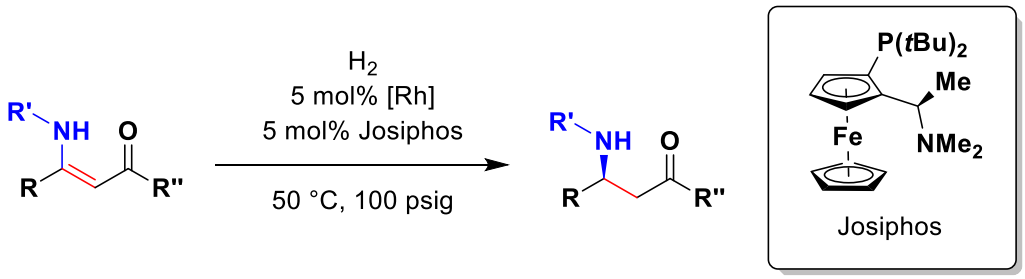
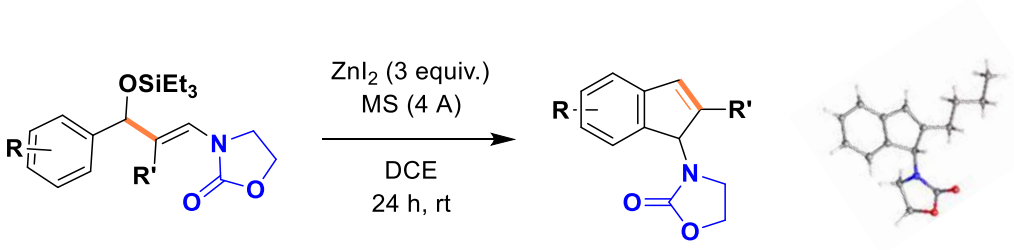
Amine-attached chiral centers are prominent in amino acids, alkaloids natural products and pharmaceuticals. Asymmetric hydrogenation of enamines provides a straightforward and atom-economic route to chiral amines. Here, we have synthesized several precursor substrates of Ezetimibe, a cholesterol-lowering drug, and demonstrated their asymmetric hydrogenation using rhodium/Josiphos catalysts. Desired hydrogenated products were obtained in moderate yields (19-67%) and high ee (62-97%).



We are exploring various routes to chiral aminoindenes using Lewis acid-catalyzed Friedel-Crafts reaction. Here, we demonstrate the efficient synthesis of aminoindenes through Lewis Acid-Catalyzed Intramolecular Friedel Crafts Alkylation of enecarbamates featuring silylated allylic alcohol. Further, we aim to show the synthesis of enantiopure indenes through zinc-based chiral phosphoric acids (CPAs)



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Palladium-Catalyzed γ-Arylation of Acylketene Synthons with Aryl Chlorides Enabled by Ylide-Functionalized Phosphines (YPhos)

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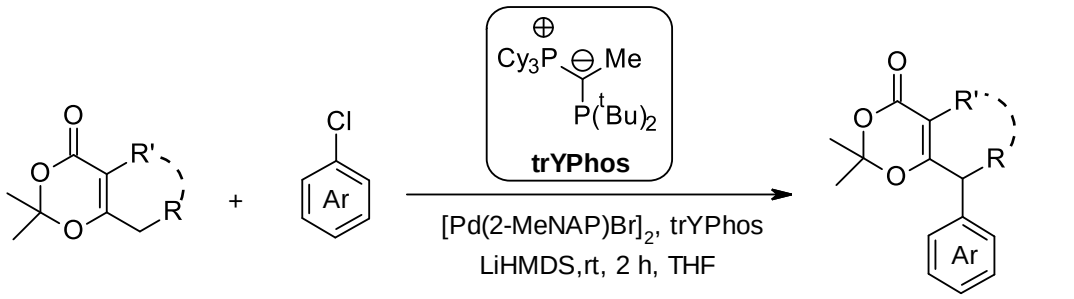
1,3-Dioxinones are versatile synthetic equivalents of acylketenes, a substructure widely encountered in pharmaceuticals and natural products. A catalyst system based on palladium 2-methylnaphthyl complexes bearing ylide-functionalized phosphines (YPhos) was found to enable the selective γ-arylation of 1,3-dioxinone derivatives with diversely functionalized aryl, heteroaryl, and vinyl chlorides. The products were further converted into 1,3-diketones and various heterocycles, highlighting their function as synthetic hubs. Experimental and computational studies revealed that bulky, electron-rich YPhos ligands are uniquely effective because they enable the oxidative addition of aryl chlorides at room temperature in the presence of the thermally sensitive enolates while at the same time efficiently promoting the rate-limiting reductive elimination step.



Scheme 1. Palladium-Catalyzed γ-Arylation of Acylketene Synthons with Aryl Chlorides Enabled by Ylide-Functionalized Phosphines (YPhos)

References: [a] S. Manna [a], F. Papp [a], Y. Hisata [b], J. Löffler [a], M. Rybka [a], V. H. Gessner*[a], Y. Hoshimoto*[b], L. J. Goossen*[a], *submitted.*

Poster Presentation (PP-44)
International Conference on Emerging Trends in Catalysis & Synthesis (IC-ETCS 2024)

Sulfonamide as Photoinduced Hydrogen Atom Transfer Catalyst for Organophotoredox Hydrosilylation and Hydrogermylation Reaction

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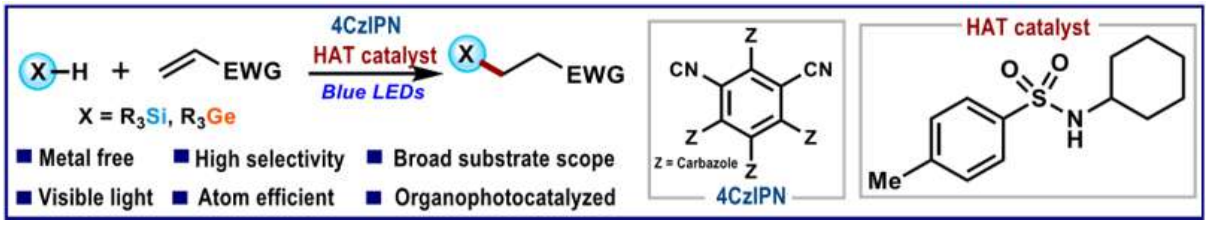
Abstract: Organosilanes are versatile intermediates in organic synthesis, and they have prevailing applications in material science, agrochemicals, polymer science, and in the pharmaceutical industry.[1a-b] Due to the high lipophilic nature of silicon, organosilanes, and silyl analogs of bioactive compounds have appreciable physiochemical properties which makes them an ideal candidate for drug discovery.[1c-e] In order to synthesize the organosilane, hydrosilylation of alkenes *via* direct activation of Si-H bond in hydrosilanes are vastly significant because of the high atom economy of the approach.[1f]



Last decade, visible light photoredox catalysis has made a significant impact in the field of synthetic organic chemistry. In addition to single electron transfer (SET) and energy transfer, hydrogen atom transfer is more frequently encountered in photocatalysis. Recent reports on selective Si-H bond functionalization of hydrosilanes under photolytic conditions suffers from site-poor selectivity[2] likely due to the similar BDEs (Si-H vs C-H)[3].

In this presentation, the synthetic utility of newly designed readily available, sterically, and electronically tunable sulfonamide as a photoinduced hydrogen atom transfer catalyst for the selective activation of Si-H/Ge-H bond (from hydrosilanes and hydrogermanes) for the hydrosilylation (Si-H) and hydrogermylation (Ge-H) of activated alkenes under visible light mediated metal free condition[4] will be discussed.

Keywords: *Hydrosilylation, Hydrogermylation, Sulfonamides, Hydrogen Atom Transfer, Radicals*

References:

1. (a) Mizoshita, N.; Tani, T.; Inagaki, S.; *Chem. Soc. Rev.* **2011**, *40*, 789; (b) Dang, T. T.; Nguyen, H. M. T.; Nguyen, H.; Dung, T. N.; Nguyen, M. T.; Dehaen,W. *Molecules* **2020**, *25*, 548; (c) For selected reviews, please see: Pooni, P.K.; Showell, G. A. *mini-rev. Med. Chem.* **2006**, *6*, 1169; (d) Franz, A. K.; Wilson, S. O. *J. Med. Chem.* **2013**, *56*, 338; (e) Taylor, R. D.; MacCoss, M.; Lawsom, A. D. G. *J. Med. Chem.* **2014**,*57*, 5845., Ramesh, R.; Reddy, D. S. *J. Med. Chem.* **2018**,*61*, 3779; (f) Zhou, R.; Goh, Y. Y.; Liu, H.; Tao, H.; Li, L.; Wu, J. *Angew. Chem. Int. Ed.* **2017**, *56*, 16621.
2. Qrareya, H.; Dondi, D.; Ravelli, D.; Fagnoni, M. *ChemCatChem* **2015**, *7*, 3350.
3. Salamone, M.; Bietti, M. *Acc. Chem. Res.* **2015**, *48*, 2895.
4. Bajya, K. R.; Kumar, M.; Ansari, A.; Selvakumar, S.; *Adv. Synth. Catal.* **2023**, *365*, 976.

Poster Presentation (PP-45)
International Conference on Emerging Trends in Catalysis & Synthesis (IC-ETCS 2024)

A Direct Stereodivergent Route to Chiral α-Aminoimines Using Allylboronic Acids: Access to Chiral α-Aminonitriles and Unsymmetrical 1,2-Di-amines

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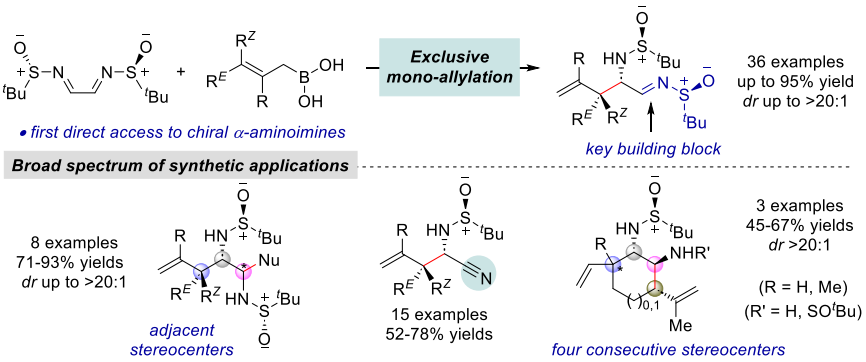
A direct asymmetric synthesis of α-aminoimines is realized for the first time, through rapid and exclusive mono-allylation of chiral bis-*N*-sulfinylimines using allylboronic acids. Notably, by varying the geometry and chiral auxiliary, all four isomers of the α-aminoimines were accessed from readily available precursors. The applicability of the products α-aminoimines were further demonstrated by accessing a range of structurally diverse chiral 1,2-diamines bearing adjacent stereocenters. Moreover, the leaving group aptitude of sulfinyl auxiliary was utilized to access valuable chiral α-aminonitriles through a non-Strecker route under thermal conditions without employing any reagents. Besides these, synthesis of optically pure cyclic 1,2-diamines having four consecutive stereocenters was accomplished through an intra-molecular Prins-type cyclization by exploiting the nucleophilicity of the tethered alkene moiety.[1] Detailed DFT studies revealed a chair-like transition state for the allylboration reaction.[2,3]



Scheme 1. Rapid and diastereoselective allylation of bis-sulfinylimines for the direct access of chiral α-aminoimines.

References: [1] S. Sahu, B. Das, M. S. Maji, *Org. Lett.* **2018**, *20*, 6485–6489. [2] S. Sahu, G. Karan, L. Roy, M. S. Maji, *Chem. Sci.* **2022**, *13*, 2355–2362. [3] M. Ghosh, S. Sahu, S. Saha, M. S. Maji, *Chem. Sci.* **2024**, Advance Article (https://doi.org/10.1039/D3SC04732F)

Poster Presentation (PP-46)
International Conference on Emerging Trends in Catalysis & Synthesis (IC-ETCS 2024)

$CsPbBr_3$ as Heterogeneous Photocatalyst in Diaryl Thio/Seleno Etherification and Chemodivergent Functionalisation of *N*-Methylalkanamides

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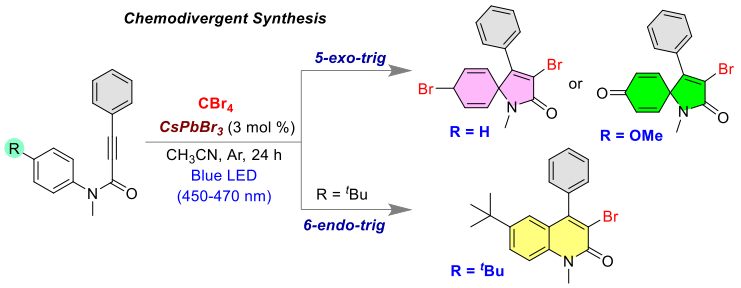
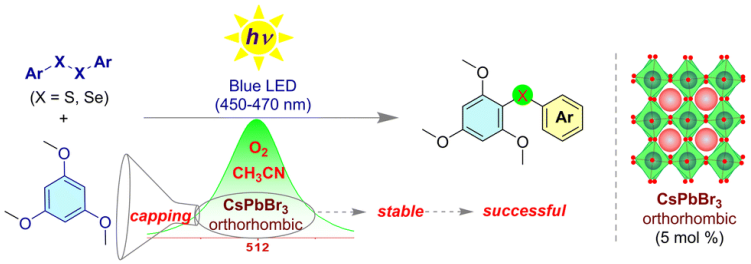
$CsPbBr_3$ holds promise as a visible light photocatalyst, but its instability in oxygen-rich and polar solvent environments poses a significant challenge for practical utilization. This study demonstrates the effectiveness of orthorhombic $CsPbBr_3$ nanocrystals (NCs) synthesized from dibromoisocyanuric acid. These NCs exhibit high efficiency as heterogeneous visible light photocatalysts (450–470 nm, 5 mol%) in a template-free aerobic thio/seleno etherification reaction involving 1,3,5-trimethoxybenzene, employing diaryl sulfides and diaryl selenides in acetonitrile ($\varepsilon \sim 37.5$). A novel surface treatment approach is proposed, utilizing electron-rich 1,3,5-trimethoxybenzene as a reactant to stabilize $CsPbBr_3$ NCs *in situ* and address stability challenges in polar solvents and open-air environments. Additionally, among the four systems, the bromide-enriched orthorhombic $CsPbBr_3$ NCs exhibit markedly enhanced photocatalytic efficiency and stability compared to the cubic systems. The orthorhombic $CsPbBr_3$ NCs, with prolonged excited state lifetime, promote efficient electron transfer, generating superoxide radical anions from the conduction band. These findings highlight the potential of perovskite nanocrystals and provide insights into their applications as visible light photocatalysts in organic transformations. Additionally, employing CBr_4 and $CsPbBr_3$ perovskite as photocatalysts, we recently reported on the chemo-divergent functionalization of *N*-Methylalkanamides.



Scheme 1. $CsPbBr_3$ photocatalyst for chemodivergent synthesis of 3,8-dibromo-1-methyl-4-phenyl-1-azaspiro[4.5]deca-3,6,9-trien-2-on or 3-bromo-1-methyl-4-phenyl-1-azaspiro[4.5]deca-3,6,9-triene-2,8-dione or 3-bromo-6-(*tert*-butyl)-1-methyl-4-phenylquinolin-2(1*H*)-one.



Scheme 2. The orthorhombic $CsPbBr_3$ perovskite NCs as photocatalysts for facilitating C–S/Se bond formation *via* C–H functionalization under an aerobic atmosphere and in acetonitrile.

References:

[a] **B. Pal**, A. Mathuri, A. Manna, P.Mal*, *Org. Lett.* **2023**, *25*, 4079-4079.

[b] A. Mathuri,‡ **B. Pal**,‡ M. Pramanik, A. Manna*, P.Mal*, *Catal. Sci. Technol.*, **2024**, Advance Article

Poster Presentation (PP-47)
International Conference on Emerging Trends in Catalysis & Synthesis (IC-ETCS 2024)

A metal-free tandem cyclisation and alkynylation using hypervalent iodine reagents

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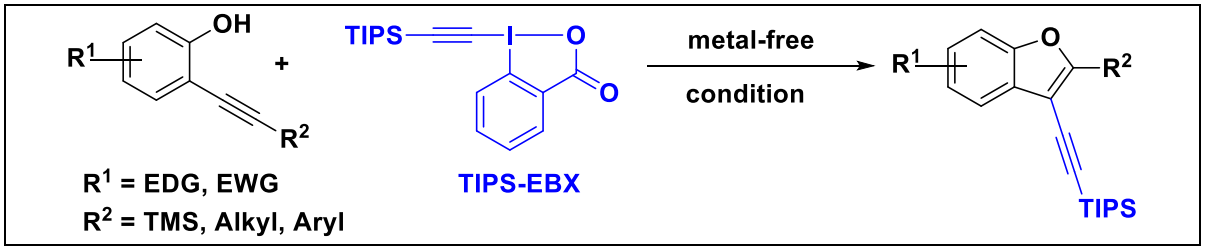
Benzofuran is one of important molecule due to its ubiquity nature in various natural products, pharmaceutical ingredients as well as functional materials.[a] Due to its broad spectrum of application provoked us to develop more environmental benign methodology to afford this moiety. We describe a unique and environmentally beneficial technique that avoids the usage of metals, which are frequently connected with environmental and toxicological concerns[b-d] The reaction employs cyclic hypervalent iodine reagents (TIPS-EBX) as potent and selective activators to activate internal alkynes (Scheme 1) of phenol derivatives. The sustainability of this protocol has been concerned while also expanding the synthetic toolbox for the creation of library of benzofuran scaffolds. This metal free tandem alkynylation followed by cyclisation can be further modified for synthetic and biological interest in near future.



Scheme 1. Tandem alkynylation followed by cyclisation using hypervalent iodine reagents.

References: [a] D. Dwarakanath S. L. Gaonkar, *Asian J. Org.Chem.* **2022**, *11*, e20220028 [b] Y. Li, G. Gryn'ova, F. Saenz, X. Jeanbourquin, K. Sivula, C. Corminboeuf , J. Waser, *Chem. Eur. J.* **2017**, *23*, 8058 – 8065. [c] J.P. Brand, C. Chevalley, J. waser, *Beilstein J. Org. Chem.* **2011**,*7*, 565-569. [d] H. Shi1, M. C. Dietl, P. M. Stein1, M. Rudolph, T. Wang1, J. Li, P. Krämer, F. Rominger, A.S. K. Hashmi, *ChemRixv* **2022**, (doi.org/10.26434/chemrxiv-2022–4vj37)

Catalytic Stereoselective Ring-opening of Vinylcyclopropanes as an Approach to functionalized δ-valerolactones

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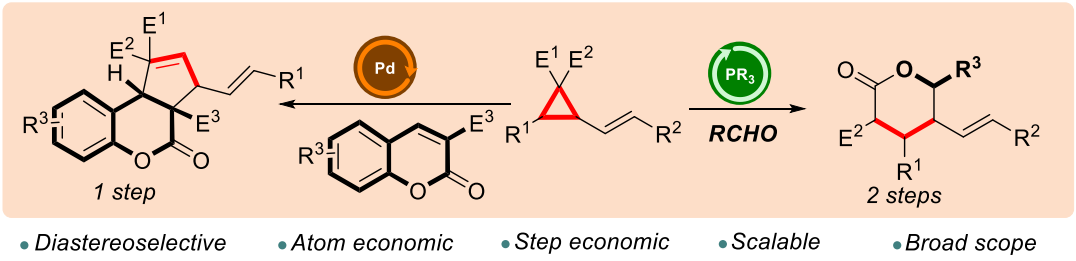
Innovative catalytic methodologies in accessing complex structures relevant to medicinal chemistry, highlights the potential impact on the development of bioactive compounds. We present a pioneering one-step palladium-catalyzed methodology to access the biologically significant cyclopenta[c]chromenone core directly from vinyl cyclopropanes and coumarin. This approach addresses the longstanding challenges associated with the laborious and intricate synthesis of this core structure.[1-2] Furthermore, we demonstrate a sustainable and efficient organophosphorus-catalyzed borylative ring-opening of donor acceptor vinylcyclopropanes affording allyl boronates through an umpolung process.[3] A facile coupling of allyl boronates with aldehydes affords homoallylic alcohols, which undergo lactonization under basic conditions to provide highly functionalized δ-valerolactones, which are important bio-feedstock chemicals used as synthons in material sciences, agrochemical industries,[4] also prominent in several biologically important molecules and commercially used drugs.[5] Further, the synthetic utility of obtained allyl boronates and homoallylic alcohol has been demonstrated. A plausible mechanism for borylative ring-opening reaction and Pd-catalyzed [3+2] type cycloaddition of VCP and coumarins has been proposed based on the control experiments and DFT studies respectively.



Scheme 1. Ring-opening of vinylcyclopropanes via palladium and phosphine catalyzed pathways to access δ-valerolactones.

References:

(1). Yang, L.; Wang, Z., *Front. Chem.* **2021,** *9*.
(2). Norman, B. H.; Dodge, J. A.; Richardson, T. I.; Borromeo, P. S.; Lugar, C. W.; Jones, S. A.; Chen, K.; Wang, Y.; Durst, G. L.; Barr, R. J.; Montrose-Rafizadeh, C.; Osborne, H. E.; Amos, R. M.; Guo, S.; Boodhoo, A.; Krishnan, V., *J. Med. Chem.* **2006,** *49*, 6155-6157.
(3). Biswas, K.; Khamrai, A.; Malik, S.; Ganesh, V., *Org. Lett.* **2023,** *25*, 1805-1810.
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Poster Presentation (PP-49)
International Conference on Emerging Trends in Catalysis & Synthesis (IC-ETCS 2024)

Harnessing The Allylic Selectivity of Vinyl Ethylene Carbonates (VECs): A Catalyst-Controlled Chemodivergent Entry to *N*-heterocycles

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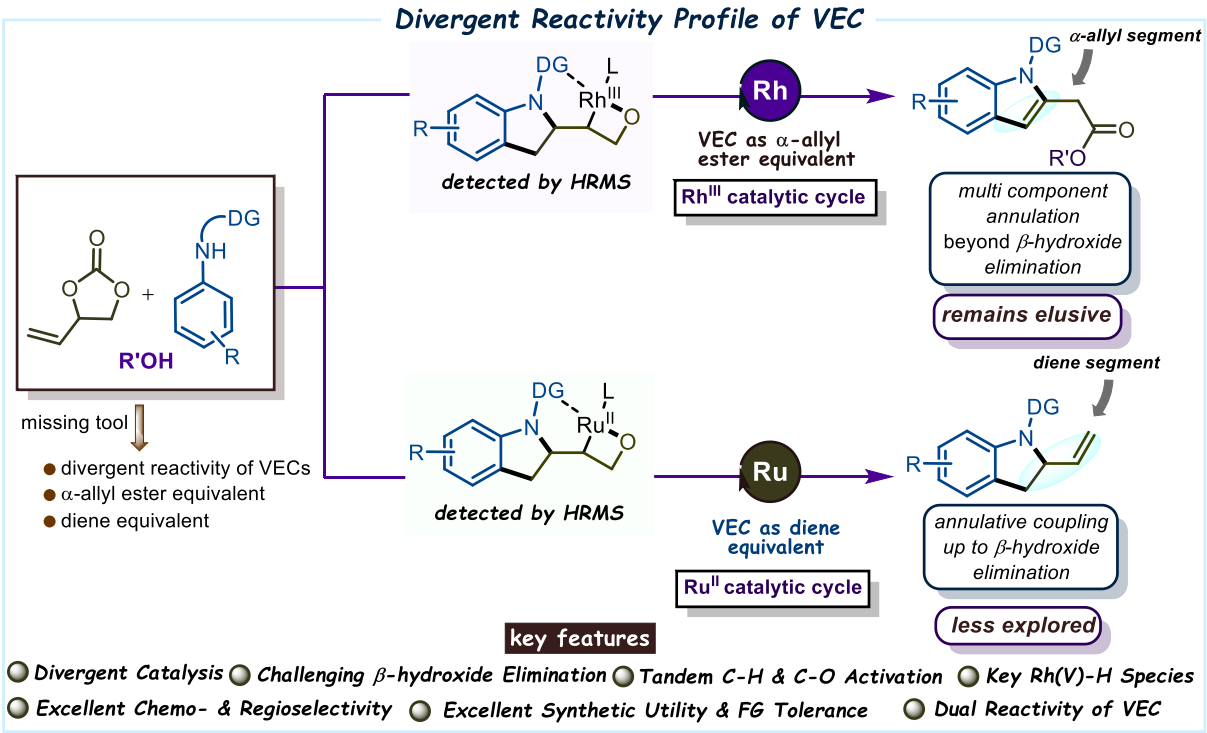
(E-mail: santosh16@iiserb.ac.in)

As a smart organic synthon, cyclic carbonates (bearing a native functional group) have witnessed increasing application in several catalytic transformations *via* strain release decarboxylative ring-opening processes.[a] Notably, VECs as a diene equivalent in catalytic reactions remain less explored whereas their reactivity mode as an □-allyl ester equivalent remains elusive.[b] A unique catalyst-controlled chemodivergent startegy to access 2-vinyl indoline and indole ester by overcoming the usual allylic reactivity of vinyl ethylene carbonates (VECs) *via* a tandem C□H/C□O activation sequence has been developed. This methodology features □-hydroxide elimination/oxidative insertion of MeOH into a Rh(III)-species to give a Rh(V)-H intermediate and provides useful scaffolds by following two distinct pathways in a highly step- and atom-economical manner. Detailed mechanistic insights unveil the unusual reactivity mode of VECs and this opens a new avenue for divergent catalysis. Post synthetic modifications of the annulated products add additional practicability to the protocol.[c]



Scheme 1. Catalyst-Controlled Chemodivergent Reactivity Profile of Vinyl Ethylene Carbonates.

References: [a] Khan, S.; Ahmed, T.; Rasheed, T.; Ullah, T. *Coord. Chem. Rev.* **2022**, *462*, 214526. [b] Zheng, Y.; Qin, T.; Zi, W. *J. Am. Chem. Soc.* **2021**, *143*, 1038. [c] Keshri, S. K.; Kapur, M.(*manuscript submitted*).

The Effect of *Meso* Substituents on the Formation of Nickel Complexes and on their Performance in the Transfer Hydrogenation of Ketones

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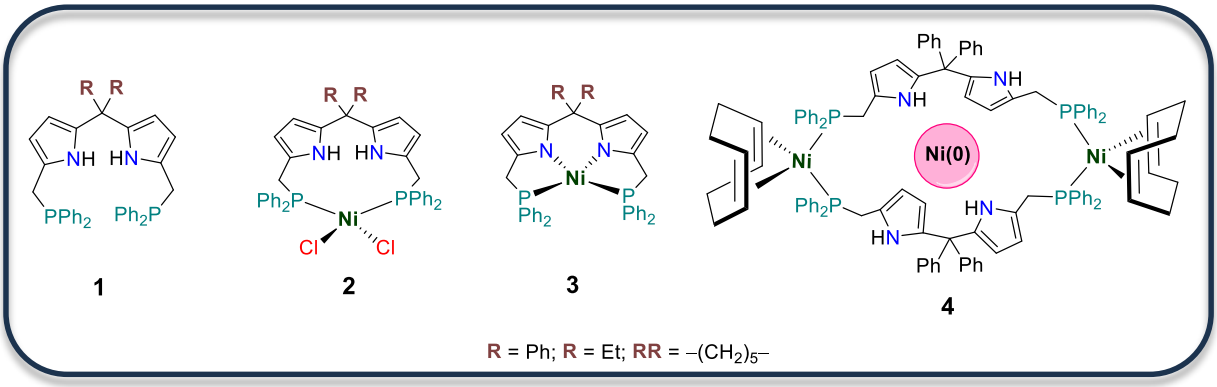
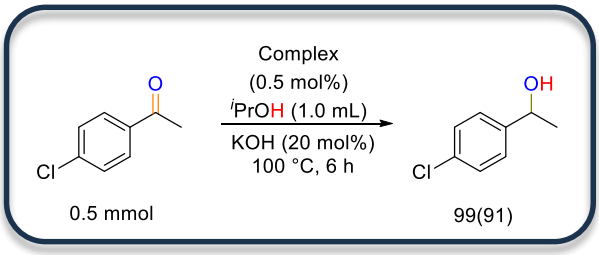
Three new dipyrromethane-based diphosphine ligands **1** containing Ph, Et, and Cy groups at the *meso* position were synthesized and characterized.[1,2] Their metalation with nickel(II) precursors afforded two types of complexes (**2** and **3**) depending upon the nature of the *meso* substituent ligand adopts κ^2-PP and κ^4-PNNP coordination modes. Their reactions with $Ni(COD)_2$ gave a novel binuclear Ni(0) complex **4**. In the presence of a strong base, only the κ^4-PNNP coordination mode of ligand was observed. These complexes (0.5 mol%) in the presence of KOH using isopropanol as a hydrogen source under N_2 atmosphere catalyze the transfer hydrogenation of a series of ketones to give their secondary alcohols (20 substrates) in overall excellent isolated yields. Spectroscopic data, X-ray structures, and salient features of the catalytic reaction with mechanism are presented in the poster.





References: [a] S. Kumar, G. Mani, S. Mondal, and P.K. Chattaraj. *Inorganic Chemistry*, **2012**, *51*, 12527-12539. [b] R. Gupta, A. Kumar and G. Mani. *Dalton Transactions*, **2023**, *52*, 18332-18341.

Organo-Soluble Colloidal MoS_2 Quantum Dots (QDs) as an Efficient Photocatalyst for α-Amino Phosphonate Synthesis

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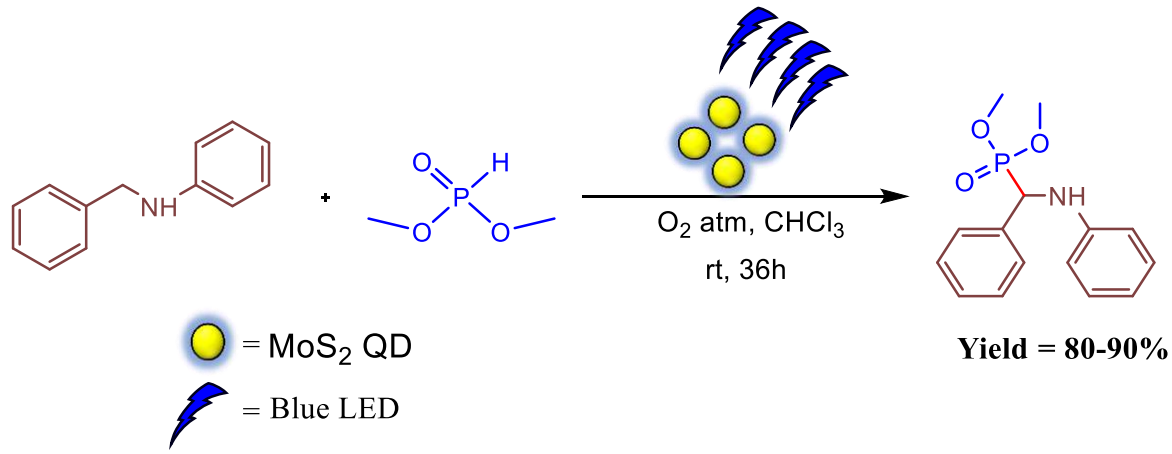
α-Amino phosphonates are bioisosteres of amino acids and have numerous indispensable biochemical activities. [a] While they are generally prepared via carbon–phosphorus bond formation using a plethora of methods[b]-[c] but using recyclable photo-catalysts and readily accessible amine and phosphites are not commonly used in synthesis. Herein, we used organo-soluble MoS_2 Quantum Dots (QDs) as an exceptionally efficient nano-photocatalyst for the synthesis of α-amino phosphonates. Our approach emphasizes on photocatalysis within organic media, providing a facile and effective method for conducting these intricate organic conversions under mild conditions. This straightforward process harnesses the power of molecular oxygen (O_2) as an oxidizing agent. To elaborate, our method is elegantly orchestrated by the inherent capability of MoS_2 QDs to enter an excited state upon absorption of blue light. This excited state bears appropriate potential energy to initiate the formation of reactive iminium ion species from N-phenyl benzylamine, thus driving the desired product formation. Mechanistic analysis has also unveiled the pivotal role of MoS_2 QDs in generating reactive superoxide radicals from O_2 through single electron transfer (SET), underscoring their significance in the process. Remarkably, this photocatalytic transformation furnishes a diverse array of functionalized products, expanding its applicability and potential implications in various contexts.



Scheme . Reaction design for the synthesis of C-P bond

References:

[a] M.F. Abdel-Megeed, B.E. Badr, M.M. Azaam, G. A. El-Hiti, *Arch. Pharm.* **2012,** *345*, 784-789.

[b] X. Jia, X. Liu, Y. Yuan, P. Li, W. Hou, K. He, *Chem. Asian J.* **2018**, *13*, 1911

[c] C. Feng, M. Ye, K. Xiao, S. Li, J. Yu, J.Am.Chem.Soc.**2013**, 135, 9322−9325

Microwave-Assisted Metal-Free C(sp^2)–H Thiocyanation of Aromatic Amines

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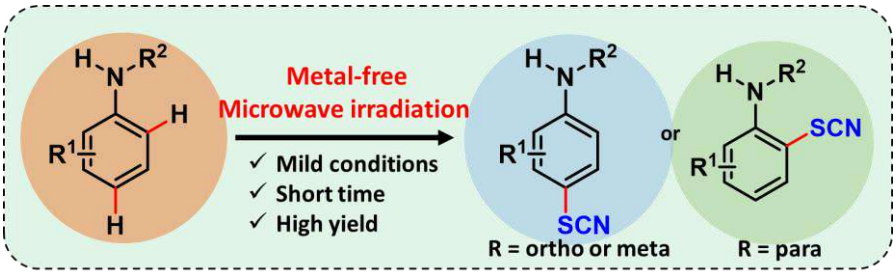
Metal-free efficient method for thiocyanation of aromatic amines under microwave irradiation for the synthesis of aryl thiocyanates using inexpensive and nontoxic NH_4SCN as thiocyanation source and $K_2S_2O_8$ as an oxidant. This protocol tolerates a wide range of substituted anilines to provide the corresponding thiocynated products in good to excellent yields. The mild reaction conditions, high yields, short reaction time, and site-selective thiocyanation of anilines make it an attractive choice for organic synthesis, medicinal chemistry, and material science. The features of this strategy include a broad substrate scope, high functional group tolerance, mild reaction conditions, good to excellent yields, and short reaction time



Scheme 1. Microwave assisted metal free C(sp^2)–H thiocyanation of amine

References: B. Desai, P. Satani, R. S. Patil, H. Bhukya, T. Naveen*, *ChemistySelect*, **2023**, *8*, e202302849.

An Electrochemical Cascade Process: Synthesis of 3-Selenylindoles From 2-Alkynylanilines with Diselenides

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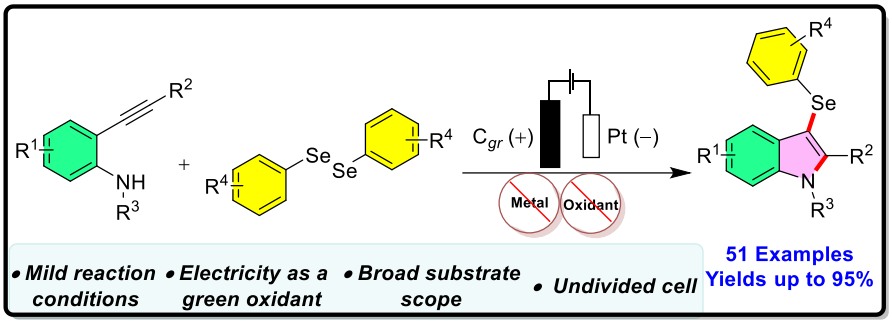
The substituted organoselenium compounds are crucial structural motifs in pharmaceutical molecules. Herein, we report a metal, oxidant, and base-free electrochemical approach to access 3-selenylindoles through an oxidative cyclization of 2-alkynylanilines with diselenides. This environmentally friendly approach demonstrates a wide range of substrate scope under mild reaction conditions in an electrochemical undivided cell setup.



(*Chem. Commun.*, 2023, **59**, 8719–8722)

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Poster Presentation (PP-54)
International Conference on Emerging Trends in Catalysis & Synthesis (IC-ETCS 2024)

Synthetic Studies Towards Naturally Occurring RALS Caryospomycin A-C

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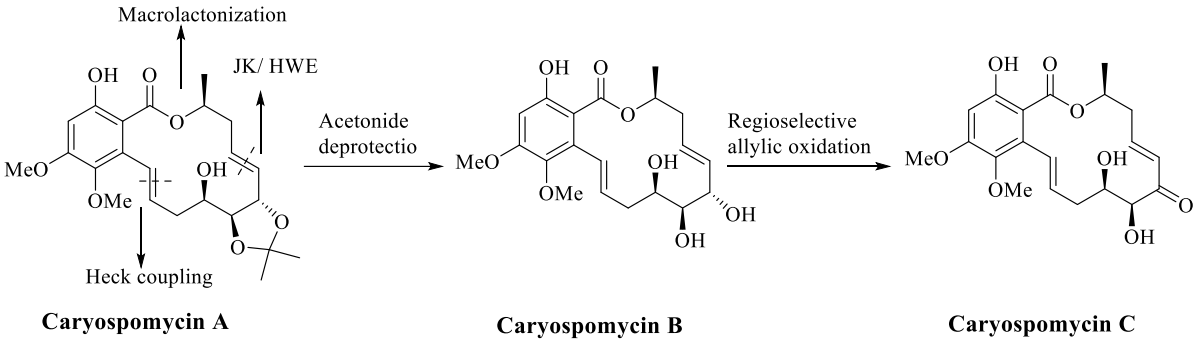
Abstract:

Resorcylic acid lactones (RALs) that contain a 14-membered macrocyclic lactone ring fused with a β-resorcylic acid moiety belong to a subclass of the benzenediol lactone family. More than hundreds of RALs have been isolated from various fungal genera. These metabolites exhibit various biological activities, like inhibitions of proteins, cytotoxic, antiviral, etc. Due to their unique structural features and biological activity, they are suitable targets for synthetic chemists. We are currently working on the total synthesis of a newly isolated class of RALs known as Caryospomycin, from commercially available starting materials, employing late-stage olefination and macrolactonization as key steps. (Scheme 1)



Scheme 1.

References:

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Asymmetric Synthesis of Hydrophenanthrenones Bearing Multiple Stereogenic Centers via Squaramide-Catalyzed Domino 1,4-/1,4-Addition Desymmetrization Sequence

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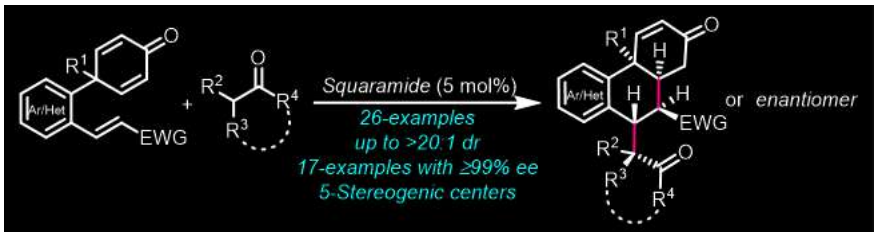
Tetrahydrophenanthren-2(1*H*)-one is a constitutive unit of a large number of important natural products including alkaloids, useful lipids and several synthetic bioactive molecules exhibiting a broad range of biological properties.[a] On top of that, it also serves as a precursor for obtaining another important core i.e., octahydrophenanthrene, which is, present in several steroids and terpenoids. [b] Acknowledging the usefulness of above-cited cores, their stereoselective synthesis is of utmost significance. In this context, an organocatalytic intramolecular 1,4-addition reaction of 2,5-cyclohexadienones appended with aromatic ring-bearing sulphone units has been established to procure enantiopure tetrahydrophenanthren-2(1*H*)-ones bearing two stereogenic center.[c] We have utilized Michael acceptor-tethered 2,5-cyclohexadienones as a new class of substrate to undergo a chiral squaramide catalyzed domino 1,4-/1,4-addition reactions with simultaneous desymmetrization of 2,5-cyclohexadienone core to obtain tetrahydrophenanthren-2(1*H*)-ones bearing five contiguous stereogenic centers including two-tetra-substituted carbon centers in excellent diastereo- and enantioselectivities.[d] The detailed findings of our research in this direction will be presented.



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Poster Presentation (PP-56)
International Conference on Emerging Trends in Catalysis & Synthesis (IC-ETCS 2024)

Three-component Carbosilylation of Alkenes by Merging Iron and Visible-Light Photocatalysis

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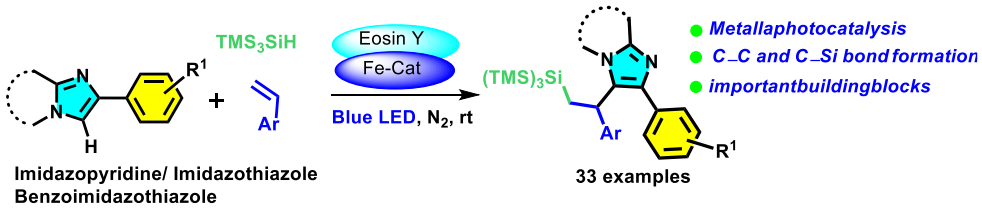
Organosilicon compounds are one of the vital synthetic building blocks in the field of organic chemistry and they have widespread applications in material science, polymer science and agrochemistry. Notably, the silicon analogues of biologically active molecules and organosilicon compounds exhibit exceptional physicochemical properties, allowing them to be extensively used in medicinal chemistry. Consequently, the development of efficient techniques for organosilicon compound synthesis is always fascinating and challenging for chemists. Herein, we have demonstrated a mild, efficient, and one-pot protocol for three-component carbosilylation of alkenes with imidazoheterocycles and silanes by merging iron(II) and visible-light photocatalysis. This concomitant C□C and C□Si bond-forming method provides functionalized organosilicon derivatives having imidazoheterocycles moieties in step- and atom-economic fashion under room temperature. The reaction possibly proceeds through a radical pathway.



Scheme 1.

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Ancillary Ligand Coordination Directed Modes of Aggregation in Mixed-Valence Tetranuclear Cobalt Complexes: Synthesis, Structure, Field-Induced SIM Behavior and Theoretical Insight

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A multidentate Schiff base ligand H_3L was synthesized by 1:2 condensation reaction of 4-methyl-2,6-diformylphenol and 2-aminobenzyl alcohol. The metal ion coordination behavior of the synthesized ligand H_3L ([2,6-bis-{(2-hydroxymethyl-phenylimino)methy}-4-methylphenol]) toward cobalt(II) ions in the presence of two different types of ancillary ligands sodium pivalte and ammonium thiocyanate resulted two different types of mixed-valence tetranuclear cobalt complexes $[Co^{III}_3Co^{II}(L)(HL)(\mu_4\text{-}O)(\mu\text{-}OH)((CH_3)_3CCOO)_2]ClO_4.H_2O$ (1) and $[Co^{III}_2Co^{II}_2(L)_2(NCS)_4(CH_3CN)_2]\cdot CH_3CN$ (2).For the former complex, the presence of pivalate anion triggered the oxido-hydroxido-bridging dual control for aggregation whereas for the later one, involvement of terminal thiocyanate leads to the dicubane like aggregates. Different numbers of connectivity around the Co^{III} and Co^{II} centers are satisfied by the water derived HO^- and O^{2-} linkers and ligand-anion-based double phenolato bridges. Alternating current (AC) / direct current (DC) magnetic studies revealed field induced slow magnetic relaxation for complex 1 arises from the single octahedral Co^{II} center whereas the other three Co^{III} ions are diamagnetic in nature. For the complex 2, among the tetranuclear $Co^{III}_2Co^{II}_2$ centers only two Co^{II} centers exhibited an antiferromagnetic interaction (J = −0.39 cm−1). The structural distortions in these two types of aggregates lead to different magnitudes of easy-axis magnetic anisotropy (D = −51.31 cm^{-1} for 1 and −31.9 cm^{-1} for 2) and a small but non-negligible transverse component (E/D = 0.263 for 1 and 0.255 for 2). The static and dynamic magnetic data were analyzed using DFT and CASSCF-based calculation.

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Visible-Light-Induced Metal and Photocatalyst Free Diastereoselective Synthesis of *trans*-2,3-dihydrofurocoumarin Derivatives

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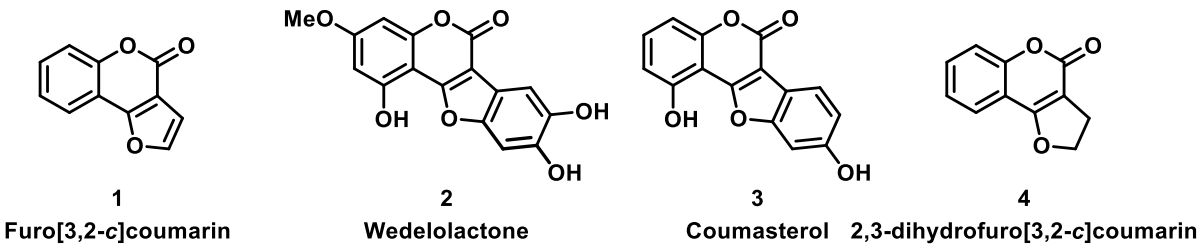
2,3-dihydrofurocoumarin derivatives (DHFC) are fused heterocyclic moiety frequently encountered in many natural products. Furocoumarin **1**-**3** and 2,3-dihydrofurocoumarin **4** exhibit several bioactivities such as anticoagulant, antibacterial, antifungal, antitumor, antiviral, anticonvulsant, anticancer, antimicrobial, antiprotozoal, insecticidal, fungicidal, antimycobacterial, antimutagenic, antioxidant, and anti-inflammatory. Till date few synthetic approaches have been taken for synthesis of DHFC scaffold.[a-d]



Scheme 1. Natural products containing furocoumarin derivatives.

Here in this contribution we have developed a novel photocatalytic strategy for the synthesis of *trans*-2,3-dihydrofurocoumarin derivatives starting from commercially available 4-hydroxycoumarin. The developed protocol tolerates wide range of substrates and provided the desired products with good to excellent yields with excellent diastereoselectivity. A thorough mechanistic study revealed that the reaction followed radical pathway. Also some synthetic transformations were achieved from the synthesised DHFC derivatives, highlighting the importance of the DHFC moiety in synthetic organic chemistry. Results from this study will be presented.

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Poster Presentation (PP-59)
International Conference on Emerging Trends in Catalysis & Synthesis (IC-ETCS 2024)

C-H Bond Halogenation using Ni (II)-Biguanide and Substituted Biguanide Complexes

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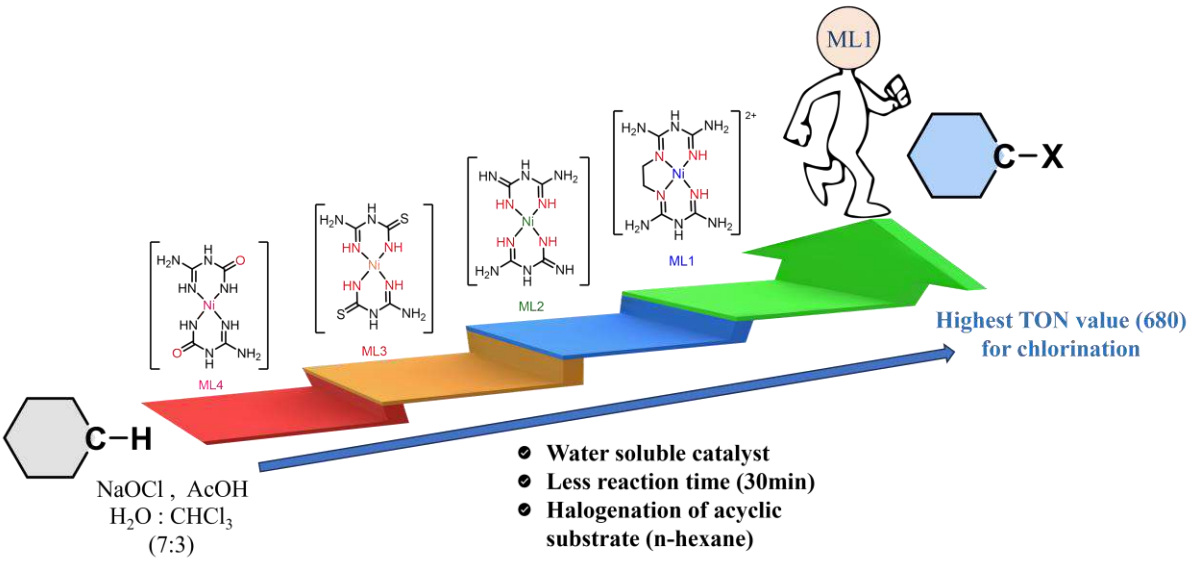
Water soluble Nickel(II)-Biguanide based complexes (ML1, ML2, ML3 and ML4,) were synthesised and characterised by various analytical techniques such as single crystal XRD (S-XRD), cyclic voltammetry (CV), ultraviolet-visible (UV-Vis) and high-resolution mass spectroscopy (HR-MS) etc.[a] These Ni-complexes successfully carried the C-H chlorination of a series of hydrocarbons using sodium hypochlorite (NaOCl) and acetic acid (AcOH) in water-chloroform mixture (7:3) at room temperature for 30 minutes. Here, NaOCl is acting as as an oxidant and a source of chlorine. The bond dissociation energy of the C(sp^3)-H bond of the substrates varies from 99.3 kcal mol^{-1} (cyclohexane) to 87 $kcal^{-1}$ (ethylbenzene).[b] Exclusively chlorinated products (TON: 680 ± 60 for cyclohexane) were obtained without any hydroxylated products, thus mimicking the activity of the halogenase enzyme. We successfully achieved C-H bond chlorination of *n*-hexane with high selectivity towards 2° products. Ni(III) species was identified by electron paramagnetic resonance (EPR) spectroscopy and the plausible mechanism for chlorination is confirmed by DFT calculation. Furthermore, C-H bond bromination of cyclohexane, *n*-hexane and toluene was also carried out using NaOCl in presence of NaBr and AcOH.



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Poster Presentation (PP-60)
International Conference on Emerging Trends in Catalysis & Synthesis (IC-ETCS 2024)

A Highly Chemically Robust 3D Interpenetrated MOF Heterogeneous Catalyst for the Synthesis of Hantzsch 1,4-Dihydropyridines and Drug Molecules

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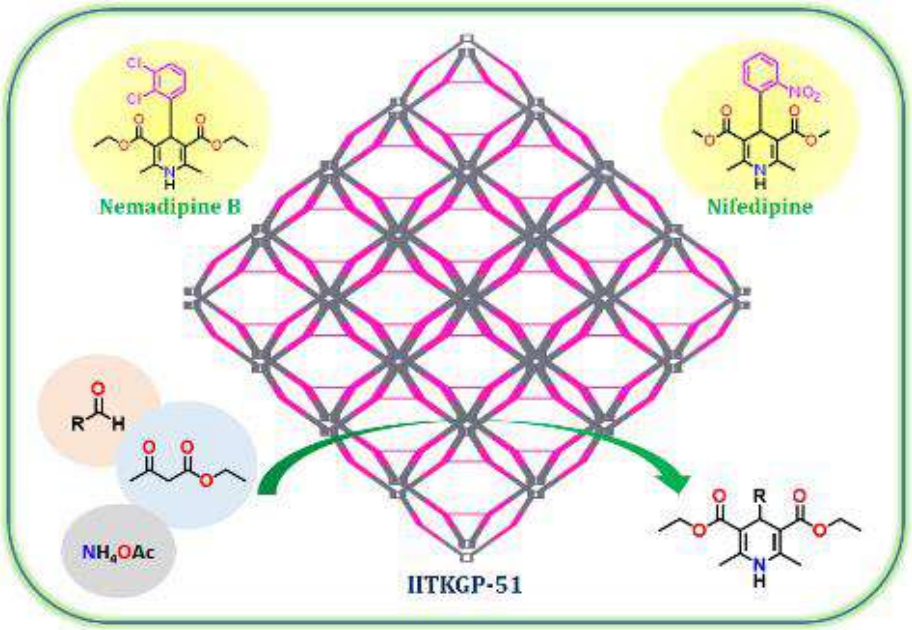
Metal-organic frameworks (MOFs) have attracted immense attention as efficient heterogeneous catalysts over other solid catalysts, however, their chemical environment instability often limits their catalytic potential.[a,b] Herein, utilizing a flexible unexplored tetra-acid ligand and employing the mixed ligand approach we have strategically developed a 3D interpenetrated robust framework, **IITKGP-51**, which retained its crystallinity over a wide range of pH solution (4-12).[c] Having ample open metal sites (OMSs), **IITKGP-51** was explored as a heterogeneous catalyst in one-pot Hantzsch condensation reaction, with low catalyst loading for a broad range of substrates. Synthesis of drug molecules remains one of the most significant and emergent areas of organic and medicinal chemistry. Considering such practical utility, biologically important Nemadipine B and Nifedipine drug molecules (calcium channel protein inhibitor) were synthesized for the *first* time by using this catalyst and fully characterized *via* SC-XRD and other spectroscopic methods. This report inaugurates the usage of a MOF material as a catalyst for the synthesis of drug molecules.



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Catalytic Enantioselective Friedel-Crafts Allenylic Alkylation

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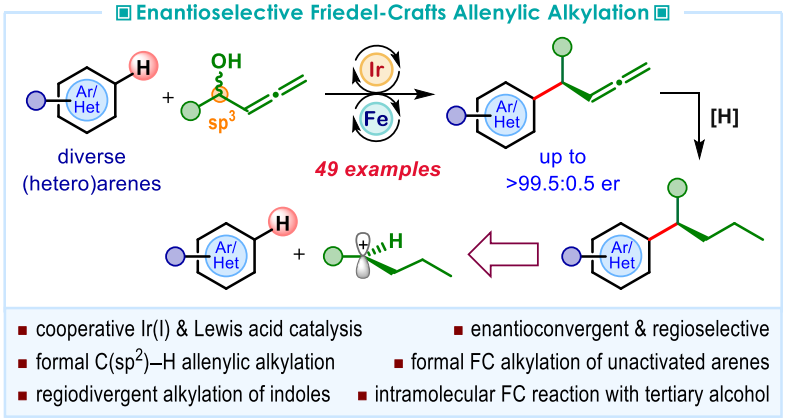
Despite the recent progress in C–H activation, Friedel-Crafts alkylation[a] remains a straightforward strategy for introducing unfunctionalized alkyl groups to (hetero)arenes. A multitude of catalytic methods have emerged for accomplishing enantioselective Friedel-Crafts reactions.[b] An overwhelming majority of these enantioselective FC reactions have mainly focused on electrophiles with sp^2 carbon centers,[b] with limited application of those with reactive sp^3 carbon centers.[c] Herein, the first catalytic enantioselective Friedel-Crafts (FC) allenylic alkylation reaction for the creation of central chirality has been developed under cooperative Ir(I)/(phosphoramidite,olefin) and Lewis acid catalysis.[d] Using racemic allenylic alcohol as the electrophile, this enantioconvergent reaction proceeds through an Ir(I)-stabilized allenylic carbocation intermediate,[e] which is intercepted with a variety of electron-rich arenes and heteroarenes. The resulting highly enantioenriched 1,1-disubstituted allenylic methanes, bearing a benzylic carbon stereocenter, are obtained with complete regiocontrol – both on (hetero)arenes as well as on the allenylic fragment. This protocol allows for the enantioselective formal introduction of 4-carbon alkyl chains into (hetero)arenes with the creation of a benzylic stereocenter. Judicious synthetic elaborations not only lead to formal enantioselective FC alkylation products of less electron-rich arenes but also of substituted arenes in *ortho*- and even *meta*-selective fashion. An intramolecular version of this FC allenylic alkylation has also been shown to proceed with promising enantioselectivity under the same catalytic conditions.



Scheme: Catalytic enantioselective Friedel-Crafts allenylic alkylation

References:

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Poster Presentation (PP-62)
International Conference on Emerging Trends in Catalysis & Synthesis (IC-ETCS 2024)

Harnessing solar driven organic transformation by metal dipyrrinato complexes

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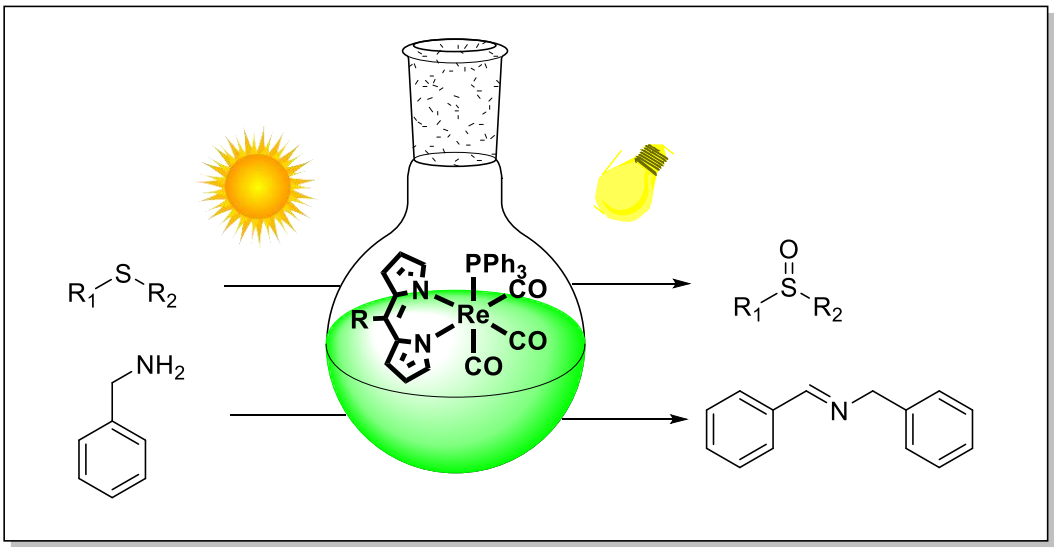
Photocatalysis has evolved as a flexible technique in recent decades, with applications ranging from environmental cleanup[1] to organic synthesis[2], as well as promising instances used for solar-driven organic transformations[3-4]. Visible-light photocatalysis has emerged as a key area offering environmentally friendly alternatives to various classic synthetic procedures[5]. The heavy metal complexes can be used as photosensitizers as it fulfils all the criteria for ideal photosensitzer. Rhenium(I)dipyrrinato complexes have emerged as promising candidates for photocatalytic applications in the light-induced aerobic oxidation of sulphides and amines due to distinctive features of these complexes, including their high absorption coefficients in the visible region, long-lived triplet excited states, and large quantum yields, endow them with remarkable photocatalytic properties[6]. This method showcases excellent conversion in presence of sunlight with low catalyst loading and reduced reaction time. The findings presented in this poster provide valuable insights into the potential of Rhenium(I)dipyrrinato complexes as innovative photocatalysts, paving the way for their application in various environmentally sustainable oxidation processes.



Scheme 1. Organic Transformation involving Metal Dipyrrinato Complex

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Enhanced Peroxidase Mimicking Catalytic Activity through Dynamic Metal Ion Crosslinked Novel Hydrogel

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Peroxidase enzymes, a diverse group of enzymes, are responsible for catalysing the oxidation of their substrate using peroxide, typically hydrogen peroxide. This process plays a crucial role in many biological systems[a], as well as bioanalytical and clinical chemistry[b]. Recently, there has been increasing interest in developing peroxidase enzyme mimics in order to overcome the limitations associated with natural enzymes such as high cost, complicated synthesis processes, and storage issues. In this study, we present the synthesis and characterization of a novel Fe^{3+}-crosslinked Poly(Acrylamide-co-Maleic acid) hydrogel, which exhibits catalytic properties similar to those of naturally occurring horse radish peroxidase (HRP) enzymes. The effectiveness of this hydrogel as a catalyst was evaluated using colorimetric assays with different substrates, including Pyrogallol and 3,3',5,5'-tetramethylbenzidine (TMB). Our results demonstrate that the Fe^{3+}-crosslinked hydrogel shows efficient catalytic performance and stability over a longer period of time, making it a promising candidate for a range of applications, such as environmental remediation and biomedical sensing. In conclusion, our study highlights the potential of Fe^{3+}-crosslinked hydrogel as a cost-effective and sustainable alternative to natural HRP enzymes. This novel hydrogel has significant implications for the development and advancement of various fields, and further research in this area could lead to ground-breaking discoveries.

Scheme 1. Fe^{3+}-crosslinked hydrogel for peroxidase like catalytic action.

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Synthesis of Quinoline-Based (NNP)Ni(II) Complexes: A Robust Catalyst System for C–H Alkylation of 2-Pyridones

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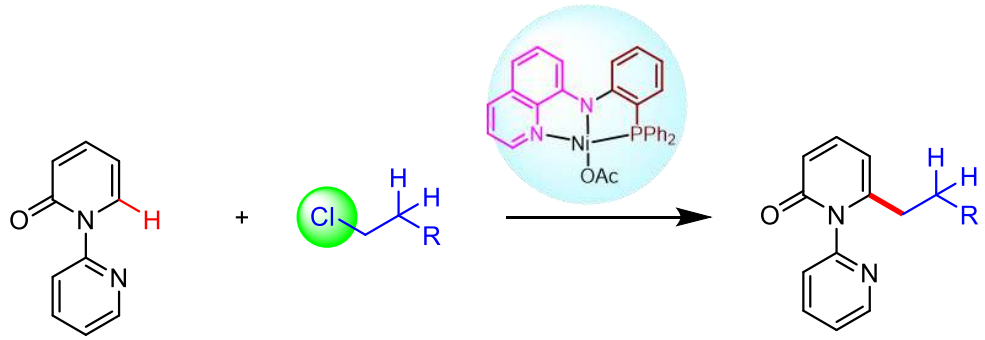
Abstract

The C−H bond alkylation of 2-pyridones has emerged as a powerful tool in organic chemistry, which helps in the improvement of chemical and biological properties of synthetically important compounds, including their lipophilicity and metabolic stability. Traditionally, C−H bond alkylation of 2-pyridones is demonstrated using activated coupling partners. Moreover, researchers have used 4d and 5d transition metals as catalysts, and most of these protocols have shown limited substrate scopes, multistep synthetic sequences and undesired products. In particular, the C6-alkylation of 2-pyridone with organic halide has not been precedented. In this presentation, we will discuss the selective C6 C(sp^2)–H bond alkylation of 2-pyridones with unactivated alkyl halides using a well-designed quinoline-based nickel pincer complex. This method shows a broad substrate scope and functional group tolerance. Alkyl halides containing alkenyl, silyl, ether, indolyl, and carbazolyl groups as well as polycyclic-steroid moiety work well under the reaction conditions. Moreover, we will discuss detailed mechanistic aspects of the reaction including the reaction scope and limitations.



Keywords: Alkylation, C–H Activation, 2-Pyridone, and Nickel Pincer Complex

Reference

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Poster Presentation (PP-65)
International Conference on Emerging Trends in Catalysis & Synthesis (IC-ETCS 2024)

Phosphite Catalyzed Atroposelective Dynamic Kinetic Asymmetric Transformations (DYKAT) of N-Aryl Isoquinolinium Salts

Pinku Saikia, [a, b] Susmita Maity, [a] Ayantika Bhattacharjya, [a] Aarthika Murugan, [a, b] Priyam Bajpai, [a, b] and Pradip Maity* [a, b]

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[b] Academy of Scientific and Innovative Research (AcSIR), Ghaziabad-201002 (India)

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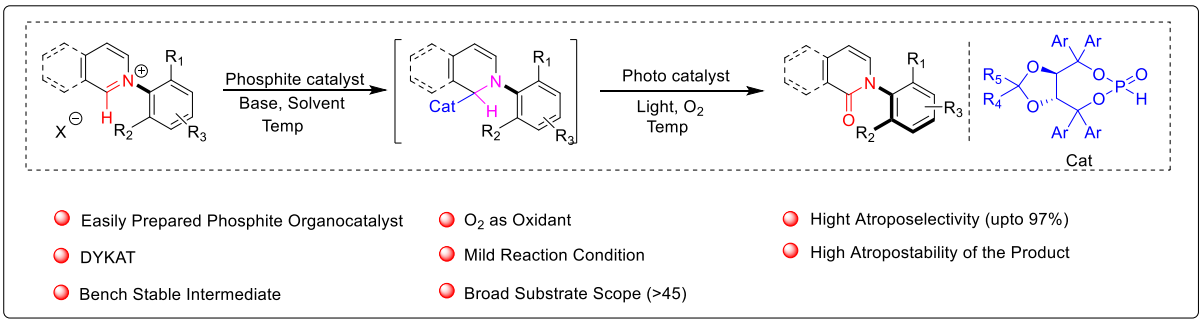
Axially chiral C-N bonds are widely found in bioactive molecules and natural products and used as chiral ligands for asymmetric catalysts. We utilized the captodative effect of phosphite catalyst to provide synergistic stability on α-radicals to explore an organocatalyst-bound alpha-amino radical formation and its subsequent catalyst-controlled functionalization. Computational studies support the atroposelective aerobic oxidation of N-aryl isoquinolinuim salt via dynamic kinetic asymmetric transformations. This strategy features easy operation, mild reaction conditions, high functional group tolerance, and very good enantioselectivities (up to 97% ee). Moreover, we were able to extend the substrate scope from isoquinolinium to pyridinium salts by changing the oxidant.



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Poster Presentation (PP-66)
International Conference on Emerging Trends in Catalysis & Synthesis (IC-ETCS 2024)

Asymmetric Construction of Vicinal All-C Quaternary and Tertiary Stereogenic Center in Acyclic Framework *via* Cu^{I} Catalyzed Claisen Rearrangement of Allyl-Vinyl Ethers

Subhransu Sekhar Pati and Jaya Prakash Das*
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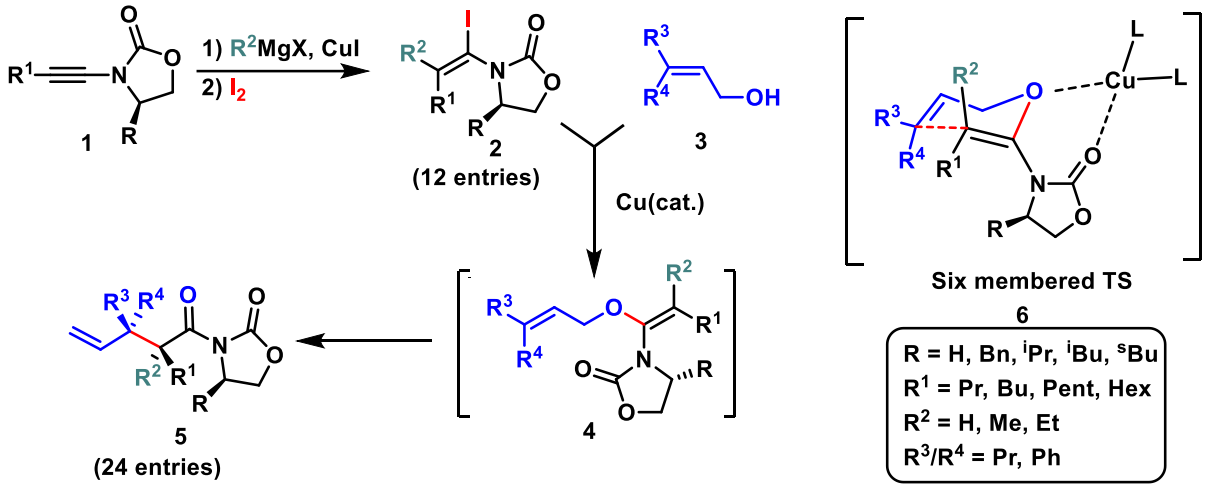
The Claisen rearrangement is considered as one of the most efficient methods for the construction of C-C single bond along with the formation of *γ, δ*- unsaturated carbonyl compounds. This reaction proceeds through a six-membered chair like (Zimmermann-Traxler) transition state with inherent diastereoselectivity. Furthermore, the construction of all carbon quaternary stereogenic centers along with contiguous stereo centers in an acyclic system is still a challenging task. This work focuses on the design of a novel domino process that consists of a metal-catalyzed C-O bond coupling and a subsequent Claisen Rearrangement with diastereo- & enantioselectivity, which leads to the construction of two adjacent stereocenters along with the desired all-carbon quaternary stereocenter. Details about this endeavour will be presented in the poster.



Scheme 1. Asymmetric Claisen rearrangement for construction of all-C quaternary and tertiary stereogenic center in 1,2-relationship

References:

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4) *Manuscript under preparation.*

Cyclometalated Ruthenium Complex Catalyzed Selective Synthesis of 2-substituted Benzimidazoles

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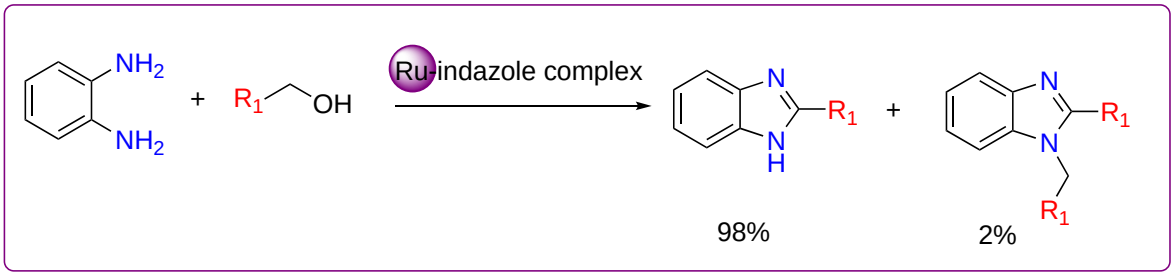
The catalytic activity of cyclometalated ruthenium complex is investigated for the selective synthesis of 2-substituted benzimidazole motifs through acceptor less dehydrogenative coupling of primary alcohols and diamines. Due to the various biological activity shown by the benzimidazole moiety, an efficient and selective method for the synthesis of benzimidazole is the need of the hour. A series of C,N-cyclometalated 2*H*-indazole Ru(II) complex bearing different substituents have been synthesized and characterized to investigate their catalytic activity. However, introducing bulkier substituent at the R_4 position of the phenyl ring of the 2*H*-indazole chelating ligand significantly enhanced the formation of 2-substituted benzimidazole over 1,2-disubstituted benzimidazole. The merit of this current catalytic protocol is advantageous due to its high selectivity over other conventional methods. Overall, the synthesis of substituted benzimidazole is achieved in excellent yield under microwave irradiation without formation of unwanted side products using the ruthenium catalyst. To the best of our knowledge, this type of selectivity and specificity have not been reported earlier in case of metal catalysed benzimidazole synthesis.



Scheme 1: Synthesis of 2-substituted benzimidazole catalysed by C,N-cyclometalated 2*H*-indazole Ru(II) complex

References: [a] R. Zhang, Y. Qin, L. Zhang and S. Luo, *Org. Lett.*, 2017, **19**, 5629–5632.

[b] X. Yi, Z. Zhao, M. Wang, W. Yu and J. Chang, *Org. Lett.*, 2022, **24**, 8703-8708.

Chemoselective Addition of Indole Derivatives to Donor Acceptor Cyclopropane: A Mechanistic Study Through Computational Approach

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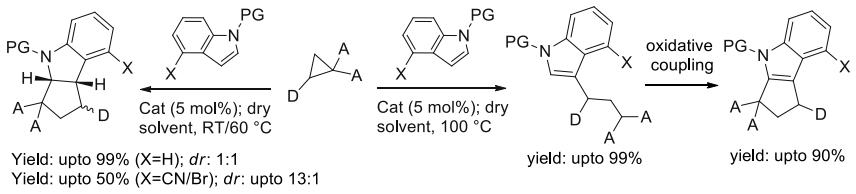
Cyclopropanes are essential building blocks in organic chemistry due to their unique reactivity and strained structure. The incorporation of donor and acceptor group at vicinal position generates the "push-pull'' effect that has been synthetically exploited to access 1,3-functionalized compounds including annulated products. During the reaction initial ring-opened products often undergoes annulation by suitably positioning of complimentary functionality. Understanding the unique electronic balance that governs the ring-opening of Donor-Accepter Cyclopropane (DAC) followed by closing or towards other competitive pathways are therefore essential with respect to various reacting partners. [1]

Indoles are ubiquitous nucleophile that are largely exploited as reacting partners to DAC leading to various indole based scaffolds.[2] Fine tuning the electronic effects of the substituents' on both cyclopropane as well as on the nucleophiles it is possible to significantly alter the reaction pathways.[3] Modern research employing advanced computational studies enables chemists to understand and manipulate between the competing reacting pathways leading to better regio- or stereocontrol of the reaction. The present work examines the reactivity of indoles *vs* 4-substituted indoles towards ring-opening or ring-opening annulation of DAC enrouting medicinally important cyclopenta[*b*]indole derivatives. The differential reactivity of indoles derivatives towards DAC has been explained with the help of computational approach. [4]



Scheme 1. Chemoselective addition of Indole derivatives towards DAC.

References:

[1] M. A. Cavitt, L. H. Phun and S. France,*Chem. Soc. Rev.*, **2014**,43, 804
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Poster Presentation (PP-69)
International Conference on Emerging Trends in Catalysis & Synthesis (IC-ETCS 2024)

Synthesis of Cyclopropane-fused Lactam *via* SET Oxidation

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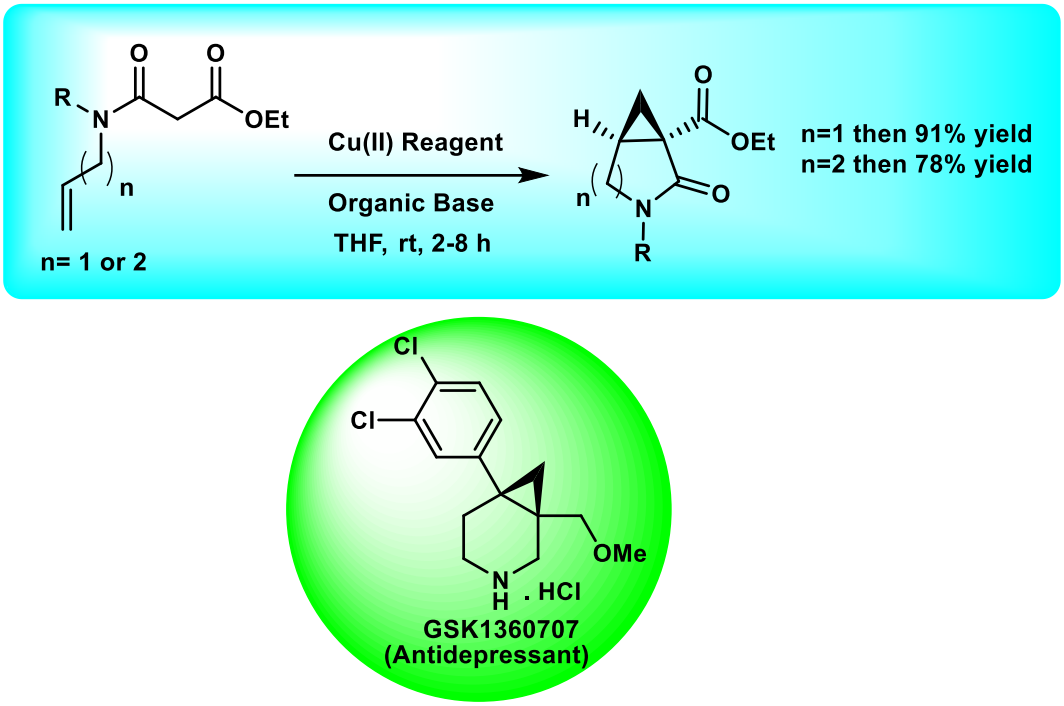
Abstract- An efficient and stereoselective synthesis of cyclopropane-fused lactam from *N*-allyl amidoester has been developed using copper (II)-mediated SET (Single Electron Transfer) oxidative cyclization as a key strategy.[1] The advantage of this unique transformation has been demonstrated with a wide variety of substrates to furnish novel cyclopropane-fused lactams in very good yields. This approach offers a convenient route to biologically active and pharmaceutically important 3-azabicyclo(n.1.0)alkane frameworks under mild conditions. The synthetic power of this methodology is exemplified in the concise synthesis of an antidepressant drug candidate, GSK1360707.[2]



Scheme 1. Synthesis of novel cyclopropane-fused lactams *via* SET oxidative cyclization.

References:

1. Zhang, N., Samanta, S. R., Rosen, B. M., Percec, V., *Chem. Rev*. **2014**, 114, 5848-5958.
2. a) Kirana, D. V., Kanak, K. D., Baskaran, S., *Angew Chem. Int. Ed*. **2017**, *56*, 16197-16201; b) Kirana, D. V., Kanak, K. D., Baskaran, S., *Chem. Comm*. **2019**, *55*, 7647-7650; c) Kirana, D. V.; Das, K. K.; Baskaran, S. *Org. Biomol. Chem.* **2021**, *19*, 4054-4059; d) Akriti, S., Lakshmanan, P., Baskaran, S., *Chem. Eur. J*. **2023**, *29*, e202300828.
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Visible Light-Enabled Decarboxylative Alkylation of Quinoxalin-2(1H)-ones using Alkyl Carboxylic Acids via Energy Transfer Process

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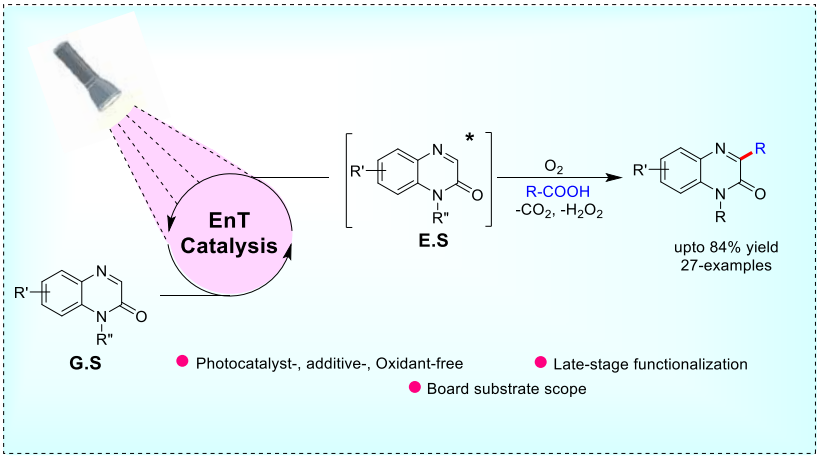
The development of efficient and sustainable methods for decarboxylative coupling processes is synthetically fascinating due to structural diversity, non-toxic nature, and vast commercial availability of carboxylic acids. However, challenges in the decarboxylation reaction persist primarily due to entailing oxidants, catalysts, and pre-functionalized conditions. Here, we described the photochemical decarboxylative alkylation of quinoxalin-2(1H)-ones using commercially accessible carboxylic acids with oxygen as sole oxidant through energy transfer process. The coupling of diverse array of alkyl carboxylic acids (1o to 3o) and bioactive acids with quinoxalin-2(1H)-ones was successfully accomplished to achieve the desired alkylated products.



Scheme 1. xxxxx

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[a] S. Singh, N. Dagar, S. R. Roy, *Chem. Commun*. **2022**, *58*, 3831–3834

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[c] M. Sun, L. Wang, L. Zhao, Z. Wang, P. Li, *ChemCatChem* **2020**, *12*, 5261–5268.

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[e] B. Sun, R. Shi, K. Zhang, X. Tang, X. Shi, J. Xu, J. Yang, C. Jin, *Chem. Commun*. **2021**, *57*, 6050–6053

Ir(III)-Catalyzed Site-Selective Introduction of Tyrosine Attached Peptides Based Diazoquinone to Oxindole at Ambient Temperature: Application in TMC-95A Synthesis

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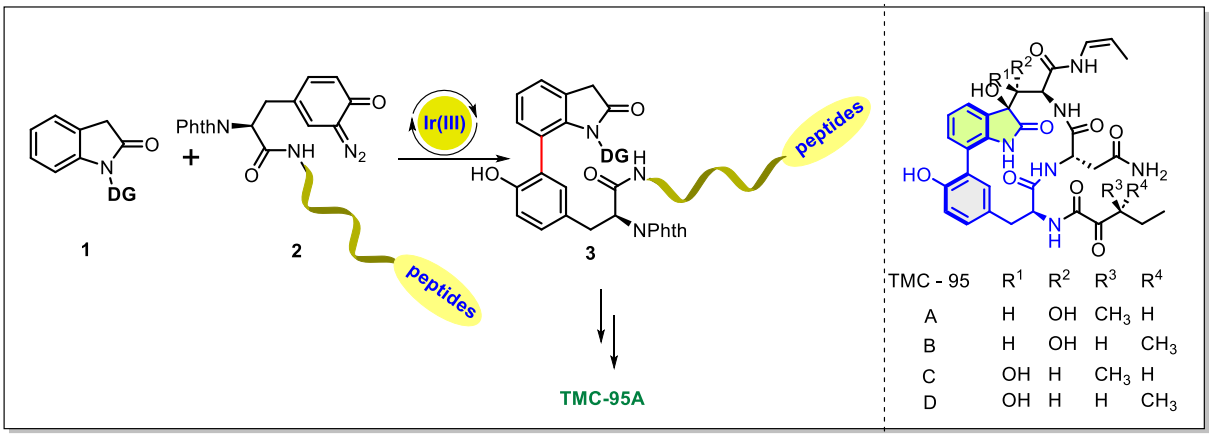
Diazoquinone is considered as one of the important coupling partner to introduce phenol/naphthol group in heterocycles.[1,2] An efficient Ir(III)-catalyzed redox-neutral method for the direct C7-arylation of oxindole using diazoquinone as coupling partner has been demonstrated. The strict regioselectivity is guided by the pyridyl substituent attached to the nitrogen of the oxindole ring. The developed method is simple, scalable and straight-forward with broad substrate scope. Also synthetic studies were done towards the construction of natural product TMC-95(A-D).[3]



Scheme 1: Ir(III)-catalyzed C7-arylation of oxindole using tyrosine attached peptide containing diazoquinone.

References:

1. a. H. T. Dao, P. S. Baran, *Angew.Chem.Int. Ed.* **2014**, *53*, 14382; b) S.Zhang, C. Jiang, J. Wu, X. Liu, Q. Li, Z. Huang, D. Li, H. Wang, *Chem.Commun.* **2015**, *51*, 10240; c) D. Das, P. Poddar, S. Maity, R. Samanta, *J. Org.Chem.* **2017**, *82*, 3612; d) K. Wu, B. Cao, C. Y. Zhou, C. M. Che, *Chem. Eur. J.* **2018**, *24*, 4815.

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Merging Photocatalytic Decarboxylative C–O/C-C Cross-Coupling from *α*, *β*-unsaturated carboxylic acid

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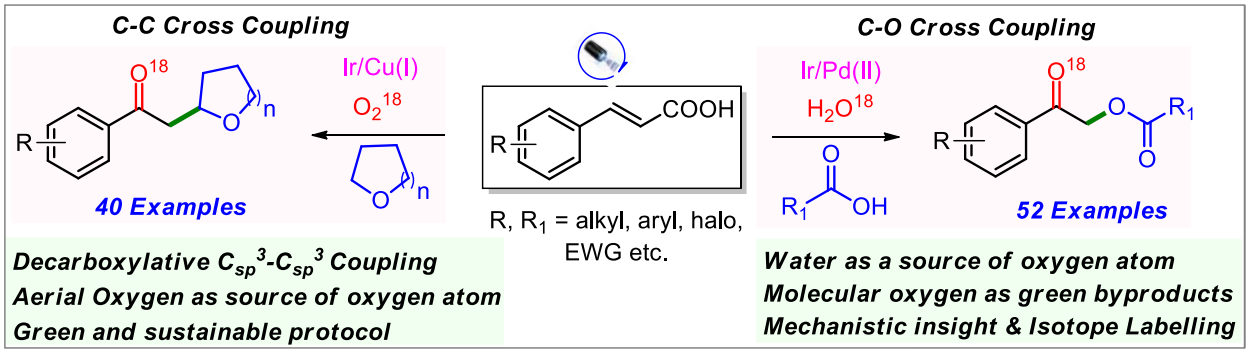
Herein, merged photocatalytic pathway for the C-O cross-coupled esterification of carboxylic acids and C-C bond formed *α*-alkylation of cyclic ether has been demonstrated. Decarboxylation of *α*,*β*-unsaturated acids promotes the formation of the *β*-ketone fragment of the desired product. Water as the source of oxygen for the ketone segment and aerial oxygen as an oxidant make esterification methodology green and sustainable. Subsequently, aerial oxygen as a source of oxygen in *beta*-ketone fragment makes alkylation pathway distinguishable from carboxylic acid. This new C=O and C-O/C-C bond-forming methodology takes place in a cascade manner under a dual Ir/Pd and/or Ir/Cu-catalytic pathway.



Scheme 1. Merging Photocatalytic Decarboxylative C–O/C-C Cross-Coupling from *α*, *β*-unsaturated carboxylic acid

References: [a] S. Mondal, S. Mondal, S. P. Midya, S. Das, S. Mondal, P. Ghosh*, *Org. Lett.* **2023,** 25(1), 184-189. https://doi.org/10.1021/acs.orglett.2c04041**. [b] S. Mondal,** S. Mondal.; S. P. Midya, P. Ghosh*. [Manuscript under preparation]

One-pot telescopic approach to synthesize disubstituted benzimidazoles in deep eutectic solvent

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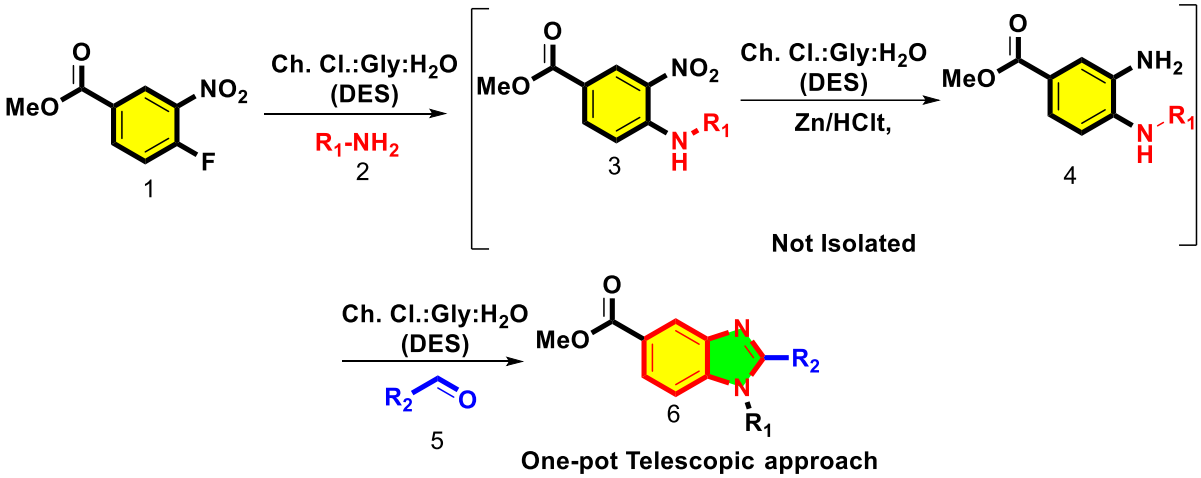
An ongoing challenge in the pharmaceutical sector is the need to find and implement novel synthetic approaches because traditional methods sometimes violate the principles of green chemistry. While benzimidazoles are of great importance as building blocks for the creation of molecules having pharmacological activity, the development of methods for their sustainable synthesis has been a challenge for organic synthesis. Herein, we have carried out a one-pot telescopic approach to the synthesis of disubstituted benzimidazole derivatives in a deep eutectic solvent (DES) medium to investigate an alternate synthetic technique. Starting with methyl 4-fluoro-3-nitrobenzoate, S_NAr reaction, reduction, and cyclization were performed with choline chloride/glycerol/H_2O as DES medium, which gave the best performance out of the five DESs examined. We report the synthesis of disubstituted benzimidazoles via one-pot telescopic approach.



Scheme 1. One pot telescopic approach for the synthesis of benzimidazole DES medium.

References:

[1] Das, S.; Chanda, K. Synthesis (Stuttg). 2023. (Published)

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Pd-Catalyzed Oxypalladation: Why does Solvent Polarity Control the Chemoselectivity?

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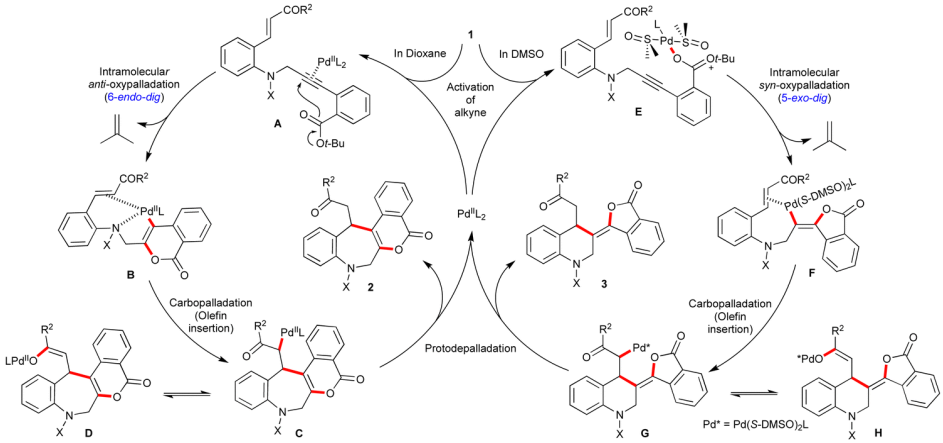
Palladium-catalyzed, chemodivergent, intramolecular, oxypalladation–initiated cascade sequences can give rise to functionalized benzazepines **2** and tetrahydroquinolines **3** from the alkynes bearing tethered nucleophilic carboxylic ester and electrophilic enone functionalities. These benzo-fused nitrogen heterocycles are the building blocks of enormous biologically active natural products and synthetic drug molecules. Particularly, the seven membered aza-heterocycle, *i.e.* benzazepine, is embedded in some bioactive molecules having antidepressant, anxiolytic, anti-obesity and neuroleptic activities. On the other side, tetrahydroquinolines containing six-membered nitrogenous heterocycle, are embedded in numerous bioactive compounds that exhibit antibacterial, antifungal, cytotoxic, antimalarial, anticancer, and anti-HIV properties. However, there is a surprising solvent-dependent selectivity found in the synthesis of these valuable heterocycles.[a] Benzazepine is formed in low polarity solvent e.g. 1,4-dioxane, while tetrahydroquinoline is formed in high polarity solvent e.g. DMSO, from the same substrate. In order to understand the molecular role of the solvent in controlling the chemoselectivity, we have performed detailed mechanistic study computationally. The olefin insertion step is found to be rate-determining, and the crucial role of the solvent molecules in controlling the energetics of this step has been identified which can be immensely helpful for further reaction design in environmentally green solvent like water.



Scheme 1. Solvent–dependent selectivity in Pd-catalyzed cascade reactions.

References: [a] A. Gupta, T. Jandial, M. Karuppasamy, N. Bhuvnesh, S. Nagarajan, C. U. Maheswari, V. Sridharan, *Chem. Commun.* **2023**, *59*, 5233.

Reactivity Studies of 4-Hydroxy-2*H*-chromene-2-thione: C=S Plays Crucial Role for the Formation of Linear Product Chromeno[2,3-*b*] chromene and Some of Their Anti-proliferative and ROS Study

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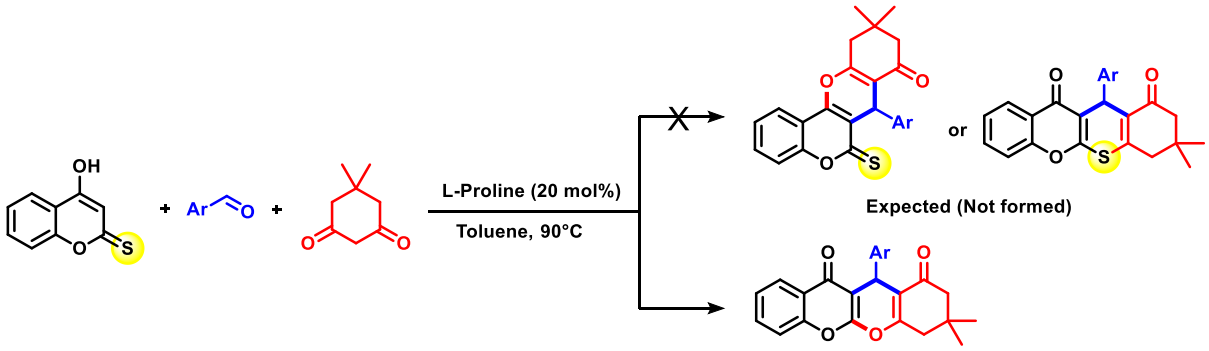
The reactivity of 4-hydroxy-2*H*-chromene-2-thione is investigated with aryl aldehydes and 5,5-dimethylcylohexane-1,3-dione (dimedone) in the presence of 20 mol% L-proline in toluene. The hitherto unreported products, 1,2-substituted chromeno[2,3-*b*]chromenes, were obtained in good to excellent yields instead of the linear product having sulphur atom in the ring provided by 4-hydroxydithiocoumarin or an angular product obtained from 4-hydroxycoumarin. The reaction proceeds through a three-component reaction via Knoevenagel condensation between dimedone with an aromatic aldehyde followed by Michael addition with 4-hydroxy-2*H*-chromene-2-thione. In addition, a molecular docking study of all derivatives was performed, and among them, four compounds exhibited anti-proliferative activity and elevated ROS generation in breast cancer (MCF7) cell lines.



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Photophysical properties of protonated and free base 5,15-bisferrocenyl-10,20-bisphenylporphyrin and 5-ferrocenyl-10,15,20-triphenylporphyrin

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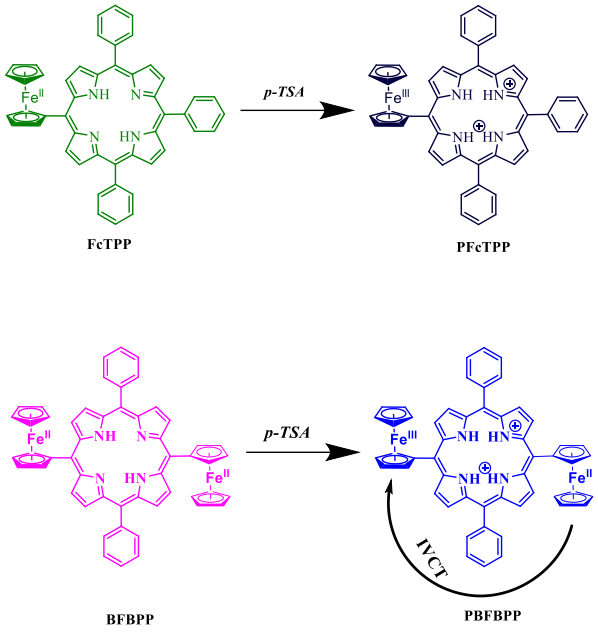
Porphyrins possess strong absorption and fluorescence in the visible region of electromagnetic radiations, which makes them more suitable in various applications[1]. Porphyrins can be protonated at acidic pH and can respond to various external stimuli such as pH, light, heat etc.[2-4] The electroic properties can be tuned by protonation of the porphyrin core. In ferrocenyl porphyrin oxidation of ferrocene results in ligand to metal charge transfer (LMCT) or inter valence charge transfer (IVCT).[3] In this work, we have synthesized 5,15-bisferrocenyl-10,20-bisphenylporphyrin(BFBPP) and 5-ferrocenyl-10,15,20-triphenylporphyrin(FcTPP). The synthesized compounds were characterized by ^{1}H-NMR spectroscopy and studied its photophysical properties in the form of protonated and free base porphyrin by UV-Visible spectroscopy. Upon protonation with *p*-toluenesulfonic acid, in FcTPP, LMCT was observed at 747 nm. Whereas IVCT was observed in BFBMP at 824 nm due to oxidation of iron Centre from Fe^{2+} to Fe^{3+} (mixed valence state) which makes the molecule to absorb in the NIR region.



Scheme 1: Synthesis of PBFBPP and PFcTPP.

References:

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Poster Presentation (PP-77)
International Conference on Emerging Trends in Catalysis & Synthesis (IC-ETCS 2024)

Design and Development of a Malachite Green-Based NIR-Responsive PRPG for Cancer Treatment

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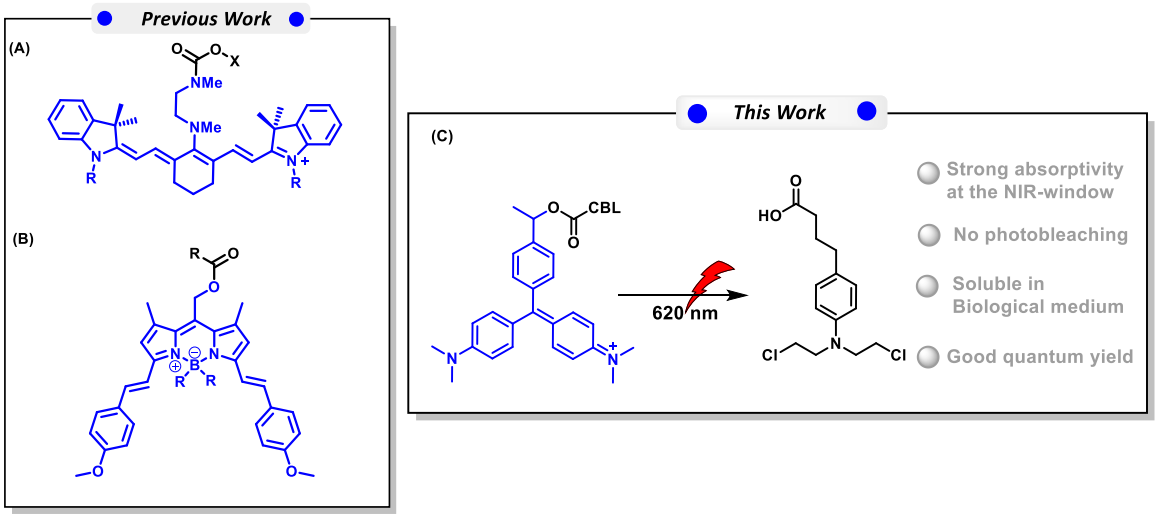
Abstract:
Photocontrolled removal of protecting groups (PRPGs) has provided a platform to the researchers for photopatterning, peptide synthesis, and drug delivery, achieving spatial and temporal control over the release process. An enormous amount of effort has been made into the design and development of visible light-activated PRPGs, which limits their applicability in terms of low tissue penetration ability and phototoxicity. In this regard, NIR light-activated PRPGs offer greater tissue penetration depth, low phototoxicity, and less scattering effect. Notably, the utilisation of cyanine and boron-dipyrromethene BODIPY-based NIR chromophores for preparing NIR-PRPGs has recently attracted attention. However, only limited NIR-responsive PRPGs are known in the literature.

Malachite Green (MG) stands out for its NIR absorptivity and resistance to photobleaching. Hence, in this manuscript, we developed MG-based PRPG. Our developed meso-MG-PRPG released the caged molecules in the NIR region (620 nm) via the formation of a carbocation intermediate. However, we observed a low photochemical quantum yield. To overcome this limitation, we redesigned secondary meso-MG-PRPG, and interestingly, we observed a clean photorelease within 3 h, having a quantum yield of 0.05. Overall, this approach expands the research path towards a futuristic photo-controlled toolbox for potential biological applications.

Figure/Scheme (if any):



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Visible Light-induced EDA-mediated C-3 Coupling reaction of Quinoxalin-2(1*H*)-ones with Unactivated Aryl Iodides

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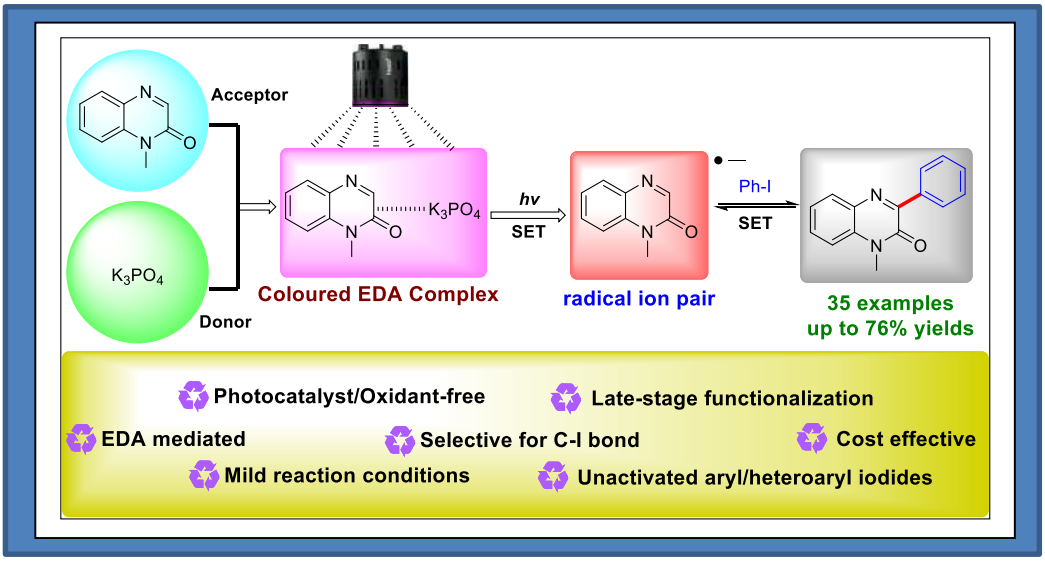
Visible light-induced C-3 arylation of quinoxalin-2(1*H*)-ones with aryl iodides with good yields *via an* EDA-complex formation has been accomplished. Both aryl/heteroaryls iodides and quinoxalin-2(1*H*)-ones possessing electron-donating as well as electron-withdrawing groups were coupled well to access the desired products in good yields. The radical scavenging, EPR, UV-visible experiments, and quantum yield revealed that the reaction went through a radical pathway *via* a SET process. Furthermore, the protocol could also be applied for late-stage functionalization, which illustrated the practicability of the present protocol.



Scheme 1. C-3 Coupling reaction of Quinoxalin-2(1*H*)-ones.

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Ru(II)-Catalyzed Deoxygenative Formal [3+1+2] Benzannulation of Allyl Alcohols and Acetylenediesters via C−H Activation and Site-Selective Carbon−Carbon Triple Bond Cleavage

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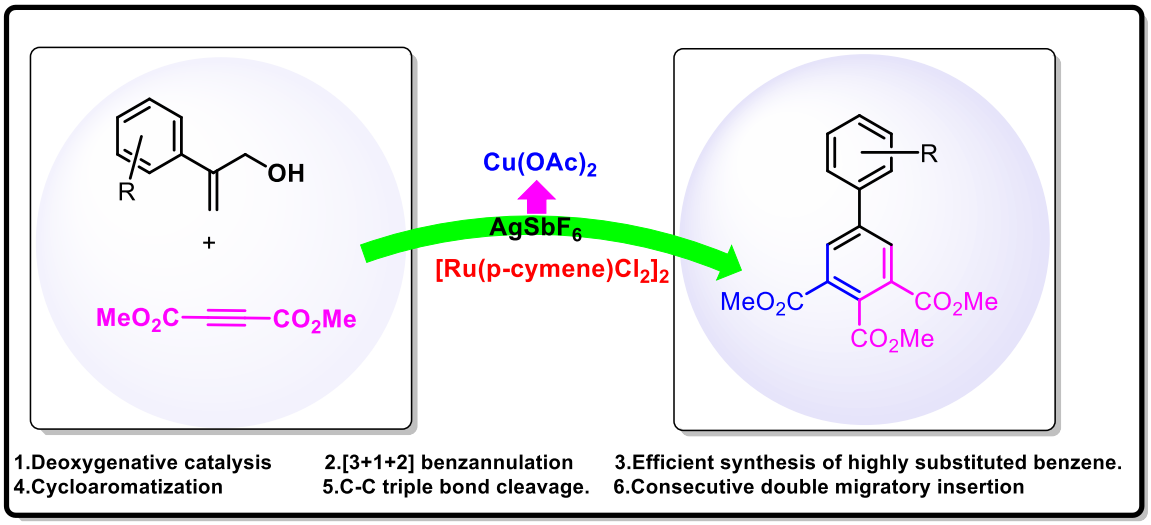
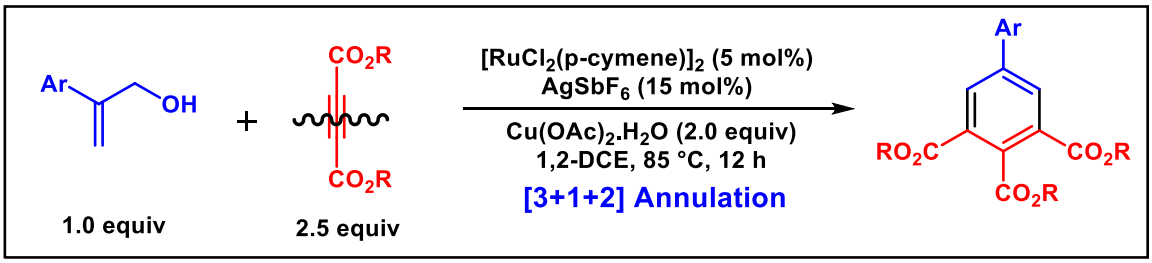
An unprecedented Ru(II)-catalyzed deoxygenative, site-selective formal [3+1+2] benzannulation reaction for the efficient synthesis of highly substituted benzene molecules is reported. This reaction between allyl alcohols and acetylenediesters proceeds via cascade C-H activation, consecutive double migratory insertion with alkynes, and cycloaromatization followed by unusually specific C-C triple bond cleavage.

Figure 1 :- Graphical Abstract.





Scheme 1. Ruthenium-catalyzed cleavage of alkyne in intermolecular annulation reactions between allyl alcohols and acetylenedicarboxylate esters.

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Brønsted Acid and Ni (II)-catalyzed C-H Oxidation/Rearrangement of Cyclotriveratrylenes (CTVs) to Cyclic and Acyclic Quinones as Potential Anti-cancer Agents

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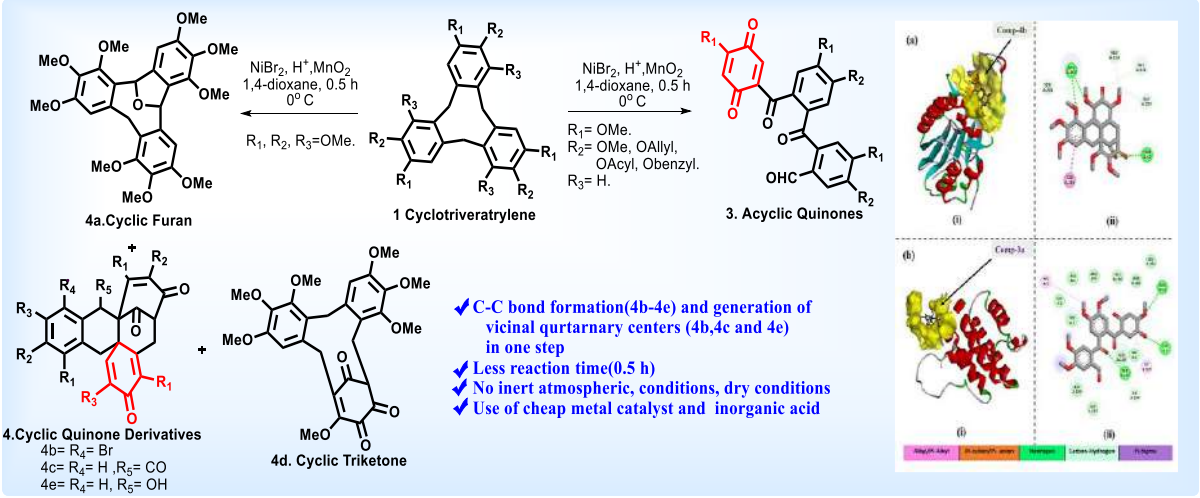
Quinones represent the most prevailing framework of numerous biologically active natural products and pigments that exhibit antioxidant, anti-inflammatory, antibiotics,[1] anti-microbial,[2] and anti-cancer [3,4] activities. Moreover, quinone-derived scaffolds are abundant in redox-active natural compounds associated with several biological processes like photosynthesis in plants and bacteria, coenzyme Q functions, vitamins K and E activities. quinones can be accessed from phenols, 1, 4-dihydroxybenzenes and dimethoxybenzenes by oxidizing agents. However, synthesizing these quinone moieties in complex molecular systems, especially in natural products, is a still challenging task.

In this work we describes a simple and practical protocol for the direct synthesis of acyclic and cyclic quinone derivatives *via* an acid-promoted nickel (II) catalyzed inner rim C-H oxidation of cyclotriveratrylene[5-7] (CTV) and its analogues. The cyclic quinone derivatives are resulted from trimethoxy-cyclotriveratrylene (TCTV) through C-C bond formation *via* intramolecular *ipso* substitution followed by subsequent anionic rearrangement containing stereo-vicinal quaternary centers. All the newly synthesized compounds were screened for their *in vitro* anti-cancer activity using colorimetric SRB assay analysis. Out of which, some compounds exhibited moderate anticancer activity against A549, HCT-116, PC-3, MDA-MB-231, HEK-293 and SW620 human cancer cell line.



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Metal–organic frameworks with open metal sites act as efficient heterogeneous catalysts for Knoevenagel condensation and the Chan–Lam coupling reaction

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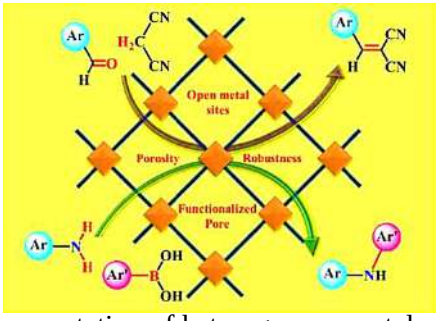
In the heart of organic synthesis, C-C and C-N bond formation reactions are of great importance due to their utility in forming biologically important entities and pharmaceutically active molecules, tailor-made therapeutics, smart optoelectronic materials etc.[a,b] Knoevenagel condensation and Chan-Lam cross-coupling are two widely studied reactions in this field for C-C and C-N bond formation, respectively. Several methods using homo- and heterogeneous catalysis are being developed for these reactions under mild and ambient condition. Owing to the drawbacks of homogeneous catalysts regarding their reuses and separations, the development of efficient, highly stable, and sustainable heterogenous catalysts for C-C and C-N bond formation reaction is of immense interest and challenge for scientists.

In this endeavour, Metal-Organic Frameworks (MOFs) are being widely explored as heterogeneous catalysts due to structural diversity, robustness, presence of Lewis acidic open metal sites, permanent porosities and functionalized pore surface [c,d]. Herein, the acylamide functionalized tetra-carboxylic acid (H_4CDA) has been successfully employed for the formation of two robust 3D-MOFs, **Cd-CDA-MOF** and **Cu-CDA-MOF**, having open metal sites with two distinct and diverse network topologies namely diamondoid and PCU. The **Cd-CDA-MOF** is shown to act as an efficient heterogeneous catalyst for the Knoevenagel condensation reaction under ambient conditions. The **Cu-CDA-MOF** demonstrates excellent catalytic activity for the Chan–Lam coupling reaction with a considerably high turnover number. The heterogeneous catalytic activity of the MOFs can be attributed to the coordinatively unsaturated open metal sites of the activated frameworks. The MOFs are found to be recyclable with almost uniform catalytic activity.



Scheme 1. Schematic representation of heterogeneous catalysis with functionalized MOFs.

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Poster Presentation (PP-82)
International Conference on Emerging Trends in Catalysis & Synthesis (IC-ETCS 2024)

Enantioselective total synthesis of Adociasulfate-1 and Merosterolic acid-A

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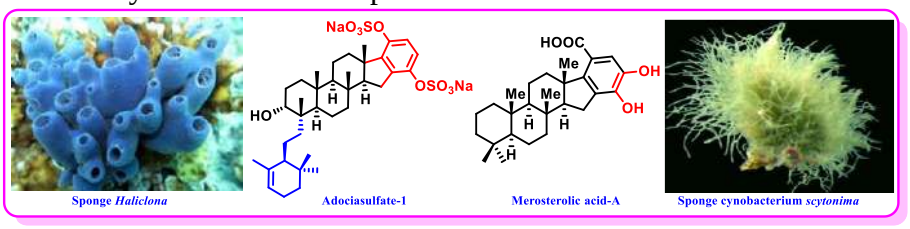
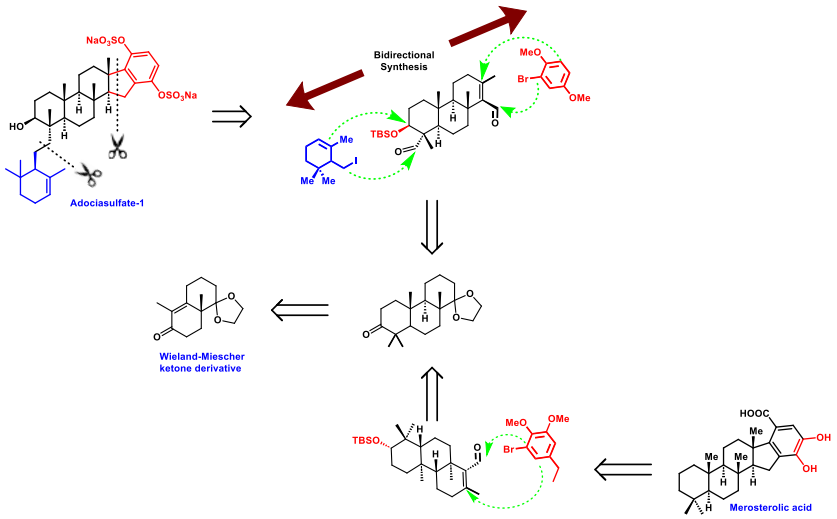
Abstract: The enantioselective total syntheses of highly complex Hexacyclic marine natural product adociasulfate-1 which inhibit members of the kinesin motor protein super family in the low micromolar range and the first kinesin inhibitors identified that are not nucleotide analogue has been achieved. Key elements of the synthetic route include the use of Robinson-type annulation reaction to construct the tricyclic terpenoid building block and lewis acid mediated friedal craft reaction for construction of indane ring and regioselective sp^3 (C–H) activation for paving the way for construction of hexacyclic framework.
The first enantioselective total synthesis of Merosterolic acid A, a pentacyclic marine meroterpenoid, has been achieved. The notable points in the synthetic route are synthesis of a highly functionalized tricyclic diterpenoid moiety starting from an enantiopure Wieland–Miescher ketone derivative in concise manner via Robinson-type annulation and an elegant hydrogen atom transfer olefin reduction followed by Lewis acid-catalyzed Friedel–Crafts reaction for C–C bond formations to construct the indane ring, resulting in completion of the pentacyclic meroterpenoid skeleton. This route also enables the determination of absolute configuration of the synthesized natural products.



Retrosynthetic Scheme:



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Poster Presentation (PP-83)
International Conference on Emerging Trends in Catalysis & Synthesis (IC-ETCS 2024)

Pd-Catalyzed Tandem Pathway for Stereoselective Synthesis of (*E*)-1,3-Enyne and 1,3,5-Tri(het)aryl Benzene from β-Nitroalkenes by Using a Sacrificial Directing Group

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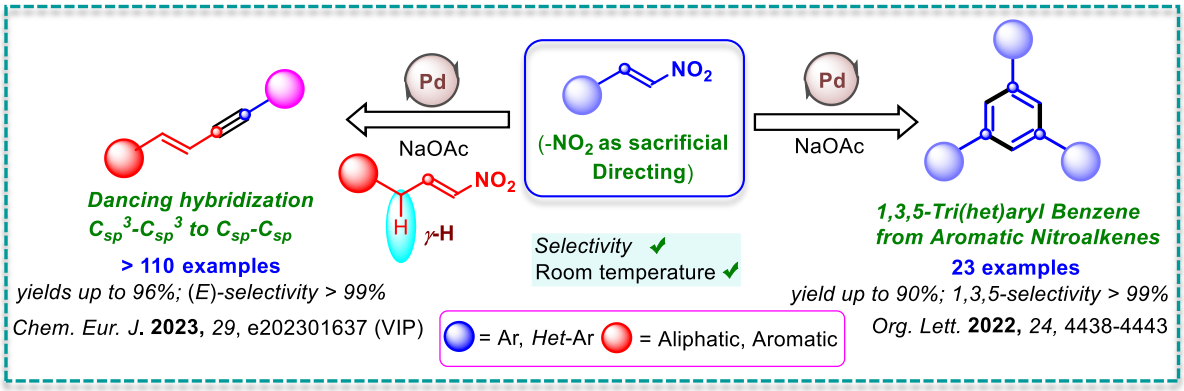
The involvement of nitroalkenes instead of minimal one alkyne motif for (*E*)-1,3-enynes and 1,3,5-tri(het)aryl derivatives synthesis through a palladium catalyzed stereoselective bond forming pathway at room temperature is presented. Implication of nitro group as a sacrificial directing group, formation of magical alkyne on a newly developed Csp3- Csp3 bond with initial palladium-MBH adduct make this methodology distinctive. This protocol features an unprecedented sequential acetate addition, carbon-carbon bond formation, isomerization of double bond and nitromethane degradation in a tandem catalytic walk via dancing hybridization. Mechanistic understanding through identification of intermediates and computational calculations furnishes complete insight into the tandem catalytic pathway. Broad substrates scope and functional groups tolerance make this synthetic methodology magnificent and dynamic. This represents the first example of stereoselective 1,3-enyne synthesis exclusively from alkene substrates by introducing the concept of sacrificial directing group.



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Poster Presentation (PP-84)
International Conference on Emerging Trends in Catalysis & Synthesis (IC-ETCS 2024)

Synthesis of D-Ribose based "*N-CH₂-C*" linked Hybrid Oligo Triazolamers using Click & Vinyl Sulfone Chemistry

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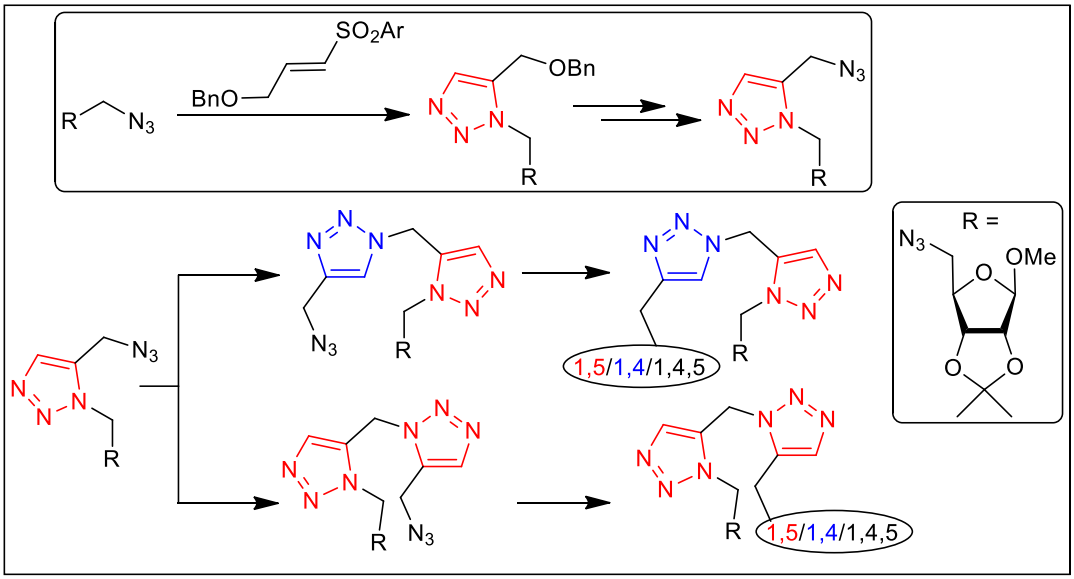
Triazolamers composed of 1,4-disubstituted triazoles (1,4-DTs) were reported as being reminiscent of a peptide β-strand conformation and had shown a broad spectrum of applications.[1] These triazole-based oligomers where monomeric triazole units are connected by "*N-(CH)n-C*" linkage forming mostly a linear chain by iterative sequential growth cycle in a one pot manner.[2] However, triazolamers constructed using 1,5-disubstituted triazoles (1,5-DTs) or in combination with differently substituted triazoles such as 1,4-DTs/1,5-DTs/1,4,5-trisubstituted triazole (1,4,5-TTs) remained under-explored. The metal free vinyl sulfone-based route[3] established in our laboratory was used to synthesize 1,5-DTs linked homo and hetero bis, tris and tetra triazolamers using sugar residues. A combination of simple Huisgen triazolylation, "Click" chemistry and vinyl sulfone chemistry afforded hetero triazolamers. Synthesis of some of these triazolamers will be presented in the poster.



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Poster Presentation (PP-85)
International Conference on Emerging Trends in Catalysis & Synthesis (IC-ETCS 2024)

Total Synthesis and Biological Evaluation of Elgonene Natural Products

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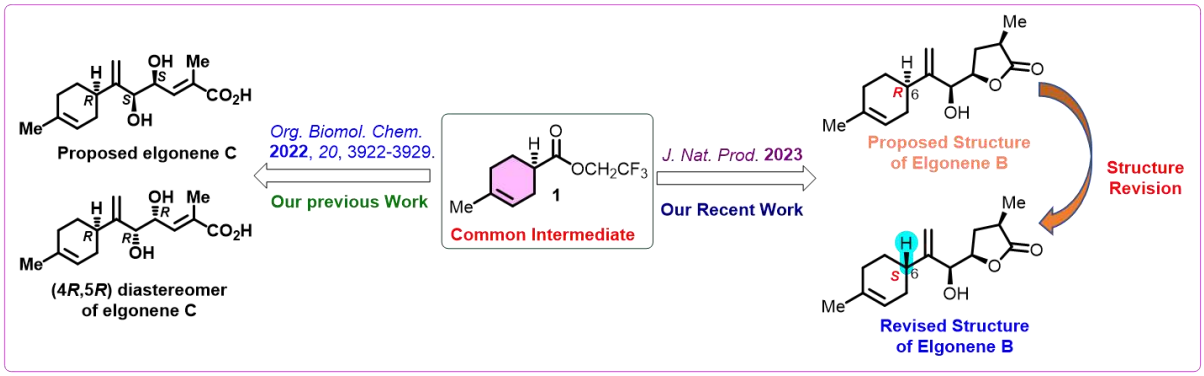
Natural products with appreciable bioactivities play a significant role in the discovery and development of new medications. A majority of FDA-approved drugs between 1981 to 2019 were inspired by natural products or synthetic molecules based on natural product pharmacophores.[1] Therefore, it is important to synthesize new biologically active natural products and determine their further activities for drug discovery and development. However, the isolation of natural products is quite often associated with immense challenges, and in many instances, only minute amounts of natural products are purified. Stadler and co-workers isolated 12 new secondary metabolites, namely, elgonenes A−L, from a Kenyan basidiomycete in 2019.[2] Among them, elgonene B was isolated in a small quantity (0.49 mg), which prevented the isolation group from studying its biological activity. The small amount of the compound also can make structure elucidation challenging. Organic chemists play a crucial role in producing a reliable and abundant supply of these natural products through total synthesis. In 2022, we completed the total synthesis of proposed elgonene C and its (4*R*, 5*R*) diastereomer using intermediate **1**.[3] But the spectral and analytical data of our synthetic compounds do not match the isolation data provided by the isolation group, which indicates that structural revision is required for the proposed elgonene C. Recently, we have completed the first total synthesis of elgonene B using the same intermediate **1**, consequently resulting in a revision of the originally proposed structure by inverting the configuration at the C-6 carbon.[4] The preliminary biological activities of revised elgonene B and its diastereomers showed no significant cytotoxic and antibacterial activities.



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Poster Presentation (PP-86)
International Conference on Emerging Trends in Catalysis & Synthesis (IC-ETCS 2024)

Asymmetric Synthesis of Oxindoles having a C3-Quaternary Stereocenter via NHC-catalyzed Desymmetrization of 1,3-Diols

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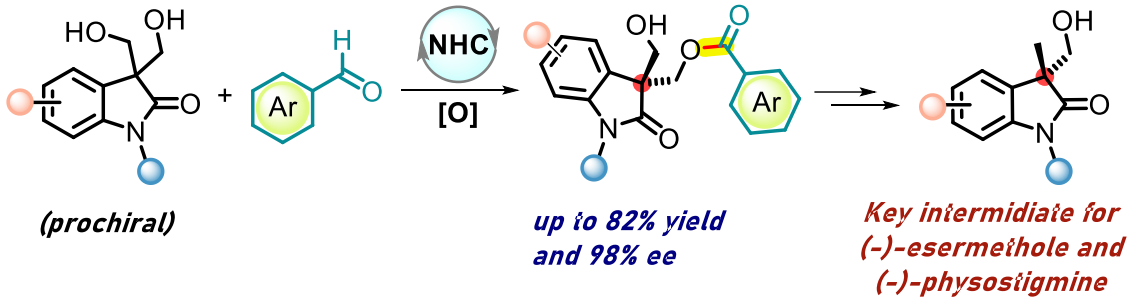
Oxindoles possessing an all-carbon quaternary stereocenter at the C3 position are privileged structural motifs. They constitute the core of many biologically relevant compounds and natural products. Consequently, different effective strategies for enantioselective synthesis of such targets have been reported. Among them, the catalytic asymmetric desymmetrization of prochiral oxindoles raises significant interest but remains highly challenging. Over the decades, oxidative NHC catalysis has emerged as a powerful strategy for asymmetric synthesis[1] and our group is actively involved in developing new asymmetric organic transformations utilizing this process.[2] Very recently, we have demonstrated an efficient strategy for NHC-catalyzed asymmetric desymmetrization of oxindoles having C3-quaternary stereocenter.[3] This process involves the selective transfer acylation of prochiral diol using oxidative NHC-catalysis, where readily available aldehydes are used as acylation agents. The reaction enables easy access to diversely functionalized C3-quaternary oxindoles with excellent enantioselectivity and good to moderate yields. The synthetic potential of the process is further illustrated by the preparation of a key intermediate for (-)-esermethole and (-)-physostigmine. During the poster presentation, reaction design, substrate scope, and synthetic utilities of the catalytic asymmetric desymmetrization process will be discussed in detail.



Scheme 1. NHC catalyzed asymmetric desymmetrization of 1,3 prochiral diol.

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Reactivity of 1,3-Enyne Boronates: Modular Access of Heteroatom-rich BCMs and Iterative Cross-Coupling Partners

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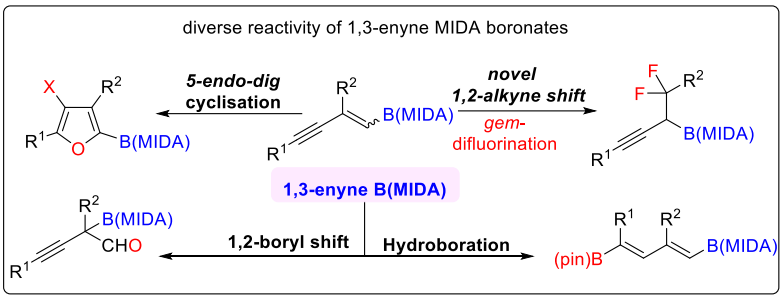
The Discovery of a new class of heteroatom-rich boron-containing molecules (BCMs) and iterative cross-coupling (ICC) partners created a toolbox for future drug developments using organoboron compounds. Herein, we report the potential utility of 1,3-enyne MIDA boronates to access diverse gem-difluoro MIDA boronates via novel 1,2-alkyne shift. Furthermore, we demonstrated the synthesis of various novel furan-based BCMs via 5-endo-dig cyclization and iterative coupling partners via copper-catalyzed hydroboration and platinum-catalyzed diboration reaction.



Scheme 1. Diverse reactivity of 1,3-enyne MIDA boronates

Poster Presentation (PP-88)
International Conference on Emerging Trends in Catalysis & Synthesis (IC-ETCS 2024)

Bi(III)-Catalyzed Synthesis of Substituted Furans from Hydroxy-oxetanyl Ketones: Application to Unified Total Synthesis of Natural Products

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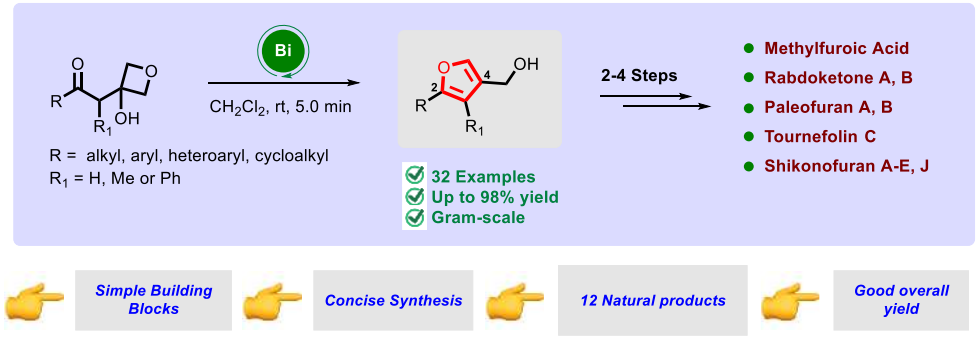
We report an improved synthetic protocol for hydroxy methyl-derived polysubstituted furans employing Bi(III)-catalyzed dehydrative cycloisomerization of α-hydroxy oxetanyl ketones. This procedure provides rapid access (within 5 min) to highly substituted furans with exceptional functional group diversity, excellent yields, scalability, and operationally simple reaction conditions. Further, it demonstrated the utility of this method in the concise total synthesis of twelve 2,4-disubstituted furan-derived natural products (including methylfuroic acid, rabdoketones A and B, paleofurans A and B, tournefolin C, and shikonofurans A-E and J). The key step includes a selective organo-catalyzed cross-ketol addition, $Bi(OTf)_3$-catalyzed dehydrative cycloisomerization of α-hydroxyoxetanyl ketones to yield furans, chiral-phosphoric acid (TRIP)-catalyzed asymmetric prenylation as a key step to induce the chirality and a hydrogen atom transfer (HAT)-mediated oxidation of primary alcohols into the corresponding acids.



Scheme 1. Graphical abstract for method development and synthesis of twelve 2,4-furan-derived natural products.

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[a] P. Kataria, S. S. Sahoo and R. Kontham* *J. Org. Chem.* **2023**, *88*, 7328−7346.

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Poster Presentation (PP-90)
International Conference on Emerging Trends in Catalysis & Synthesis (IC-ETCS 2024)

Synthesis, Characterization and Bioactivity Studies of Novel 1,4,5-Trisubstituted Triazoles Derived from Cycloaddition of Azides and Chalcones

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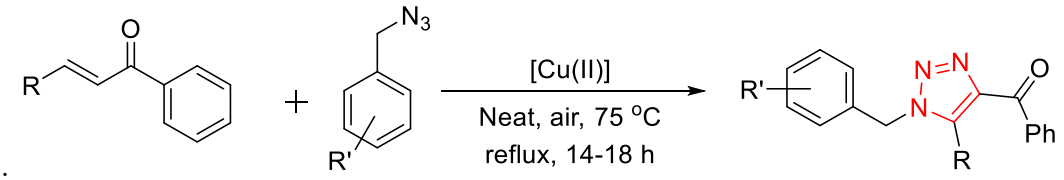
Abstract: The synthesis of various substituted triazoles has attracted organic chemists due to their interesting structural aspects and versatile biological significance. In this regard, investigations were carried out to synthesize new 1,4,5-trisubstituted triazoles using Cu(II)-catalysis through the cycloaddition of different chalcones with azides under neat methodology. A series of triazole derivatives was prepared from moderate to excellent yields. All the products were structurally characteized bt analytical and spectroscopic techniques. The influence of externally added ligands on catalysis reactions of $Cu(NO_3)_2$ is discussed. Notably, these derivatives exhibited potential cytotoxic characteristics against MCF-7 cancer cell lines.



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Photocatalyzed C(sp3)-H functionalization for Synthesis of α, β-unsaturated Ketones

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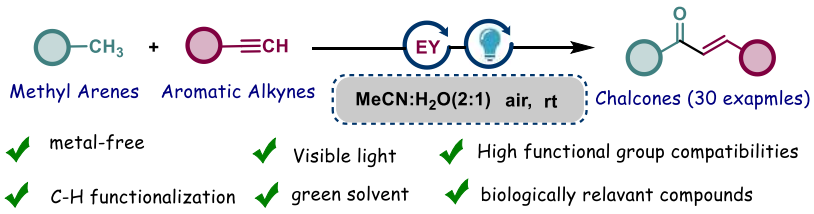
Despite significant progress in the last decade in forming carbon-carbon bonds through transition metal-catalyzed cross-coupling processes, there remains a scarcity of and high demand for metal-free cross-coupling reactions in the hydroacylation of aromatic alkynes via Csp3-H functionalization. In this context, we present a reliable metal-free approach for synthesizing α, β-unsaturated ketones (chalcones) through Csp3-H functionalization. This method utilizes MeCN:H_2O as a green solvent, Eosin Y as an organic photocatalyst, and ambient air as an oxidant. Notably, this strategy effectively transforms various methyl arenes and aromatic alkynes into the desired product. With its high atom efficiency, use of green solvents, metal-free nature, environmental friendliness, and reliance on visible light as a renewable energy source, this approach is compatible with biologically active molecules.



Synthesis of Vinyl-1,5-Disubstituted 1,2,3-Triazoles as an Efficient Building Blocks: Metal Free Route from Vinyl Sulfones

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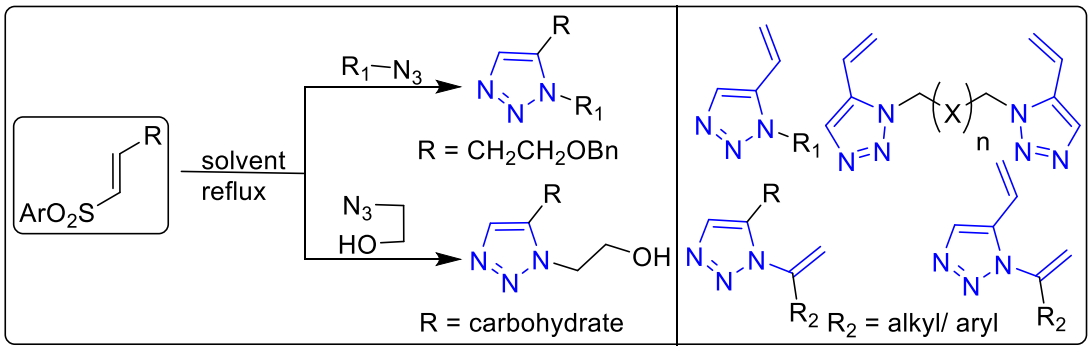
Vinyl sulfones are now oftenly used for the regioselective and metal-free synthesis of 1,5-disubstituted 1,2,3-triazoles (1,5-DT's) from our lab.[1] Suitably functionalized vinyl sulfones can be used to synthesize 1,5-DT's with various biological and material application.[2] Recently, we have identified vinyl sulfone **1** containing CH_2CH_2OBn group as a highly useful building block for the synthesis of a wide range of 1,5-DTs. The vinyl sulfone **1** on reactions with various mono-, bis-organic azides at elevated temperature afforded 1,5-DTs. Further functionalization lead to the selective introduction of vinyl and functionalized vinyl groups into the C- and N- positions of 1,5-DTs.[3] Using this synthetic strategy carbohydrate modified vinyl sulfones afforded carbohydrate functionalized N-vinyl-1,5-DTs.



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Unveiling catalyst-free electro-photochemical reactivity of aryl diazoesters and facile synthesis of oxazoles, imide-fused pyrroles and tetrahydro-epoxy-pyridines *via* carbene radical anions

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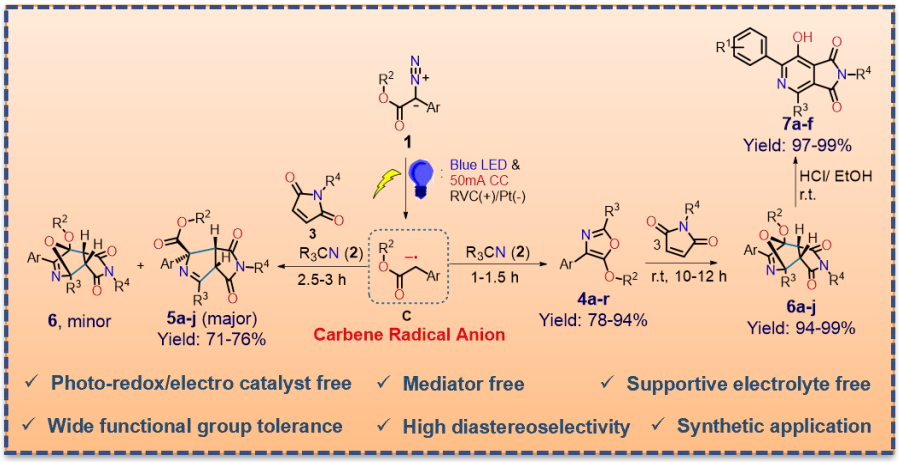
Electrochemistry has played a pivotal role in driving various organic transformations in recent past. Simultaneously, photochemistry has served as a potent energy source for diverse organic reactions over an extended period. However, in recent years, the synergistic combination of electrochemistry and photochemistry has emerged as a powerful strategy to facilitate and modulate organic transformations through single-electron redox pathways. Towards this venture, while thermal and photochemical decomposition of aryl diazoesters, with or without metal catalysts, has been extensively explored in synthetic organic chemistry, the electro-photochemical reactivity of aryl diazoesters has remained underexplored., In an effort to bolster the concept of Electro-Photochemistry EPC and to explore the electro-photochemical reactivity of diazoesters, we reported[a] an EPC reaction of diazoesters driven by electricity (50 μA) and a blue LED (5 W) to produce radical anions which on subsequent reactions with acetonitrile or propionitrile and maleimides, resulted in the formation of diverse oxazoles, diastereoselective imide-fused pyrroles, and tetrahydroepoxy-pyridines (Scheme 1). The reaction is reagent free (devoid of catalyst, supporting electrolyte, oxidant and reductant) with excellent atom economy, high yield and good diastereoselectivity. Our comprehensive mechanistic investigation, including a 'biphasic e-cell' experiment, supports a reaction mechanism involving a carbene radical anion. Notably, the tetrahydro-epoxy-pyridines obtained can be smoothly converted into fused pyridines resembling vitamin B6 derivatives. Importantly, the electric current required for the EPC reaction can be supplied by a simple cell phone charger, making the process easily accessible. Furthermore, the scalability of the reaction to the gram level has been demonstrated, and the product structures have been confirmed through crystal structures, 1D and 2D NMR, and HRMS data



Scheme 1.

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SYNTHESIS, CHARACTERIZATION AND APPLICATIONS OF NOVEL FUNCTIONALIZED TERPYRIDINES

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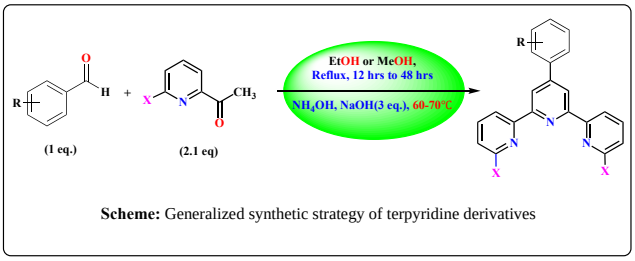
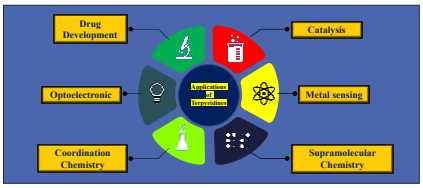
Abstract:

Terpyridine derivatives have garnered substantial attention due to their versatile utility in various domains, including coordination chemistry, catalysis, and supramolecular chemistry. 2,2':6',2''-Terpyridine and its functionalized derivatives are classified as Pincer-type ligands, featuring three binding sites with low lower-lying unoccupied molecular orbitals (LUMO). This characteristic earns them the reputation of being NNN-tridentate ligands, and their complexes serve as catalysts in challenging transformations. As researchers persist in their pursuit of novel synthesis approaches and application domains, terpyridine derivatives are poised to make noteworthy contributions to the advancement of diverse scientific frontiers. However, terpyridine ligands, when combined, form closed-shell octahedral complexes with enormous applications in supramolecular chemistry. This abstract highlights the synthesis and characterization of innovative terpyridine derivatives and their potential implications in catalytic organic transformations and bio-activities. The creation of terpyridine derivatives involves modifying the fundamental terpyridine molecule through a spectrum of chemical reactions, including substitution, addition, and complexation transformations. These alterations are orchestrated to customize the attributes of terpyridine for precise applications. Typical paths of synthesis include the functionalization of pyridine rings or the integration of substituents into the terpyridine framework. The scrutiny of terpyridine derivatives is crucial to validate their structures and characteristics. Diverse analytical methodologies are harnessed, encompassing nuclear magnetic resonance (NMR) spectroscopy, mass spectrometry, infrared spectroscopy (IR), and X-ray diffraction (XRD).



Scheme: Generalized synthetic strategy of terpyridine derivatives



Scheme: General synthetic strategy of functionalized terpyridines and **Figure:** Possible applications in different fields.

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First-Row Transition Metal Complexes Utilising Amido-Based Ligand Frameworks: Application in C-H, O-H Activation and Asymmetric Catalysis

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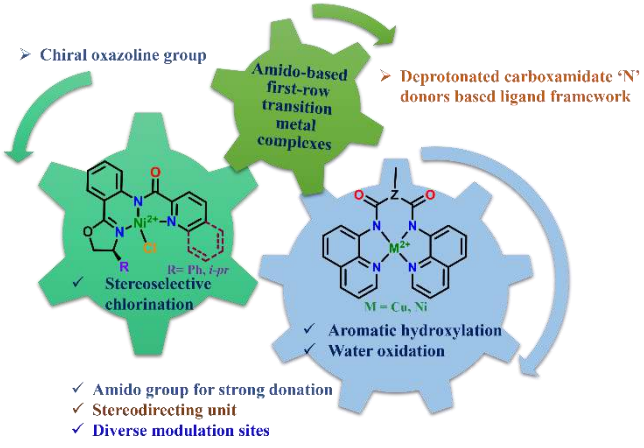
The incorporation of deprotonated carboxamidate 'N' donors into the ligand framework imparts distinctive properties that can significantly influence the reactivity, stability, and selectivity of metal complexes.[a] Taking this into account, Ni(II) and Cu(II) complexes consisting of tetradentate-amido quinoline ligands (L1 and L2) were synthesized and characterized by various analytical methods. Cu(II) complexes effectively catalysed the single-step hydroxylation of aromatic C-H bonds using H_2O_2 as an oxidant without using an external base and afforded greater than 90% selectivity for phenol with a TON of 810 for benzene. Based on our experimental findings (KIE value, Hammett plot, EPR, etc.) DFT calculations, a plausible mechanism for aromatic C-H hydroxylation was proposed Where Cu(II)-OOH was the reactive intermediate.[b] In case of Ni (II) complexes, a metal-based II/III oxidation process was observed at 1.07 V and a ligand-based electron oxidation process at 1.67 V, associated with a large electrocatalytic water oxidation (WO) wave in a non-aqueous solvent to which water has been added as a limiting reagent.[c] The non-innocent behaviour of the ligands helps to enhance the multielectron catalysis by facilitating electron–proton transfer. Moreover, the KIE value also indicates an atom–proton transfer (APT) mechanism.



A chiral catalyst of Ni(II) complexes using chiral tridentate amido-oxazoline ligands were developed to synthesize enantiomerically pure chiral organic molecules. Chlorination of benzylic C-H bonds using NaOCl as an oxidant in the presence of acetic acid catalysed by these chiral Ni(II) complexes showed excellent enantiomeric excess within a short reaction time of 30 minutes.

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Alkoxide Assisted Secondary Selective Functionalization of 1,2-Bis-boronic Esters Under Photoredox Catalysis

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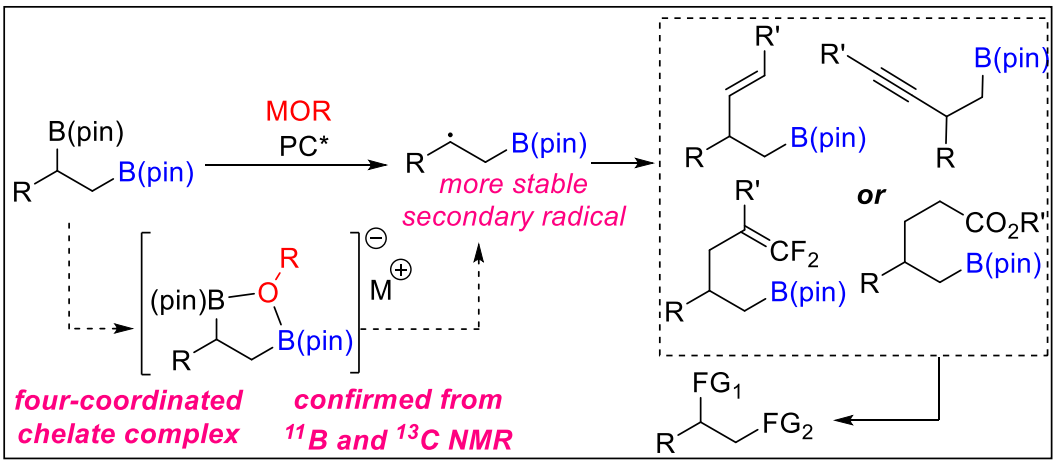
Organoboron compounds have been playing an increasingly important role in organic synthesis due to their low toxicity, commercial availability, stability and easy synthesis from available starting materials.[1] Site-selective functionalization of the C-B bond of 1,2-bis-boronic esters has been proven to be an important method for the generation of 1,2-functionalized compounds in a highly stereoselective manner.[2] Herein, we introduced a photoredox activation of the chelated complex generated from the 1,2-bis-boronic esters and an alkoxide base for the generation of secondary radicals over primary for the diverse stereoselective transformations.[3] We have explored previously unknown site-specific alkenylation, allylation, alkynylation and 1,4-addition to aryl vinyl trifluoromethane. The realization of such site-specific transformations, followed by downstream manipulations, holds promise for accessing homoallylic and homopropargylic compounds, which are present in a large number of marketed drugs and bioactive compounds. Furthermore, straightforward transformations of the resultant products can be seamlessly converted into natural products, substituted tetrahydrofurans, and bioactive compounds. Also, details ^{11}B-NMR & DFT studies have been conducted to elucidate the mechanistic detailed.



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Tandem Acylation and Aromatization of Vinylogous Esters for the Regiospecific Synthesis of 6-Acyl Resorcinols

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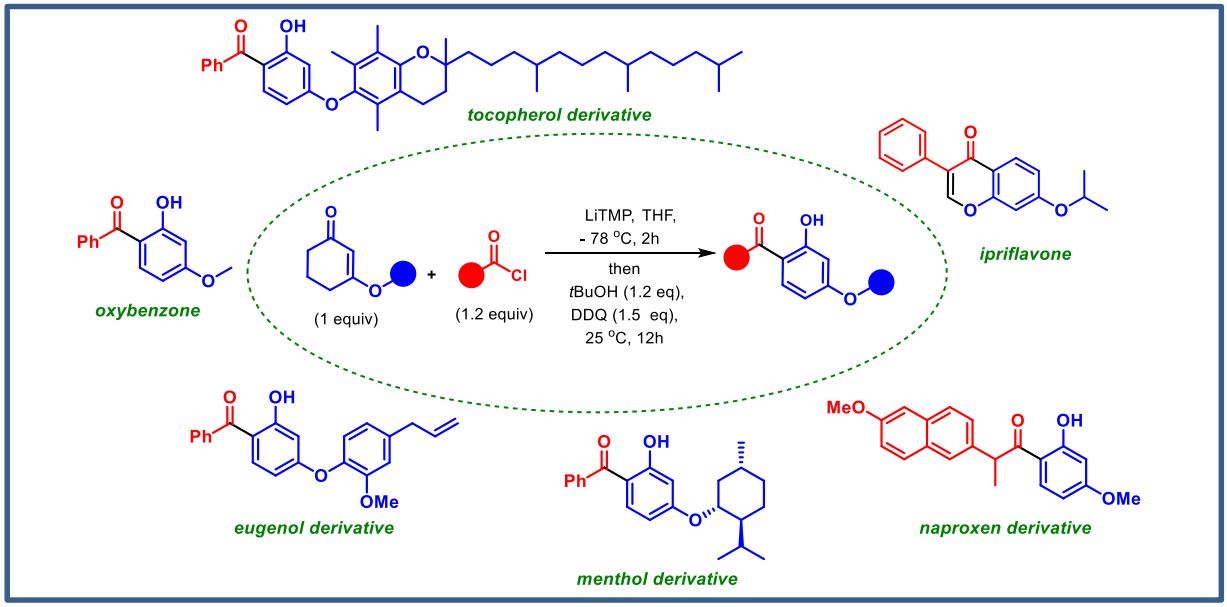
A new methodology was proposed for the direct conversion of vinylogous esters into monoprotected 6-acyl resorcinols (4-alkoxy-2-hydroxy arylketones) in a regiospecific manner. Vinylogous esters, derived from 1,3-cyclohexadione, underwent sequential one-pot acylation and oxidative aromatization, resulting in selectively variously protected 6-acyl resorcinols. Acylation of vinylogous esters poses a challenge as the reactive intermediates, namely 6-acyl/4-acyl 3-alkoxy cyclohexenones, are highly sensitive, undergoing retro-Claisen condensation and reverting to its starting materials. Inorder to overcome this challenge an oxidizing agent was directly added to acylating mixture to obtain 6-acyl resorcinols. DDQ and $PhI(OAc)_2$ were identified as excellent reagents for aromatization. The application of this method has been extended to the total synthesis of natural products. Additionally, the method has been adapted for vinylogous thioesters, yielding 6-acyl 3-thio phenol derivatives in a regiospecific manner.



Scheme 1. Synthesis of 6-acyl resorcinols from vinylogous esters

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Poster Presentation (PP-97)
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Metal-free Approaches Towards C-N Bond Formation

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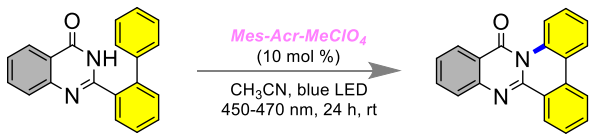
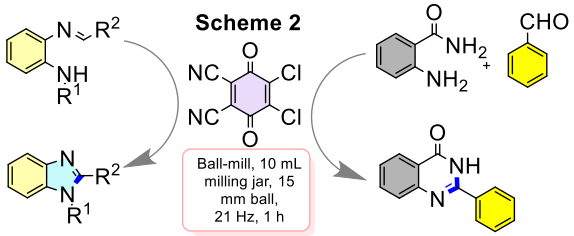
The demand for sustainable energy sources and mild metal-free reaction techniques in synthetic organic chemistry have surged due to growing environmental concerns and global warming. To combat with issues associated with metal catalysed reactions like poor atom economy, extreme sensitivity for moisture and air, difficulties in purifications etc., metal free strategies have emerged as alternatives. Visible light photocatalysis is the most pronounced one which can selectively transform substrates by avoiding the use of high thermal energy and stochiometric amount of reagent. Similarly, solvent-free mechanochemical procedures are another greener alternative that can make the world more sustainable by following the "Twelve Principles of Green Chemistry".[1] Here, a straightforward photocatalytic regioselective intramolecular C-N coupling reaction is illustrated for the construction of 14*H*-quinazolino[3,2-f]phenanthridin-14-one employing the Mes-Acr-MeClO$_4$ (9-mesityl-10-methylacridinium perchlorate) as a visible light organoredox photocatalyst (Scheme 1).[2] In addition to that 2,3-Dichloro-5,6-dicyano-1,4-benzoquinone (DDQ) mediated oxidative C-N coupling toward the synthesis of 1,2-disubstituted benzimidazoles and substituted quinazolin-4(3*H*)-one derivatives under the solvent-free mechanochemical (ball milling) condition is also discussed (Scheme 2).[3]

Scheme 1



Bhanja, R.; Bera, S. K.; Mal, P., Chem. Commun. 2023, 59, 4458

Scheme 2



Bera, S. K.; Bhanja, R.; Mal, P., Beilstein J. Org. Chem. 2022, 18, 646

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Cu doped Carbon Dot for highly efficient catalyst for alkyne-azide cycloaddition

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In recent years, carbon dots (CDs), a quasi-spherical 0D carbon- based nanoparticle have emerged as the rising star of the carbon nanomaterial family due to their tunable photoluminescence property, non-toxic nature, abundance of surface functional group and excellent photo stability[1]. Due to the formation of the exciton-PL semiconductor, CDs possess photoexcited electron which could be efficiently transferred from CDs to other molecule, showing potential in electron transfer assisted catalytic reactions. The Cu-catalysed Huisgen 1,3 dipolar cycloaddition reaction between terminal azides and alkynes is the most elegant example of click chemistry has wide range of application in organic synthesis and electrochemical and biological uses[2]. However, difficulties in purification during the formation of Cu (1) from Cu (II), and high cost of Cu (1) releasing ligands and complexity in catalyst synthesis limit the scope of the Click chemistry. Herein, we report Cu doped carbon dot as an effective catalyst for Click reaction. The sample was synthesized using 0.1 mmol of benzyl azide, 0.12 mmol of alkyne and 20 mg catalyst, stirred in the presence of UV light. Precipitation of the solid product confirmed the formation of the product, with a conversion percentage of 90%.

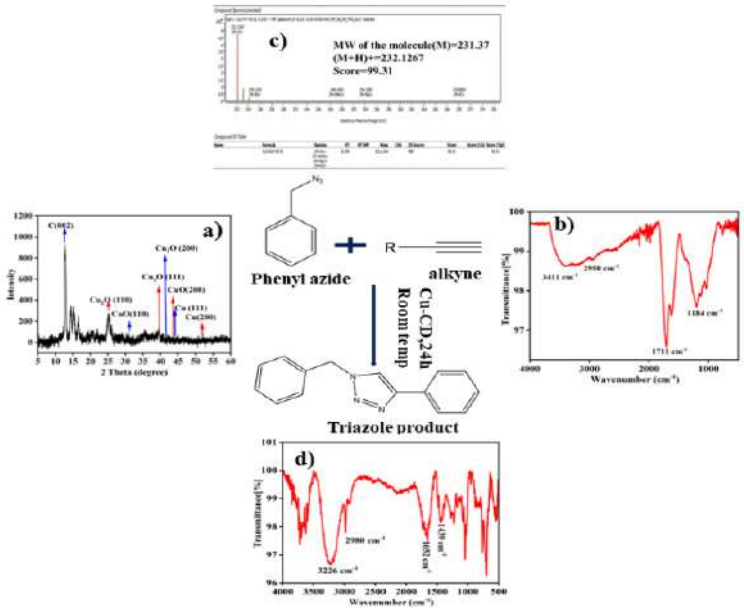

Fig 1. (a) PXRD data of synthesized Cu-CD b) FTIR spectra of Cu-CD c) HRMS profile of obtained product from the click reaction d) FTIR of obtained click product

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Blue LED induced direct site-selective functionalization of various 1,4-quinones with different diazoesters

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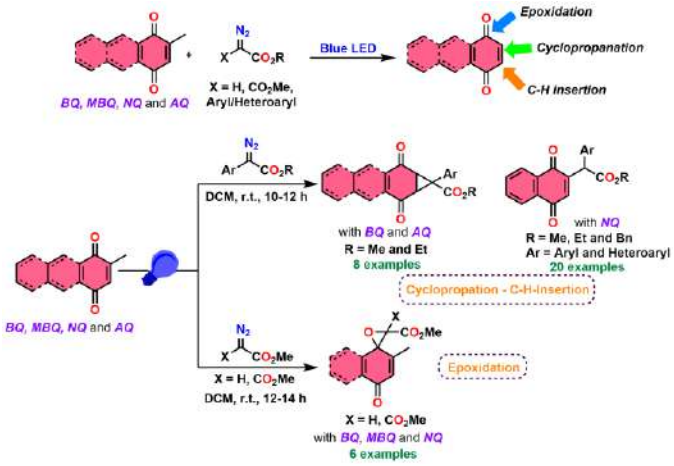
Site selective functionalization of a readily accessible starting material into myriad products is a crucial but challenging task in organic synthesis. Blue LED has been established as a sustainable, robust and controlled form of energy to orchestrate organic reactions. The high reactivity and ease of availability of diazo compounds make them a valuable reagent in organic syntheses. In the majority of these reactions, diazo compounds function as carbene precursors. 1,4-Quinones frameworks represent an important class of ubiquitous compounds which are found in several bioactive natural products and pharmaceutical molecules,[1] which show a broad range of biological activities including anticancer, antibacterial, antiviral, anti-inflammatory, neurological and trypanocidal activities.[2] Synthesis of diversely substituted quinone based compounds remains arduous and generally consists of multiple step sequences. The methods so far developed for direct functionalization of quinones are scarce and still limited in diversity, efficiency, and economy.[3-5] We herein demonstrated the site selective functionalization of a wide range of 1,4-quinones with electronically different alkyl aryl diazo acetates (electron donor-electron acceptor), methyl diazo acetates (electron acceptor) and dialkyl-2-diazomalonate (electron acceptor-electron acceptor) under visible light employing an environmentally green solvent and in the absence of base/acid/catalyst. Depending on the substrate-reactant combination the reaction either happens at the C=C region or C=O region of the 1, 4-quinones to provide a diverse variety of spiro epoxides, cyclopropanated and CH-alkylated quinones. DFT calculations and UV-Vis absorption experiments delineated the potential overall outcome of the reactions which were further used to predict the regioselective pathway.[6]



Scheme 1 Blue LED induced site-specific functionalization of 1,4-quinones with numerous diazo acetates.

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Poster Presentation (PP-100)
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Formic Acid, A Convenient Hydrogen Carrier, and Its Catalytic Dehydrogenation by Palladium Hydrides

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Hydrogen has emerged as a possible clean energy carrier as the world seeks alternatives to conventional fossil fuels. Formic acid (HCOOH) is a simple carboxylic acid that has garnered consideration as a potential hydrogen carrier in the hunt for a liquid organic hydrogen carrier (Figure 1). Exploring various catalysts for on-demand and on-site H_2 production from formic acid has been an ongoing topic of research. In this regard, bis(phosphinite)-palladium hydrides [Ref. a] were found to be an effective catalyst (Figure 2).

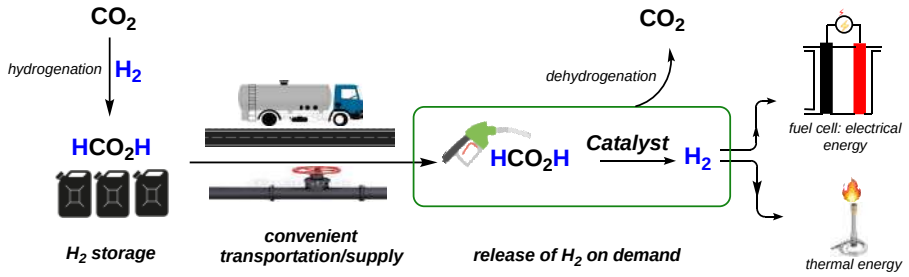

Figure 1: Formic acid storage and applications

After thorough investigation, a greener method is developed, where air stable catalyst can be used in commercial ethanol medium. We are successful to demonstrate the controllable release of dihydrogen under ambient condition and feeding it in fuel cell to produce electricity.

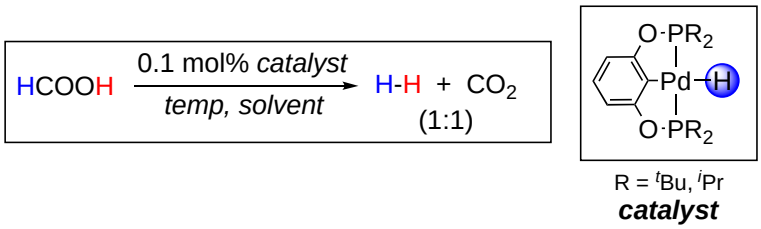

Figure 2: Formic acid dehydrogenation using palladium hydride complexes

References: [a] Adhikary, A.*; Saha, S.; Kumar, N. S.; Oliver, A. G.; Krause, J. A.; Guan, H.* *Organometallics* **2023**, *42*, 1525-1537.

Poster Presentation (PP-101)
International Conference on Emerging Trends in Catalysis & Synthesis (IC-ETCS 2024)

Enantiospecific Static Resolution of Racemic Benzoins and synthesis of Anti-Tumor Benzoyloxydiphenylethanones via *Chincona* Surfactant Stabilized Ferrite Nanoparticles

Pranshu K. Gupta [a], Neeraj Kumar [a], Abir Mujumdar [b], Manisha Pandey [a], Vasu P.V. Reddy [c], Kalluri V. S. Ranganath [a]*

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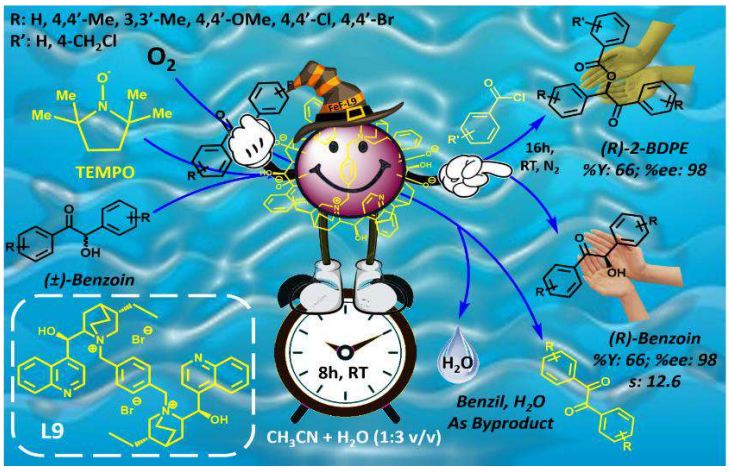
[b] *Department of Chemistry, KGTM, North Bengal University, Darjeeling-734104, Assam, India*
[c] *Department of Chemistry, Yogi Vemana University, Kadapa-516005, Andhra Pradesh, India*

Abstract

The static or dynamic resolution of racemic mixtures offer facile and affordable mode of enantioselective separation. Pharmaceutically relevant enantiopure α-hydroxy ketones like benzoins have been resolved through static resolution with significant selectivity, but with poor catalyst recollection and almost no synthetic extension. We report novel chiral hydrocinchonine gemini surfactant modified magnetite heterogeneous nanohybrids that could afford the room temperature mediated oxidative kinetic resolution of racemic benzoins with high resolution selectivity (*s* = 12.6) and enantiomeric excess (up to 98%), within 8 h, in semi-aqueous binary solvent mixture, for up to 10 catalytic cycles with no magnetic loss, releasing water as the sole byproduct. Additionally, the nanohybrid could afford one-pot enantiopure benzoylation for synthesis of tumor-suppressing benzoyloxy-1,2-diphenylethanones with ~99 % ee and ~60% yield, within 16 h under N_2 atmosphere. The 1st order kinetics, 8 h past racemization, no enantiopure-racemization, and hot-filtration effect coined the presence of chiral cleft over nanohybrid surface that showed affinity towards R-benzoin for 8 h, thereby oxidizing S-benzoin to benzil. However after 8 h, R-benzoin can either be collected or benzoylated to obtain enantiopure counterparts.



References

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3. P.K. Gupta, N. Kumar, A. Mujumder, M. Pandey, P.V. Reddy, K.V.S. Ranganath, **2023**, *Asian J. Org. Chem.*, e202300325.

Cu(II) Promoted C(sp^3)-H Activation in Unactivated Cycloalkanes: Oxo-Alkylation of Styrenes to Synthesize □-Disubstituted Ketones

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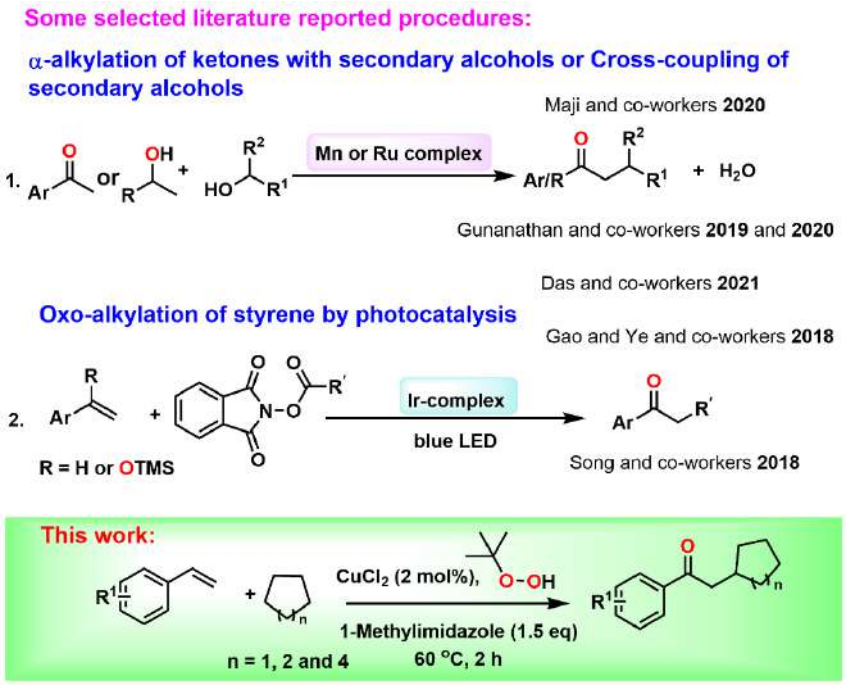
We report the Cu(II) catalyzed synthesis of *β*-disubstituted ketones from styrene *via* oxo-alkylation with unactivated cycloalkanes as the alkylating agent in presence of *tert*-butylhydroperoxide (TBHP) and 1-methylimidazole as oxidant and base respectively. *β*□disubstituted ketones are known to be synthesized by using either expensive Ru/Ir complexes, or low-cost metal complexes (*e. g.*, Fe, Mn) with activated species like aldehyde, acid, alcohol, or phthalimide derivatives as the alkylating agent, however, use of unactivated cycloalkanes directly as the alkylating agent remains challenging. A wide range of aliphatic C-H substrates as well as various olefinic arenes and heteroarene (35 substrates including 14 new substrates) are well-tolerated in this method. Hammett analysis shed more light on the substitution effect in the olefinic part on the overall mechanism. Furthermore, the controlled experiments, kinetic isotope effect study, and theoretical calculations (DFT) enable us to gain deeper insight of mechanistic intricacies of this new simple and atom-economic methodology.



Scheme 1. Comparison of literature reported procedures for synthesis of *β*-disubstituted ketones with our synthetic strategy.

References: K. M. Das, A. Pal, L. Surya T, L. Roy, A. Thakur*, *Chem. Eur. J.* **2023**, *e202303776*.

Nitrogen doped carbon dots (NCDs) as metal-free catalyst for Knoevenagel-Doebner Condensation

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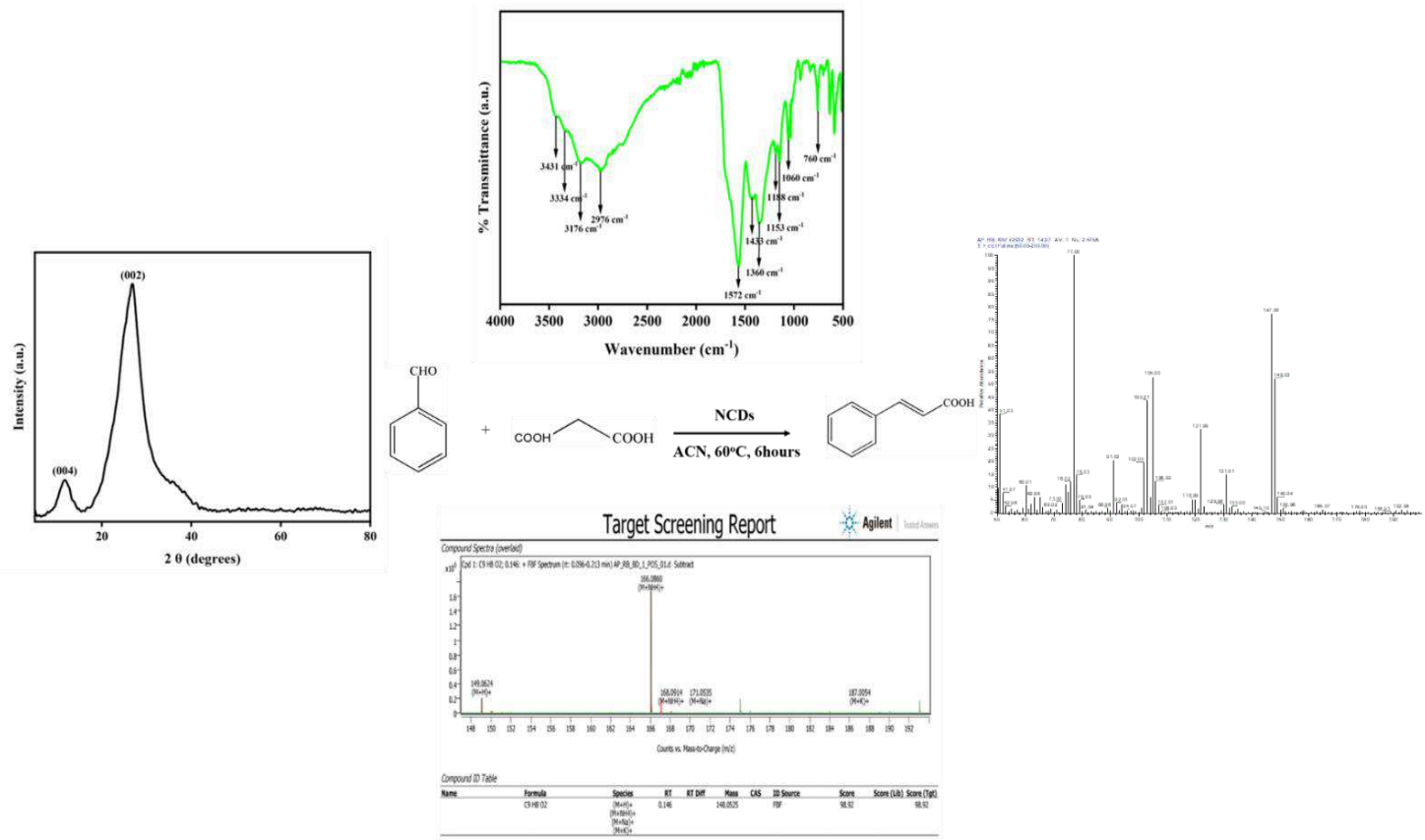
Formation of carbon-carbon (C= C) double bond from α, β- unsaturated carbonyl compound is a frequently used method for achieving cinnamic acid and its derivatives. Cinnamic acid is considered to be a privileged molecule in organic synthesis because it is an important intermediate and final product in organic synthesis for the production of cosmetics and perfumery products.[2] In the field of biological chemistry, it occupies a dominant position because of its antibacterial and antifungal activities. Among various available methods, some significant approaches for the preparation of cinnamic acid are the Knoevenagel-Doebner condensation, Perkin reaction, Claisen condensation and Heck reaction. In this work we report nitrogen doped carbon dots (NCDs) as an effective metal free catalyst for Knoevenagel Doebner Condensation. The carbon dots have been synthesized through one-pot thermolysis of citric acid and urea at 140ºC for 6 hours. The catalytic reaction was carried out in a 50 mL round bottom (RB) flask with constant magnetic stirring of 250 rpm at ambient temperature. For the reaction, 1 mmol of Benzaldehyde, 1 mmol of Malonic acid, 30 mg of NCDs (catalyst), and 5 mL of Acetonitrile (solvent) were taken in a round bottom flask and stirred at 60ºC for 6 hours. Precipitation of the solid product confirmed the formation of the product. The conversion percentage was found to be 75% from GC-MS data.



Outer-Coordination Sphere Interaction in a Molecular Iron Catalyst Allows Selective Methane Production from Carbon Monoxide and Carbon Dioxide

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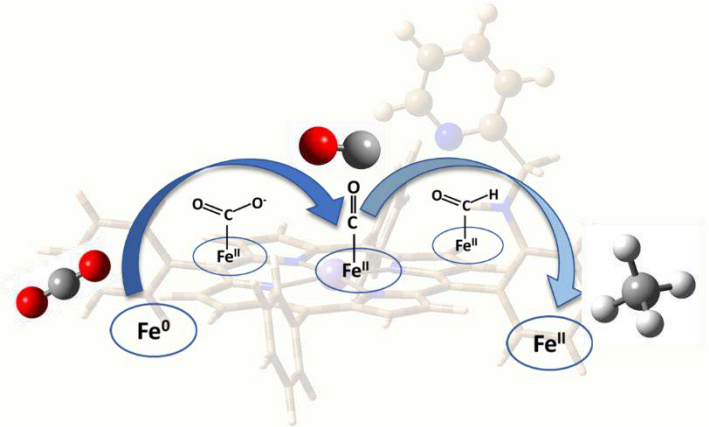
Reduction of oxides of carbon (CO and CO_2) into fixed forms of carbon is desirable to achieve sustainable and clean energy. Carbon monoxide (CO), an intermediate product in CO_2 reduction, is challenging to reduce which, in turn, jeopardizes the direct reduction (both electrochemical and photochemical) of CO_2 by $8e^-/8H^+$ to CH_4. Iron porphyrins can efficiently reduce CO_2 to CO by $2e^-/2H^+$ but further reduction is halted by rapid dissociation of CO from the reduced iron centre. This work show that CO can indeed be reduced upon inclusion of a pendent pyridine in the second coordination sphere of an iron porphyrin complex efficiently and selectively to CH_4 using water as the proton source. In-situ spectro-electrochemistry and theoretical modelling indicate that the pendent pyridine moiety imposes a hydrogen bonding interaction between the bound CO and adjacent water molecule which stabilizes two low-valent CO adducts i.e., Fe(I)-CO and Fe(0)-CO porphyrins, allowing its complete reduction, via a Fe(II)-CHO species, to CH_4. The ability to activate and reduce CO by ne^-/nH^+ via second sphere hydrogen bonding interaction in a mononuclear iron porphyrin opens newer pathways to valorise both CO and CO_2 to valuable C_1 products.



References: Dey A, Bhunia S, Patra S, Saha D, Ghosh S. Second Sphere Interaction Allows Selective Reduction of CO and CO2 to CH4. ChemRxiv. Cambridge: Cambridge Open Engage; 2022.

Variation in Catalytic Efficacies of a 2D pH-stable MOF by Altering Activation Methods

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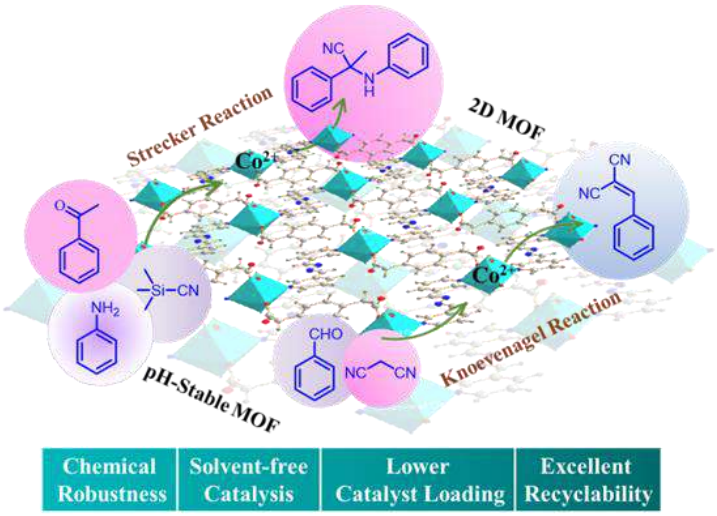
Easy accessibility of strong Lewis acidic sites onto 2D Metal-Organic Frameworks (MOFs) by using proper activation methods can be a cornerstone in attaining desired catalytic performance. Herein, we report a new 2D chemically stable MOF[a], which displayed excellent framework robustness over a wide pH range (2-12)[b]. Benefiting from the abundant open metal sites (OMSs) and framework robustness, the catalytic activity of the developed material was explored in one-pot three-component Strecker reaction and Knoevenagel condensation reaction. A comparative catalytic study was conducted using different activation methods (chloroform and methanol exchanged activated samples), highlighting the significant effect of activation methods on its catalytic performances. The sustainable synthetic pathway under *solvent-free* conditions for a broad scope of substrates using low catalyst loading and excellent recyclability made the developed pH-stable framework a promising heterogeneous catalyst.



Scheme 1. Schematic Representation of Streaker and Knoevenagel Reaction Catalyzed by a 2D MOF.

References: [a] J. Behera, A. Pal, R. Sahoo, M. C. Das, Manuscipt submitted.
[b] B. Pramanik, R. Sahoo, M. C. Das, *Coord. Chem. Rev.* **2023**, *493*, 215301.

Poster Presentation (PP-106)
International Conference on Emerging Trends in Catalysis & Synthesis (IC-ETCS 2024)

A Metal-free and Operationally Simple Radical Trifluoromethylative Borylation of Unactivated Alkenes

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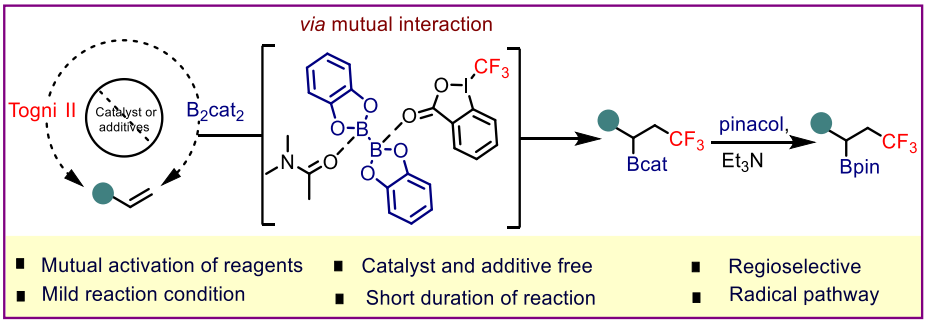
The trifluoromethyl and boronic ester groups are privileged moieties by themselves in the field of medicinal and synthetic chemistry because their attributes offer versatile tunability to the molecule. [a,b] Within the past 20 years, the FDA has approved more than 20 trifluoromethyl group containing drugs and 5 boron containing drugs, reflecting the importance of both groups in medicinal chemistry. [c,d] In this rapid development, incorporating the trifluoromethyl and boron moieties in a single operation can be a potential strategy for constructing synthetically valuable complex molecules. Herein, we described a synthetic protocol of regio selective trifluoromethylative borylation of unactivated alkenes to obtain trifluoromethyl alkyl boronates by the mutual activation of the Togni II and the Bis(catecholato)diboron reagents in the absence of catalyst, additives, and light. [e] Under the optimized condition, a range of trifluoromethyl alkyl boronates were obtained using unactivated alkenes, including natural products and drug derivatives. Moreover, the derivatization of the boronic ester present in the product allows access to a range of trifluoromethyl-containing compounds. The radical trapping and gas detection experiments reveal that the more Lewis acidic diboron reagent determines the rapid formation of trifluoromethyl and boron centered radicals.



Scheme 1. Regioselective Trifluoromethylative Borylation of Unactivated Alkenes

References:

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b) P. C. Trippier, C. McGuigan, *Med.Chem.Commun.* **2010**, *1*, 183–198.

c) B. C. Das, N. K. Nandwana, S. Das, V. Nandwana, M. A. Shareef, Y. Das, M. Saito, L. M. Weiss, F. Almaguel, N. S. Hosmane, T. Evans, *Molecules* **2022**, *27*, 2615.

d) A. S. Nair, A. K. Singh, A. Kumar, S. Kumar, S. Sukumaran, V. P. Koyiparambath, L. K. Pappachen, T. M. Rangarajan, H. Kim, B. Mathew, *Processes* **2022**, *10*, 2054.

e) K. Keerthika, B. M. Sathar, K. Geetharani, *Chem. Eur. J.*, **2023**, e202303468.

Poster Presentation (PP-107)
International Conference on Emerging Trends in Catalysis & Synthesis (IC-ETCS 2024)

Visible-Light Induced Intramolecular Cyclopropanation of *N*-Tosylhydrazones

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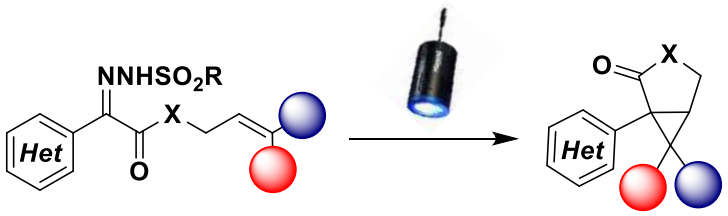
Abstract:

Cyclopropane ring is a versatile building block in many biologically active compounds.[1] Cyclopropane ring construction, either inter or intramolecular, is readily available from diazo compounds and alkenes. However, one needs to use expensive metal catalysts and explosive diazo compounds. Most of these reactions developed intermolecularly;[2-3] metal-free intramolecular cyclopropanation reactions are underdeveloped.[4] Here, we report the visible-light-induced intramolecular cyclopropanation reaction of the alkene-tethered *N*-tosylhydrazones. In the presence of a base and light *N*-tosylhydrazone precursor for carbenes, it would undergo cyclopropanation reactions. We have synthesized fused-cyclopropane ring compounds under metal-free conditions.[5] The details will be presented during the conference.



Scheme: Visible-light induced intramolecular cyclopropanation.

References:

1. K. B. Wiberg, *The Chemistry of the Cyclopropyl Group-Chapter 1* (Ed.: Z. Rapport), Wiley, New York, **1987**.
2. Pons, L. Delion, T. Poisson, A. B. Charette, P. Jubault, *Acc. Chem. Res*. **2021**, 54, 2969-2990.
3. Babbar, A. Yamini, P. Saleem, M. Yadagiri, D., *Org. Biomol. Chem.*, **2023**, 21, 7062-7078.
4. Zhang, J. Xu, W. Xu, M-H. *Angew. Chem. Int. Ed*. **2023**, 62, e2022167.
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Design strategy and synthesis of double Z-scheme photocatalyst for CO_2 reduction

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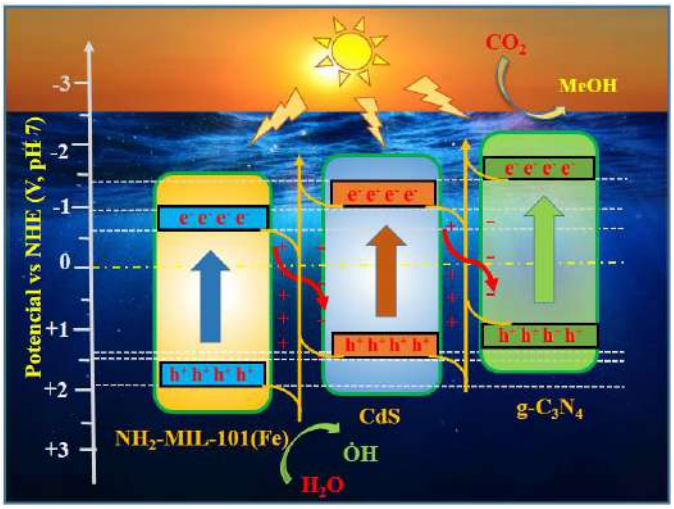
Due to the recombination of photo-exited electron-hole (e^-, h^+), inefficient use of irradiation light, and decreased CO_2 adsorption capacity, the photocatalytic CO_2 reduction reaction utilizing diverse semiconductors is quite challenging. The NH_2-MIL-101(Fe) metal-organic framework (MOF) has proven to be exceptionally effective in CO_2 adsorption and reduction due to its wide surface area, effective charge separation capacity, and ligand-to-metal charge transfer effect (LMCT). This study examines the combined effects of metal-organic framework, g-C_3N_4, and CdS semiconductors on effective photocatalytic CO_2 conversion to CH_3OH [1]. The excellent photocatalytic performance of a dual Z-scheme NH_2-MIL-101(Fe)/CdS/ g-C_3N_4 ternary hetero-nanostructured system (THS) was demonstrated through the successful synthesis and design of the system. CdS nanoparticles and NH_2-MIL-101(Fe) are deposited on the surface of g-C_3N_4 to form a Dual Z-scheme mechanism. This work is one of the pioneer for constructing double Z-scheme for extensive photocatalytic applications.



Scheme 1: Graphical presentation for double Z scheme.

References:

[1] W. Yu, D. Xu, T. Peng, Enhanced photocatalytic activity of g-C_3N_4 for selective CO_2 reduction to CH_3OH via facile coupling of ZnO: A direct Z-scheme mechanism, J Mater Chem A Mater. 3 (2015) 19936–19947.

Faculty Participants

Biographical Sketch of Professor D. Mal

Born in 1952 in a family of freedom fighters of Contai, Professor Dipakranjan Mal attended Banamalichatta High School, graduating in 1969 as valedictorian of his class. He received his BSc-Hons (valedictorian, RKM Vidyamandira, Belur) and MSc (Science College, Kolkata) degrees from the Calcutta University and PhD degree under the tutelage of Professor Layton L McCoy from the University of Missouri-Kansas City with GPA 4/4. Following 3 years of post-doctoral research with Professor Frank M Hauser at the Oregon Graduate Center, USA, he returned to India in 1984 to join Bose Institute, Kolkata as a faculty member. In 1987, joined IIT Kharagpur in a reader position and continued the remainder of his career teaching and advising graduate students at IIT for the next thirty years. During 2011-2014, he served as the head of the department. For a semester in 1998, he was a visiting professor at SUNY Albany, USA. He has published over 130 international research publications, and several book chapters and a book. Over his career, he mentored 32 PhD theses and more than 60 MSc theses.

His research interests were focused on the total synthesis of natural products using annulation strategies and pericyclic reactions. He has sole-authored the book "**Anionic annulations** in organic synthesis (Elsevier)". He has also developed a 40-lecture video course: Heterocyclic Chemistry (YouTube). He served as the sectional Scientist-in-Charge for organic chemistry section of the Indian Chemical Society for three years (2020-2022).

He is a recipient of Phi Kappa Phi Honor certificate, University of Missouri, USA (1978), and became Fellow of West Bengal Academy of Science and Technology (2012) and Fellow of the Royal Society of Chemistry, UK (2013). He is a life member of the Indian Chemical Society and the Chemical Research Society of India.

Besides professional activities, he served as the president of the IIT Kharagpur Teachers' Association for 2 years. He also served the campus school committee as the chairman for about 7 years.

Bio-Sketch of Participant

Professor Krishna C. Majumdar
(Former Professor & HOD)
Department of Chemistry
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Krishna C. Majumdar received his B.Sc. (1966) and M.Sc. (1968) degrees from the **University of Calcutta** and Ph.D.(1972) from the **University of Idaho** under the direction of Professor B. S. Thyagarajan and continued in the same University as a research associate till mid 1974. He also carried out postdoctoral work (**University of Alberta**) with Professor J. W. Lown till mid. 1977. He joined **BITS, Pilani** as an Assistant Professor in 1977 and then he was associated with **University of Kalyani**, lecturer (1977), reader (1984), Professor (1995-2010). He superannuated in 2005 and joined as UGC Emeritus Fellow in 2012 at the same University. He had also served **North-Eastern Hill University** (**NEHU**) as a visiting Professor (1996), **Indian Institute of Technology (Kharagpur)** as Associate Professor during 1990–1991, and **Tezpur University** (2011) as professor of Eminence. His research interests centred around synthetic organic chemistry and design and synthesis of liquid crystals with over 423 publications including review articles and book chapters. He has also edited a Wiley-VCH publication "Heterocycles in natural product synthesis".

Awards & Honors:

- Govt. of India National Scholarship
- CSIR Research Fellowship
- Pre-doctoral Fellowship (University of Idaho)
- Chemical Research Society of India Silver Medal (2004)
- Fellow of the West Bengal Academy of Science and Technology (2004)
- Professor A. S. R. Anjaneyulu 60th Birthday Commemoration award of the Indian Chemical Society (2006)
- Dr. S. Mukherjee Memorial Lecture Award (2012)

Representative Publications:

[1] Majumdar, K. C.; Kundu, U. K.; Ghosh, S. K. *Org. Lett.* **2002**, *16*, 2629-2631.
[2] Majumdar, K. C.; Alam, S. *Org. Lett.* **2006**, *18*, 4059-4062.
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[4] Majumdar, K. C.; Das, U. *J. Org. Chem.* **1998**, 63, 26, 9997-10000.
[5] Roy, B.; Hazra, S.; Mondal, B.; Majumdar, K. C. *Eur. J. Org. Chem.* **2013**, 4570-4577.
[6] Majumdar, K. C.; Mondal, S. *Chem. Rev.* **2011**, *111*, 7749–7773.

Bio-Sketch of Participant

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Department: Chemistry
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Dr. Adhikary grew up in Purba Medinipur district of WB. After completion of doctorate in 2015, he started his independent career as an Assistant Professor at the College of Saint Benedict / Saint John's University (CSB/SJU), USA. Then his career took a turn and he returned to India and joined Regional Institute of Education – Mysore. In 2018, he moved to Vellore Institute of Technology – Andhra Pradesh (VITAP) University and currently he is serving as an Assistant Professor Senior at the institute. His research is focused on developing novel dehydrogenation methods through transition metal catalysis.

Academic Background:

B.Sc.: Ramakrishna Mission Residential College, Narendrapur (2004-07)

M.Sc.: Indian Institute of Technology, Kharagpur (2007-09)

Ph.D.: University of Cincinnati, Ohio (2009-2015)

Awards / Honors:

i. Inorganic Chemistry-Travel Award, American Chemical Society (ACS) (2014)

ii. Visiting Researcher, University of Cincinnati (2022)

Bio-Sketch of Participant

Dr. Abhishek Dewanji
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School of Chemical Sciences
Indian Institute of Technology Mandi
Kamand, Mandi, Himachal Pradesh.
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About me

Myself, Abhishek Dewanji, currently appointed as an Assistant Professor in the School of Chemical Sciences (SCS) at IIT Mandi. After graduating from IIT Kharagpur with M.Sc., I did my Ph.D. with Prof. Armido Studer at the University of Münster, Germany and consequently two postdocs with Prof. Magnus Rueping, RWTH Aachen University, Germany and with Prof. David Procter, University of Manchester, UK, respectively.
Our research group at IIT Mandi is a vibrant team with passion for cutting-edge organic synthesis and catalysis. We are highly interested in exploring co-operative dual catalysis involving various redox and transition metal-catalytic systems to realize modular synthesis of useful organic scaffolds and important building blocks.

Professional

- **Assistant Professor** (2023-present) — **Indian Institute of Technology Mandi**, School of Chemical Sciences
- **Senior Research Investigator** (2022-2023) — **Syngene International Ltd.**, Integrated Drug Discovery
- **Postdoctoral Research Associate** (2020-2022) — **The University of Manchester, UK**, with Prof. David Procter
- **Postdoctoral Researcher** (2017-2020) — **RWTH Aachen University, Germany**, with Prof. Magnus Rueping

Academic

- **Doctor of Philosophy** (2012-2016) — **University of Münster**, with Prof. Armido Studer
- **Master of Science** (2010-2012) — **Indian Institute of Technology Kharagpur**, Chemistry
- **Bachelor of Science** (2007-2010) — **University of Calcutta**, Chemistry (Hons.)

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Dr. Alakananda Hajra graduated (M.Sc) from the Department of Chemistry, Indian Institute of Technology, Kharagpur India in 1998. After completing his Ph.D in 2002 under the supervision of Prof. B. C. Ranu from Indian Association for the Cultivation of Science (IACS), Kolkata he joined in SUNY at Albany, USA as a postdoctoral research fellow with Prof. Frank M. Hauser (2002-04). He was also a JSPS research Fellow in the University of Tokyo and worked with Prof. Eiichi Nakamura and Prof. Masaharu Nakamura from November 2004 to May, 2006. He also worked with Prof. N. Yoshikai, NTU, Singapore for one year (2011-2012) as a visiting scientist. He has published more than 200 peer-reviewed articles with more than 10,000 citations, giving him a *h*-index of 55.

Research Interest: Development of new synthetic methodologies and green synthetic procedures; Visible light mediated functionalization of heterocycles.

Awards / Honors / Membership:

- Professor D Nasipuri Memorial Award for the year 2019 by Indian Chemical Society
- Chemical Research Society of India (CRSI) Bronze Medal Award for the year 2018
- Prof. D. K. Banerjee Memorial Lecture Award for the year 2015 from Indian Institute of Science

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University of Calcutta, WB, India.
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Dr. Ramananda Maity completed his MSc in Chemistry from IIT Madras in 2009. He has obtained his Ph.D. in 2013 from University of Münster under the guidance of Professor F. E. Hahn. After the first postdoctoral studies with Professor Biprajit Sarkar at Freie Universität Berlin, he joined Prof. S. Inoue at Technische Universitatät Berlin for his second postdoctoral studies. He started his first independent carrier as an Assistant Professor at Dibrugarh University in 2015. In 2016 he moved to University of Calcutta as an Assistant Professor.

Research Areas:

- Synthesis and catalytic application (tandem catalysis) of homo- and heterobimetallic complexes possessing Poly-N-heterocyclic carbene (NHC) donor ligands
- Chiral-NHC complexes and their applications in asymmetric catalysis
- Poly-NHC ligand design for superior catalytic activity and for possible cooperative applications

Awards / Honors / Membership:

- Early Career Research (ECR) Award from DST-SERB.

Website: https://sites.google.com/view/dr-ramananda-maity/home

Bio-Sketch of Participant

Dr. Chandi C. Malakar
Associate Professor
Department of Chemistry
National Institute of Technology Manipur
Langol, Imphal 795004, India
E-mail: cmalakar@nitmanipur.ac.in
M.: 9366605025

Dr. Malakar is currently working as an Associate Professor, and Dean Research & Consultancy at National Institute of Technology Manipur. His current research interests are C-H activation, asymmetric synthesis, transition-metal catalysis and organocatalysis.

Academic Background:

B.Sc.: Vidyasagar University (2000-03)

M.Sc.: Indian Institute of Technology Kanpur (2004-06)

Ph.D.: University of Hohenheim, Stuttgart, Germany (2006-2011); Supervisor- Prof. (Dr.) Uwe Beifuss

Post-Doctoral Research:

University of Heidelberg, Germany (2012–2014); Supervisor: Prof. (Dr.) Guenter Helmchen.

University of Antwerp, Belgium (2011–2012); Supervisor: Prof. (Dr.) K. A. Tehrani.

IIT JAM: AIR- 8 (2004)

Awards / Honors / Membership:

(1) Awarded PBC FELLOWSHIP in 2014: Council for Higher Education of Israel.
(2) Awarded PEGASUS MARIE CURIE POSTDOCTORAL FELLOWSHIP in 2012: Research Foundation - Flanders (FWO), Belgium.
(3) Awarded POSTDOCTORAL FELLOWSHIP in 2012 at University of Heidelberg, Germany.
(4) Awarded IWS BOF UA POSTDOCTORAL FELLOWSHIP in 2011: University of Antwerp, Belgium.
(5) Awarded MERIT-CUM-MEANS (MCM) SCHOLARSHIP in 2004: Indian Institute of Technology (IIT), Kanpur.

Website: https://www.avikkumarbagdi.com/

Bio-Sketch of Participant

Dr. Raj K. Nandi
Assistant Professor
Department of Chemistry
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West Bengal, India
e-mail: rkn.chemistry@jadavpuruniversity.in
Office: 033 24573043

Dr. Nandi is working as an Assistant Professor in the Department of Chemistry, Jadavpur University, India. He was also served as Assistant Professor in Department of Chemistry at Diamond Harbour Women's University (DHWU) from February 2019 to February 2023, before joining at Jadavpur University. His current research interest is synthesis of pharmaceutical interested molecules by exploitation of weak bond of cyclic hypervalent iodine reagent.

Academic Background:

B.Sc.: University of Kalyani (2006) (First class with 1st Rank)

M.Sc.: University of Kalyani (2008) (First class with 2nd Rank)

Ph.D.: University of Kalyani (January, 2014); Supervisor- **Prof. K. C. Majumdar**

Post-Doctoral Research:

(i) Kobe Pharmaceutical University, Kobe, Japan (April 2014-December 2014) With **Prof. Okiko Miyata.** (ii) Universite of Paris Sud, Orsay, France (February 2015-February 2017); With **Dr. Guillame Vincent**. (iii) EPFL, Lausanne, Switzerland (March 2017-October 2018) with **Prof. Jerome Waser**.

Awards / Honors / Membership:

- **2018**: Best oral presentation at ICCHD-2018.
- **2017**: Scientific Collaborator Position at EPFL, Switzerland.
- **2015** : Postdoctoral position at Université Paris Sud, France.
- **2014**: Marie Curie International Incoming Fellowship by REA-European Commission FP7 framework Program.
- **2013**: KPU-Postdoctoral fellowship, Japan
- **2008**: CSIR-National Eligibility Test Awarded JRF(UGC) (CSIR-UGC-New Delhi)
- **2008**: First Class second in Master of Science (University of Kalyani, India)
- **2008**: Graduate Aptitude Test in Engineering (GATE), **2008**, AIR-55, 99.12 percentile
- **2007**: CSIR-National Eligibility Test Awarded JRF(UGC) (CSIR-UGC-New Delhi)
- **2007**: Professor Ashima Chatterjee endowment silver medal for obtaining 1st Class first position in B.Sc examination (University of Kalyani, India).

DR. SUDIPTA RAHA ROY

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Website: https://sites.google.com/view/srr-lab

***Research Interest*:** Cost Effective Catalysis for Small Molecule Activation

Academic Details:

Ph. D.	**Medicinal Chemistry (2012)**
Title of thesis:	Applications and Mechanistic Investigations of Ionic Liquid Catalysis
Supervisor:	Prof. Asit K. Chakraborti, National Institute of Pharmaceutical Education and Research (NIPER), India
M. Sc.	**Chemistry (Aug 2004 - July 2006)**
Specalisation:	Organic Chemistry, Visva Bharati University, West Bengal, India

Professional Experience:

Mar 2023-Present: Associate Professor, Department of Chemistry, IIT-Delhi
Nov 2018-Feb 2023: Assistant Professor, Department of Chemistry, IIT-Delhi
Postdoctoral Research (Jan 2017-Jan 2018) and (May 2018-Nov 2018):
Supervisor: Prof. Paolo Melchiorre; ICIQ, Tarragona, Spain
Postdoctoral Research (May 2014-Jan 2017):
Supervisor: Prof. Ilan Marek; Schulich Faculty of Chemistry, Technion, Israel
Research Associate (Mar 2012-Mar 2014):
Supervisor: Dr. Swadhin K. Mandal; Chemical Science, IISER-Kolkata, India.

Honours and Accolades:

- Awarded **Marie Curie Individual Fellowship** in **2018**
- Awarded **Fulbright Nehru Postdoctoral Research Fellowship** in **2014** (Declined)
- Awarded **PBC Fellowship** in **2014** for pursuing postdoctoral study in Israel
- Recipient of **Research Associate Grant 2013** from **CSIR**, Govt. of India.
- Selected for the **1st Prize** of **"2012 Eli Lilly and Company Asia Outstanding Thesis Awards**".
- Recipient of **International Travel Grant** from **DST**, Govt. of India for attending "Young Chem-2010", Reda, **Poland** from **6-10th Oct, 2010**.

Human Resource Development:

- Current PhD Students: **10** (2 Students given Synopsis)
- Current MSc Thesis students: **2** (MSc Thesis Completed: **8**)

Selected Publications (h-Index: 20; Citations: 1987, as on 15th Jan 24, Google Scholar):

1. ***ACS Catalysis***, *2024, 14, 907–920*. (*Link for PDF*)
2. ***Chemical Science***, 2023, *14*, 12541-12547. (*Link for PDF*)
3. ***Organic Letters***, 2023, *25, 923-927*. (*Link for PDF*)
4. ***Chemical Communication***, 2022, *58*, 3831-3834. (*Link for PDF*)
5. ***Green Chemistry***, 2021, *23*, 5687-5695. (*Link for PDF*)

Bio-Sketch of Participant

Md. Firoj Hossain
Assistant Professor
Department of Chemistry
University of North Bengal
Raja Rammohunpur, Siliguri, Darjeeling-734013, W.B., India
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Introduction, Academic, Awards / Honors / Membership, website, etc

Dr. Md. Firoj Hossain received his B.Sc. honours degree in Chemistry from Krishnath College, Berhampore in 2004 under Kalyani University and M.Sc. with organic special in 2006 from Kalyani University. His PhD research was conducted at the Indian Association for the Cultivation of Science (IACS) Kolkata, India under the supervision of Prof. Subrata Ghosh and was focused on the asymmetric synthesis of bioactive compounds with sugar as chiral adjuvents. Dr. Hossain employed tandem ring opening-ring closing metathesis, cross metathesis, intramolecular Diels-Alder reaction and [2+2] photocycloaddition reaction to achieve the highly structurally and stereochemically complex natural products. In 2013, he went to South Africa for his Post Doctoral (as NRF & URC Fellow) research with Prof. Charles de Koning (School of Chemistry) and Prof. Patrick Arbuthnot (Wits Medical School) at the University of Witwatersrand. In 2015 he returned to India and joined in the Department of Chemistry, Sripat Singh College as Assistant Professor. Then Dr. Hossain moved to the Department of Chemistry, University of North Bengal as Assistant Professor in 2018 and currently working there. His current research interest includes Photocatalysis, Electrocatalysis, DES mediated small molecule synthesis, and Molecular Recognition.

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Professional Position

Assistant Professor, IIT Tirupati, India 2022 – present

Education and Training

Postdoctoral Research Associate, EPFL, Switzerland 2018 – 2021
Advisor: Prof. Xile Hu
Ph.D. in Chemistry, University of Muenster, Germany 2013 – 2017
Advisor: Prof. Armido Studer
M.Sc. in Chemistry, IIT Kanpur, India 2011 – 2013
Advisor: Prof. Parimal K. Bharadwaj
B.Sc. in Chemistry, University of Calcutta 2008 – 2011

Honors and Awards

- Postdoctoral fellowship funded by SNSF (2018)
- Doctoral research fellowship from the NRW International Graduate School of Chemistry, Muenster (2013)
- INSPIRE Scholarship by DST, India (2008 – 2013)
- Dr. Shailendra Jha Memorial Prize in B.Sc. (2011)

Research Interests

Asymmetric Base Metal Catalysis, N-Centered Radical Chemistry, Molecular Editing

Selected Publications

1. Enantio- and Diastereoselective Construction of Vicinal C(sp^3) Centers via Nickel-Catalyzed Hydroalkylation of Alkenes. Srikrishna Bera, Chao Fan, and Xile Hu* *Nat. Catal.* 2022, 05, 1180–1187.
2. Enantioselective C(sp^3)–C(sp^3) Cross-Coupling of Non-activated Alkyl Electrophiles via Nickel Hydride Catalysis. Srikrishna Bera, Runze Mao, and Xile Hu* *Nat. Chem.* 2021, *13*, 270–277.
3. Nickel-Catalyzed Regioselective Hydroalkylation and Hydroarylation of Alkenyl Boronic Esters. Srikrishna Bera, and Xile Hu*, *Angew. Chem. Int. Ed.* 2019, 58, 13854-13859.
4. Oxidative *N*-Heterocyclic Carbene Catalyzed Dearomatization of Indoles to Spirocyclic Indolenines with Quaternary Carbon Stereocenter. Srikrishna Bera, Constantin G. Daniliuc, and Armido Studer*, *Angew. Chem. Int. Ed*. 2017, *56*, 7402-7406.
5. Asymmetric Synthesis of Highly Substituted β-Lactones via Oxidative Carbene Catalysis with LiCl as Cooperative Lewis Acid. Srikrishna Bera, Ramesh C. Samanta, Constantin G. Daniliuc, Armido Studer*, *Angew. Chem. Int. Ed.* 2014, *53*, 9622-9626.

Bio-Sketch of Participant

Dr. Tapas Ghosh
Assistant Professor
Department of Chemistry
(Organic Chemistry Section),
Jadavpur University,
Kolkata 700 032, West Bengal, India
Email: tapasg.chemistry@jadavpuruniversity.in

Dr. Ghosh did his Ph.D. in the group of Professor K. C. Majumdar in the University of Kalyani, India. In 2014, he was awarded TÜBITAK postdoctoral fellowship from Govt. of Turkey and worked at Izmir Institute of Technology, Izmir, Turkey in the group of Professor Levent Artok. He then moved to the Kobe Pharmaceutical University, Kobe, Japan for his next postdoctoral research stay with Professor Okiko Miyata Group (2014-2015). In 2015, he joined the research group of Professor Matthias Lehmann in University of Würzburg, Germany with prestigious **Alexander von Humboldt** postdoctoral fellowship. In 2018, he joined as an Assistant Professor in the Department of Natural Sciences, Maulana Abul Kalam Azad University of Technology (MAKAUT), West Bengal, India. Since, August 2022, he has been working as an Assistant Professor in the Department of Chemistry (Organic Chemistry Section), Jadavpur University. Dr. Ghosh is recipient of several prestigious National and International fellowships namely **TARE** fellowship from SERB, India; **Alexander von Humboldt** postdoctoral fellowship; **Marie-Skłodowska-Curie** actions postdoctoral fellowship; **BELSPO** postdoctoral fellowship, Belgium; **TÜBITAK** postdoctoral fellowship, Turkey; Research Associateship (RA), CSIR; and CSIR-JRF & CSIR-SRF, India. He was awarded *ACS Best Oral Presentation* award in '*International Conference on Chemistry for Human Development*' (ICCHD), Kolkata, 2020. Dr. Ghosh is Life Member of Humboldt Club, Kolkata and has been member of American Chemical Society, USA. He is Associate Editor of Frontiers in Soft Matter (Liquid Crystals). Dr. Ghosh has more than 45 international publications in reputed journals. His research interest includes the development of new synthetic methodologies to design and synthesis of small drug molecules of biological relevance along with the application of advanced liquid crystalline materials in organic photovoltaic.

ORCID: https://orcid.org/0000-0002-3949-885X
Google Scholar: https://scholar.google.com/citations?user=jfCR7yQAAAAJ&hl=en
Groupsite: https://ghoshresearchgroup.wixsite.com/tapas-ghosh

Bio-Sketch of Participant

Dr. Uttam Kumar Ghorai
Assistant Professor & Head
Department of Industrial & Applied Chemistry
Ramakrishna Mission Vidyamandira,
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Introduction, Academic, Awards / Honors / Membership, website, etc

Dr. Ghorai has established vibrant research programs in the field of Materials Science & Nanotechnology at Swami Vivekananda Research Centre, Ramakrishna Mission Vidyamandira Institution, Belur Math, Howrah. He has completed his MTech in Nanoscience and Technology in 2011 and PhD in Materials Science & Nanotechnology in 2016, both from Jadavpur University, Kolkata. Dr. Ghorai has been devoted to promoting the development of sustainable processes and products as an independent researcher. His study focuses mostly on electrochemical methods for the synthesis of ammonia, urea, and nitric acid under ambient conditions. As the main source of nitrogen, the macronutrient used in fertiliser, these three compounds are particularly significant. He could develop novel electrochemical conversion catalysts for these three important compounds and successfully demonstrate pilot plant-scale manufacture of these catalysts. Importantly, he used these electrocatalysts in his unique electro-catalytic procedures to obtain industrial-scale current density and a high yield rate with 100% Faradaic efficiency. Transition metal-phthalocyanine nanotubes (FePc, CoPc, CuPc, etc.) are the source of these catalysts (in a kilogram/batch reaction). He has published 120 research papers in peer-reviewed international journals (H-index: 32 and total citations ~ 3271) and has been the co-inventor of seven patents.

In recognition of his contributions in the field of Materials Science & Engineering, Dr. Ghorai has received with *"Young Engineer Award' (2019)* from the Indian National Academy of Engineering (INAE). Other noteworthy recognitions include, *Young Scientist Platinum Jubilee Award* from The National Academy of Sciences (NASI) in 2020, *Young Scientist Award (2017)* from the Indian Chemical Society; *Young Scientist Award (2018)* from the Materials Research Society of India; *Teachers Associateship for Research Excellence (TARE) Fellowship (2018-2021)* and *SERB International Research Experience (SIRE) Fellowship (2022-23)* from Indian Government;" Additionally, he was awarded the *BRICS Young Innovator Prize* for 2022. He has been elected to be an Associate Fellow of the Indian National Academy of Engineering (in 2019) and the Indian Academy of Sciences (in 2021). He has been awarded the prestigious Merck Young Scientist Award (2023) in Chemical Sciences. Furthermore, he is serving as the guest editor of a special issue of Catalysis Today, an esteemed worldwide journal published by Elsevier.

Prof. (Dr.) Sk. Manirul Islam
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manir65@rediffmail.com
Web URL: https://scholar.google.com/citations?hl=en&user=5OHnPtYAAAAJ

Awards and Honours:
(i) FRSC in Chemical Science in 2023 (ii) Name included in top 2% Scientists of the world according to the updated list published by Stanford University in 2020, 2021,2022,2023 in Chemical Science (iii) Fellow of West Bengal Academy of Science and Technology in 2024.

Summary of Research Output/ Professional Record:

- Published 170 research articles in reputed international journals
- H-index of 43; Total citation of 7197
- Invited Talk / Oral Presentations at various conferences: 25
- No of major projects implemented 10 (DST, CSIR, UGC)
- Number of Ph.D. students already awarded Ph.D. degree under Prof. Islam: 24

Education/Position: Prof. Islam did his M.Sc. in Pure Chemistry, from University of Calcutta during 1991-1993. **He did his Ph.D. from IIT Kharagpur during 1994-1999** and postdoctoral research from State University of New York, USA during 2000-2001. **At present he is serving as a Professor in the Dept. of Chemistry, University of Kalyani.**

Current Research Area: The major focus of our research is to design and synthesis of functionalized porous materials, COFs, MOFs, POPs, and their catalytic applications towards CO_2 chemistry, **CO_2 fixation to value-added chemicals,** *in situ* transformation of CO, catalytic conversion of CO into value-added chemicals, **CO_2 reduction reactions**. etc.

Prof. Islam has published his research work in various reputed journals mentioned below and he is a reviewer of various reputed journals.

Chemical Communications, Green Chemistry, Journals of Materials Chemistry. Dalton Transactions, Chem Cat Chem, Catalysis Science and Technology, Tetrahedron Letter, J Organometallic Chemistry, J. of Colloid and interface Sciences, New Journal of Chemistry, Journal of Molecular Catalysis, Applied Catalysis, A General, Catalysis Letters, Material Advances, ACS Sustainable Chemistry and Engineering, etc.; **Total no of Publication in reputed international journals- 170.**

Bio-Sketch of Participant

Dr. Lijina MP
Assistant Editorial Development Manager
Royal Society of Chemistry
World Trade Centre, Malleshwaram,
Bangalore- 560054
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lijina@rsc.org

Dr. Lijina MP obtained her MSc and PhD from the Indian Institute of Science Education and Research Thiruvananthapuram. In 2023, she joined the Royal Society of Chemistry where she is currently the Assistant Editorial Development Manager and involved in managing the journal portfolio and their growth in India. As a part of her role, she works with the scientific community, various Indian chemical societies, and researchers across various disciplines of Chemical Sciences and support the journal teams.

Bio-Sketch of Dr. Amit Kumar Simlandy

Contact

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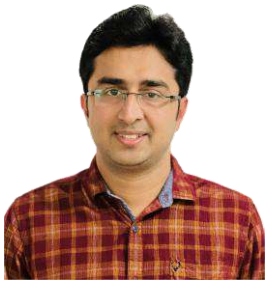

Employments

1/2024–present	**Assistant Professor**, Department of Chemical Sciences, Indian Institutes of Science Education and Research (IISER) Berhampur, INDIA
8/2021–12/2023	**Postdoctoral Research Associate**, Department of Chemistry, The Scripps Research Institute, La Jolla, San Diego, USA Advisor - Professor Keary M. Engle
1/2019–7/2021	**Postdoctoral Fellow**, Indiana University, Bloomington, USA Advisor - Professor M. Kevin Brown
8/2018–11/2018	**Research Associate**, Indian Institute of Science, Bangalore, INDIA Advisor - Professor Santanu Mukherjee

Education

8/2013–7/2018	**Ph.D.** in Chemistry, Indian Institute of Science, Bangalore, INDIA Advisor - Professor Santanu Mukherjee
8/2011–5/2013	**M.Sc.** in Organic Chemistry, Visva-Bharati Central University, Santiniketan, INDIA Advisor - Professor Alakananda Hazra
8/2008–5/2011	**B.Sc.** in Chemistry (Honours), Visva-Bharati Central University, Santiniketan, INDIA

Awards & Scholarships

2018	GRC Carl Storm International Diversity (CSID) Award to attend the 2018 GRC in Stereochemistry, USA
2013	Graduate Aptitude Test in Engineering (GATE) with All India Rank (AIR) 22
2012	Junior Research Fellowship (JRF) from the Council of Scientific and Industrial Research (CSIR) in National Eligibility Test (NET) with All India Rank (AIR) 10
2013	Fellowship from Visva-Bharati Central University for securing 1st position in M.Sc.
2011	Fellowship from Visva-Bharati Central University for securing 3rd position in B.Sc.

Bio-Sketch of Participant

Dr. Ajoy Kapat
Assistant Professor

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Shiv Nadar Institution of Eminence
School of Natural Science;
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Gautam Buddha Nagar
Uttar Pradesh - 201314-India;
Email: ajoy.kapat@snu.edu.in;
Ph: 9599626674
Website: **https://kapatgroup.org**

Professional Experience:

7/2019	Assistant Professor at Shiv Nadar Institution of Eminence
4/2019-7/2019	Visiting Research Scientists, Institute of Organic Chemistry, RWTH Aachen University, Germany.
11/2014-3/2019	Postdoctoral fellow, Institute of Organic Chemistry, RWTH Aachen University, Germany.
5/2014-10/2014	Research Associate-I, Department of Organic Chemistry, Indian Association for the Cultivation of Science, India.
8/2012 – 1/2014	Postdoctoral fellow, Frick Chemistry Laboratory, Princeton University, USA.
9/2011 – 3/2012	Assistant –I, Department of Chemistry and Biochemistry at University of Bern, Switzerland.

Academic:

9/2007 – 8/2011	PhD. Organic Chemistry, University of Bern, Switzerland.
7/2004 – 7/2006	M.Sc Chemistry, Indian Institute of Technology Madras.
8/2001 – 7/2004	B.Sc Chemistry (Honours), First Class, University of Calcutta.

Awards & Honors: Certificate of Appreciation from the American Chemical Society (ACS) as a peer reviewer 2023; SERB Special Call on Fluorine Chemistry 2022; SERB-SRG 2020.
Membership: ACS & AAAS

Bio-Sketch of Participant

Dr. Dharmendra Kumar Tiwari
Assistant Professor
Center of Biomedical Research (CBMR)-SGPGIMS Lucknow

Dr. Dharmendra Tiwari earned his Ph.D. from CSIR-NCL, Pune under the guidance of Dr. Ganesh Pandey. Following this, in April 2012, he undertook a postdoctoral research position in Prof. Michel Vaultier's group at the University of Bordeaux-1, France. In April 2013, Dr. Tiwari joined CSIR-IICT, Hyderabad as a DST-INSPIRE Faculty. Later, in January 2019, he assumed the role of Assistant Professor at the Centre of Bio-Medical Research (CBMR), Lucknow, India.

- **Assistant Professor at Center of Biomedical Research, SGPGIMS, Lucknow, U.P. INDIA.**
- **DST-INSPIRE Faculty at CSIR-IICT Hyderabad (2013-2018).**

AWARDS AND HONOURS:

1. Young scientist award: from SERB New Delhi- Augus-2015-August-2018.

2. DST-INSPIRE Faculty Award: from DST-New Delhi; April 2013.

3. SERB-Research Scientist: from SERB New Delhi: January-2019

4. Indo-French Post-Doctoral Fellowship sponsored CEFIPRA

Bio-Sketch of Participant

Dr. Anup Biswas
Assistant Professor (Grade-II)
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Hooghly Women's College, 1, Vivekananda Road; Pipulpati; Hooghly, West Bengal, India
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Dr. Anup Biswas is currently working as Assistant Professor in the Department of Chemistry of Hooghly Women's College. His research interest is asymmetric organic synthesis, organocatalysis.

Academic Background:

Dr. rer. nat in Chemie (Ph.D in Chemistry) from University of Münster, NRW, Germany (10/2009-11/2012)

M. Sc. in Chemistry from Indian Institute of Technology Kharagpur, India (08/2007-06/2009).

B. Sc. in Chemistry (Honours), Mathematics, and Physics from The University of Burdwan, India (2004-2007).

Higher Secondary (10+2) with subjects Physics, Chemistry, Mathematics, and Biology from West Bengal Council of Higher Secondary Education, India (2001-2003).

Secondary (10) with subjects Science, Humanities and Literature from West Bengal Board of Secondary Education, India (1999-2001).

Website:

http://hooghlywomenscollege.org/Science/Chemistry/

Bio-Sketch of Participant

Dr. Ujjawal Kumar Bhagat
Assistant Professor
Department of Chemistry
Professor's Colony, Block-A, Flat No. A/2
S.K.R. College Barbigha, Sheikhpura, Pin- 811101, Bihar
e-mail: ujjawalk78@gmail.com
M.: 91+ 9634899229

Introduction: I am currently working as Assistant Professor and Head in the Department of Chemistry at S.K.R. College Barbigha, Sheikhpura (A constituent unit of Munger university, Munger) for the last six years.

Academic Background:

Degree	Year	Division/Class	Institute / University / Board
Ph.D (Organic Chemistry)	2017	Awarded	IIT Roorkee, Roorkee
M.Sc. (Organic Chemistry)	2010	1st Class	Patna University, Patna
B.Sc. (Chemistry)	2008	1st Class	Magadh University, Bodh-Gaya
I.Sc	1999	1st Division	BIEC, Patna
10th	1997	1st Division	BSEB, Patna

Achievements:

Degree: Ph.D (Organic Chemistry); IIT Roorkee, Roorkee, Uttarakhand.

Date of Award of Degree: 24th September, 2017.

Title of the Thesis: Reactions of 4-Aryl-1*H*-1,2,3-Triazoles: Synthesis of Disubstituted 1,2,3-Triazoles.

Qualified CSIR-UGC-NET Examination in Chemical Science, December **2010**.

Qualified GATE Examination **2010** in Chemistry.

Awards / Honors

1. **"Young Scientist Award"** by CFOS-2017 at IIT Roorkee, Roorkee (Uttarakhand), India.
2. **"Best Oral Presentation Award"** by 7th Bihar Science Conference during 4-6 December, 2018 held at College of Commerce, Arts and Science, Patna, (Bihar).
3. **"Best Oral Presentation"** in "National Seminar on Future India and Technology" (NSFIST) Organized by "Indian Science Congress Association" (ISCA), Patna chapter during 3-4 April, 2019 held at Manger University, Munger (Bihar).
4. **"INDO ASIAN–ROBERT BOYLE DISTINGUISHED SCIENTIST AWARD"** in Chemistry by The International Multidisciplinary Research Foundation (IMRF) in recognition of participation in the United Nations 75th Anniversary Dialogue on UN Goals – Quality Education – The Future on dated 15th December, 2020**.**

Membership:

1. Regular Member - American Chemical Society (07-25-2017 to 04-28-2021).
2. Life Member - The Indian Science Congress Association (L 37555).
3. Life Member - Chemical Research Society of India (LM 3742).

Bio-Sketch of Participant

Dr. Amrit Krishna Mitra

Assistant Professor [West Bengal Education Service, Gr: A] and Founder Head
Department of Chemistry
Government General Degree College, Singur
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M.: 9432164011

Controller of Examinations (Addl. Charge)
Rani Rashmoni Green University (State Aided)
Hooghly, West Bengal

Introduction:

Dr. Amrit Krishna Mitra is an Assistant Professor (under West Bengal Education Service Gr: A) and founder Head in the Department of Chemistry, Government General Degree College – Singur. He has also been appointed the Controller of Examinations of Rani Rashmoni Green University by the Higher Education Department, Government of West Bengal. He is also serving as the Coordinator (Academic) of the Postgraduate course in Chemistry at the Rani Rashmoni Green University, West Bengal since 2020. He acquired his Honours degree in Chemistry from St. Xavier's College, Kolkata under University of Calcutta and his Master's degree from Indian Institute of Technology, Kharagpur. Dr. Mitra was awarded Ph.D. in Organic Chemistry by the University of Calcutta [Place of work: Saha Institute of Nuclear Physics]. His area of research is based on 'Synthesis and Photophysical Studies of Heterocyclic Compounds'. With thirty publications in numerous reputed international scientific journals to his credit, Dr. Amrit Krishna Mitra has also penned a book and several book chapters. He is the Editorial Board member of several research journals of international repute. He is also involved as a member of the Board of Studies and the Syllabus Committee for the postgraduate course in Chemistry. He has received several recognitions and awards from numerous reputed organisations of India. Dr. Mitra is involved in various activities related to Chemistry Education. At present, he is also a Member of Executive Council, Association of Chemistry Teachers (ACT) [C/o: Homi Bhabha Centre for Science Education (HBCSE)**,** Tata Institute of Fundamental Research (TIFR) – Mumbai]. Dr. Mitra has been involved as a resource person in various activities related to Indian National Chemistry Olympiad (INCHO), organised by Homi Bhabha Centre for Science Education (HBCSE)**,** Tata Institute of Fundamental Research (TIFR) – Mumbai, nodal centre for INCHO, Government of India. He has also been recognised as a resource person for the Vigyan Pratibha Teachers' Workshops, an initiative of DAE, Government of India. Apart from these, Dr. Mitra is frequently assigned with several confidential responsibilities by the Ministry of Education, Government of India.

Academic Background:

B.Sc.: Calcutta University (St. Xavier's college)
M.Sc.: Indian Institute of Technology, Kharagpur
Ph.D.: Calcutta University [Place of work: Saha Institute of Nuclear Physics, Kolkata]

Website: http://singurgovtcollege.org/dr-amrit-krishna-mitra-dept-of-chemistry.html

Bio-Sketch of Participant

Dr. Shubhankar Samanta
Assistant Professor
Department of Chemistry
Bidhannagar College, Salt Lake, Kol-64
e-mail: chemshubha@gmail.com
M.: 9123758774

Introduction:

Synthesis of variety heterocyclic and carbocyclic molecule in doctoral studies, and the synthesis of florescence heterocyclic molecule and their photophysical, biological study is his current ongoing research work. He has published 37 international journals, among them 24 international journals as a corresponding author. He has guided four PhD students till now (Suresh Kumar Mondal, Susanta Kumar Manna have completed doctoral degree from Vidyasagar University, and Sk. Asraf Ali awarded doctoral degree from Calcutta University and Mr. Anirban Bera completed his PhD degree from Jadavpur University). He has guided project of master's students in his department in each year. The guidance of each student molded as an independent researcher with good confidence. His synthetic skills and the familiarity with the above-mentioned techniques align very well with the current project and this will be very helpful in carrying out the proposed research work.

Academic Background:

i) B.Sc from Vidyasagar University, 2004
ii) M.Sc from Vidyasagar University, 2006
iii) PhD from IIT Kharagpur, 2011

Thesis title : ***Synthesis of Carbocyclic and Heterocyclic Compounds by Heck and Michael Reactions***

Guide's Name: Prof. Jayanta Kumar Roy

Work experience (in chronological order).

i) Assistant Professor, Haldia Govt. College, 2016
ii) Assistant Professor Stage III, Bidhannagar College, till now

Awards / Honors / Membership:

i) Winning Prize for Best Oral & Poster Presentation inNational Seminar at Vijaygarh Jyotish Ray College, Jadavpur. 2020
ii) 1st prize from 26th West BengalScience Congress, 2019
iii) 2and rank in B.Sc examination 2004 from Vidyasagar University

Website: https://www.bidhannagarcollege.org/dr-shubhankar-samanta.htm

Bio-Sketch of Participant

Name: Dr. Tapan Kumar Pradhan
Designation: Assistant Professor
Department: Department of Chemistry
Address: Krishnath College, 1, Sahid Surya Sen Road, Gorabazar, Murshidabad, Berhampur, West Bengal, 742101
e-mail: tapaniict@gmail.com
M.: +917432952882

Introduction:

Dr. Tapan Kumar Pradhan presently working as an Assistant Professor of Department of Chemistry, Krishnath College, Murshidabad, West Bengal since 2020. Dr. Pradhan received his Ph.D. degree form Osmania University in 2011 as fellow of Indian Institute of Chemical Technology (IICT), Hyderabad, India. Then Dr. Pradhan appointed as a Junior Scientist at Aurigene Discovery Technologies Ltd., Hyderabad, India. He was a postdoctoral fellow at the University of National Yang Ming Chiao Tung University and National Tsing Hua University, Taiwan. Soon after his postdoctoral studies, he was appointed as a research fellow at Genovior Biotechnology Ltd., Miaoli, Taiwan. In 2021, he was awarded as a SERB-TARE fellow, DST India. His research interests include total synthesis of natural products and KDO oligosaccharides.

Academic Background:

2005 – 2010	Ph. D. Osmania University Department of Chemistry, Hyderabad, India Work Done: CSIR-Indian Institute of Chemical Technology (IICT), Hyderabad, India
2003 – 2005	M. Sc. University of Calcutta, Kolkata, India
2000 – 2003	B. Sc. (Hons.) Ramakrishna Mission Vidyamandira, Belur Math, Howrah, India

Awards / Honors / Membership:

2015 Taiwan Ministry of Science and Technology (MOST) Fellowship for postdoctoral research
2012 Taiwan National Science Council (NSC) Fellowship for postdoctoral research
2005-10 CSIR-Fellow (JRF & SRF)
2005 Recipient of National Scholarship from Calcutta University
2003 Recipient of Somnath Banerjee Memorial Awards: (RKMV, Belur)

Website: https://krishnathcollege.ac.in/Chemistry.aspx

Bio-Sketch of Participant

AJAY SINGH YADAV, Ph.D.

Group Leader, Discovery Chemistry (Product Innovation)
PI Industries LTD, Udaipur, Rajasthan, India
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Ajay Singh Yadav is working as Deputy General Manager & Group Leader in discovery chemistry department (Product Innovation vertical) at PI Industries Udaipur. In his current role, he supports agrochemical discovery program, focussed on identifying new active ingredients for crop protection research. At PI Industries, Ajay has led a range of hit-to lead and lead to development phase (candidate) projects spanning a number of target classes. He has contributed significantly to advancing an insecticide from research to developmental phase (crop protection research). Prior to PI industries, he worked as Assistant Director & Group Leader at Daiichi Sankyo Research Center India & Ranbaxy Laboratories LTD where he has taken 2 drugs to clinical trials. In total, he has over 20 years of pharmaceutical & agrochemical research experience working in multinational industry in India and Japan.

He received his Master's in pharmaceutical chemistry from Lucknow University & secured industry sponsored PhD degree in synthetic organic chemistry from University of Jamia Millia Islamia, New Delhi.

Ajay authored and co-authored more than 20 patents (PCT) and 8 research papers. His research interests include Agrochemicals, medicinal chemistry design, data analytics and compound safety with a particular focus on computer-aided molecular property prediction and target-based discovery.

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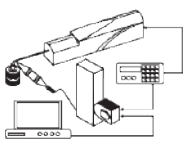

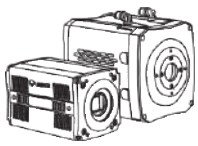

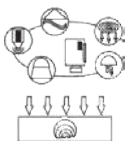

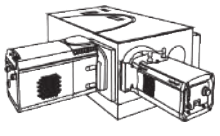

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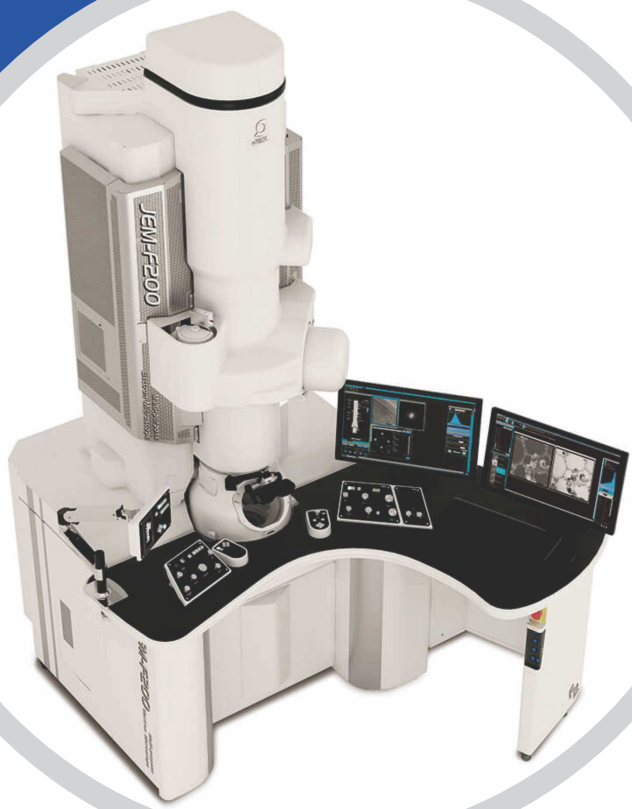

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