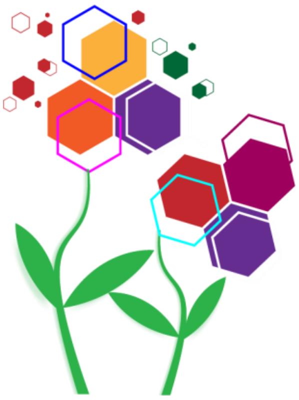
काशी हिन्दू विश्वविद्यालय
BANARAS HINDU UNIVERSITY

AN INSTITUTION OF NATIONAL IMPORTANCE ESTABLISHED BY AN ACT OF PARLIAMENT

National Symposium on Emerging Trends in Chemical Sciences

ETCS 2023



December 15-16, 2023

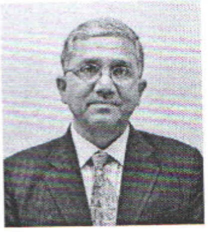
BOOK OF ABSTRACTS

Organized by
Department of Chemistry
Institute of Science
Banaras Hindu University
Varanasi 221 005 U.P., India

काशी हिन्दू विश्वविद्यालय
BANARAS HINDU UNIVERSITY
AN INSTITUTION OF NATIONAL IMPORTANCE ESTABLISHED BY AN ACT OF PARLIAMENT

प्रो.अनिल कुमार त्रिपाठी, निदेशक, विज्ञान संस्थान
Prof. Anil Kumar Tripathi
FNA, FASc, FNASc, FNAAS
Director, Institute of Science
Professor, School of Biotechnology
Banaras Hindu University, Varanasi-221005
(Formerly Director, CSIR-CIMAP, Lucknow)

Dated: 13.12.2023



MESSAGE

I am extremely happy to learn that the Department of Chemistry at the Institute of Science, Banaras Hindu University, Varanasi, India, will be hosting a National Symposium on "Recent Trends in Chemical Sciences (ETCS-2023)" on December 15-16, 2023. This symposium, featuring a broad and comprehensive theme, holds the promise of bringing together scientists and researchers from diverse disciplines within the realm of chemical sciences. Their collective purpose will be to evaluate recent advancements in research, anticipate forthcoming challenges and opportunities, and facilitate the convergence of various facets of Chemical Sciences to foster their synergistic growth.

I fully anticipate that the symposium will create new avenues for collaboration and prove to be an immensely productive endeavour. I extend my heartfelt best wishes and congratulations to the Chemistry Department for spearheading such a meaningful event. I wholeheartedly welcome all participants to the Symposium and wish for its resounding success.

(Anil K Tripathi)
Director

Email: director.inst.science@gmail.com
tripathianil@rediffmail.com
Website: www.bhu.ac.in
Varanasi 221005, UP, India
T : 91-542-2369670
T : 91-8887161518

काशी हिन्दू विश्वविद्यालय
BANARAS HINDU UNIVERSITY
ESTABLISHED BY PARLIAMENT BY NOTIFICATION NO. 225 OF 1916

प्रो0 सुख महेंद्र सिंह
संकाय प्रमुख, विज्ञान संस्थान,
काशी हिन्दू विश्वविद्यालय
Prof. Sukh Mahendra Singh
DEAN, Faculty of Science, BHU

Date: 13.12.2023

MESSAGE

I am extremely happy to learn that the Department of Chemistry at the Institute of Science, Banaras Hindu University, Varanasi, India, will be hosting a National Symposium on "Recent Trends in Chemical Sciences (ETCS-2023)" on December 15-16, 2023. This symposium, encompassing a wide range of topics within the field of chemical sciences, promises to bring together scientists and researchers from diverse backgrounds to delve into recent research advancements, identify upcoming challenges, and foster collaboration across various facets of Chemical Sciences, thereby promoting their collective growth.

I anticipate that this symposium will serve as a platform for forging new collaborations and prove to be a highly productive endeavour. I would like to extend my heartfelt best wishes and congratulations to the Department for orchestrating such a valuable event. I eagerly welcome all participants to the Symposium and wish for its resounding success.

(Sukh Mahendra Singh)
Dean
Faculty of Science

BHU
capital of knowledge

Varanasi - 221005, UP, INDIA
Mob. : 8052664273
E : dean_sci@bhu.ac.in
Twitter: @DeanScienceBHU
W : www.bhu.ac.in

काशी हिन्दू विश्वविद्यालय
BANARAS HINDU UNIVERSITY
AN INSTITUTION OF NATIONAL IMPORTANCE ESTABLISHED BY AN ACT OF PARLIAMENT

Prof. M. S. Singh (FNA, FASc, FNASc)
JC Bose Fellow/CNR Rao Chair Professor
HEAD
Department of Chemistry
Institute of Science
Banaras Hindu University
Varanasi-221005 (U.P.) India

Phone: +91-9415372614 (Mob) +91-542-2227001 (Off)
E-mail: mssingh@bhu.ac.in, mayashankarbhu@gmail.com

Message from the Head, Department of Chemistry

I am delighted to announce the forthcoming National Symposium on "Recent Trends in Chemical Sciences (ETCS-2023)" being organized by the Department of Chemistry, Institute of Science, Banaras Hindu University, Varanasi on December 15 and 16, 2023. Chemistry is having a much broader viewpoint today than it had a few decades ago. The knowledge integration through interdisciplinary areas of chemistry has invariably invigorated breakthrough discoveries for providing solution to present day problems. This conference is aimed at extending a platform to facilitate critical discussions on recent developments in various areas of all aspects of chemistry. Leading Chemists from all over India will deliver lectures on their most recent findings, and will exchange ideas which will motivate the young minds and help them to find the new paths for the future. We trust this conference will turn out to be a wonderful platform for insightful discussions among academicians, researchers, and industrialists who are dealing with chemical science and industry. With great pleasure and honor I welcome all the participants and delegates to the Department of Chemistry for the ETCS-2023 symposium. We hope this meeting will have a viable impact on its more than 200 participants and will encourage them to break out of stale thinking pattern and translate their ideas to major scientific advances.

(M. S. Singh)
Head

Prof. Satyendra K. Pandey
Department of Chemistry
Institute of Science
Banaras Hindu University
Varanasi-221 005 India

काशी हिन्दू विश्वविद्यालय
BANARAS HINDU UNIVERSITY
AN INSTITUTION OF NATIONAL IMPORTANCE ESTABLISHED BY AN ACT OF PARLIAMENT

December 13, 2023

Message from the Convener, ETCS-2023

We are delighted to announce the forthcoming National Symposium, "Recent Trends in Chemical Sciences (ETCS-2023)," meticulously organized by the Department of Chemistry at the Institute of Science, Banaras Hindu University, Varanasi. This esteemed event is scheduled to take place on December 15 and 16, 2023.

Chemistry has evolved significantly, adopting a broader perspective than it held a few decades ago. Presently, it encompasses a multitude of interdisciplinary areas that directly address contemporary challenges. These comprise core branches such as Analytical Chemistry, Inorganic Chemistry, Organic Chemistry, and Physical Chemistry, alongside emerging sub-disciplines including Biological Chemistry, Materials Chemistry, Industrial Chemistry, Catalysis, and more. The primary objective of this conference is to provide a platform for the discussion of recent developments across all facets of chemistry.

Distinguished chemists from India will deliver lectures on their latest discoveries, fostering the exchange of innovative ideas that will inspire young minds and guide them towards new horizons in the field. We firmly believe that this symposium will serve as a valuable forum for meaningful interaction among academics, researchers, and industrialists deeply engaged in the realms of chemical science and industry.

It is our distinct honor and pleasure, on behalf of the Organizing Committee, to extend a warm welcome to all participants to the world's one of the oldest living cities, Varanasi, for ETCS-2023. With an anticipated gathering of more than 200 participants, we foresee this meeting as an academically rewarding, intellectually stimulating, and enjoyable experience for all involved.

(Satyendra K. Pandey)
Convener, ETCS-2023

BHU
capital of knowledge

Varanasi 221 005, UP, INDIA
T: +91-8437908745 (M)
+91-7009346528 (M)
E-mail: skpandey.chem@bhu.ac.in
skpncl@gmail.com

Prof. Sudhir K. Jain, Vice-Chancellor, BHU (Chief Patron)

Organizing Committee
ETCS 2023

Prof. Sudhir K. Jain, Vice-Chancellor, BHU (Chief Patron)
Prof. Anil K. Tripathi, Director, Institute of Science (Co-patron)
Prof. Sukh Mahendra Singh, Dean, Institute of Science (Co-patron)
Prof. M. S. Singh, Head, Department of Chemistry (Co-patron)
Prof. Satyendra K. Pandey (Convener)
Dr. Roop Shikha Singh (Co-convener)
Dr. Ashok K. Basak (Secretary)
Dr. Kanak Roy (Jt. Secretary)
Dr. Manivannan S (Treasurer)

Distinguished Professors
Prof. G. Pandey, Prof. B. Singh, Prof. L. Mishra

Local Organizing Committee

Prof. D. S. Pandey
Prof. K. N. Singh
Prof. K. K. Upadhyay
Prof. V. P. Singh
Prof. R. N. Rai
Prof. A. Misra
Prof. V. Ganesan
Prof. P. Srivastava
Prof. P. Prakash
Prof. M. D. Pandey
Prof. B. K. Kuila
Prof. V. Prasad
Prof. S. Krishnamoorthi
Dr. L. B. Prasad
Dr. A. Kumar
Dr. N. Goel
Dr. R. Lalneihpuii
Dr. K. Kumar
Dr. K. C. Bharadwaj
Dr. A. Manna
Dr. V. K. Das
Dr. S. Kushwaha
Prof. M. S. Singh
Prof. R. Venkatesh
Prof. S. Bhattacharya
Prof. B. Ray
Prof. I. Tiwari
Prof. R. Kumar
Prof. A. K. Tewari
Prof. S. Saha
Prof. R. K. Mishra
Prof. K. V. S. Ranganath
Prof. V. K. Tiwari
Prof. B. Maiti
Dr. M. K. Bharti
Dr. D. Guin
Dr. P. R. Prasad
Dr. J. Singh
Dr. S. Rakshit
Dr. Abhishek Kumar
Dr. S. Trivedi
Dr. A. K. Kharwar
Dr. S. Garai
Dr. M. Pal

MMV Faculty Members

Prof. M. Singh
Prof. S. Pratap
Dr. D. Kushwaha
Prof. S. Pokharia
Dr. S. S. Sunkari
Dr. B. Mahanti
Prof. D. Katiyar
Dr. P. Sonkar
Dr. S. K. S. Patel

NATIONAL SYMPOSIUM ON
Emerging Trends in Chemical Sciences (ETCS 2023)

Department of Chemistry, Banaras Hindu University, Varanasi-221 005
December 15 and 16, 2023
Schedule

Day 1 (15/12/2023)

Registration		8:00 to 9:00 AM	
Inaugural Function		9:00 to 9:30 AM	
Inaugural High Tea		9:30 to 10:00 AM	
Technical Session I Chaired by Prof. Ganesh Pandey	KL	10:00 to 10:45 AM	Prof. H. Ila JNCASR, Bangalore
	IL1	10:45 to 11:15 AM	Prof. Santosh Gharpure IIT Bombay
	IL2	11:15 to 11:45 AM	Prof. Akhila K. Sahoo University of Hyderabad
	IL3	11:45 to 12:15 PM	Prof. S. S. V. Ramasastry IISER Mohali
	FP1	12:15 to 12:45 PM	Prof. M. S. Singh Banaras Hindu University
Lunch & Poster presentation		12:45 to 2:15 PM	
Technical Session II Chaired by Prof. K. N. Singh	IL4	2:15 to 2:45 PM	Prof. Nandita Madhavan IIT Bombay
	IL5	2:45 to 3:15 PM	Dr. Ravindar Kontham CSIR-NCL Pune
	IL6	3:15 to 3:45 PM	Dr. Sudipta Raha Roy IIT Delhi
Evening Tea		3:45 to 4:00 PM	
Technical Session III Chaired by Prof. S. Bhattacharya	IL7	4:00 to 4.30 PM	Dr. E. Gnanamani IIT Roorkee
	IL8	4:30 to 5:00 PM	Dr. Mahipal Ganji IISc Bangalore

	IL9	5:00 to 5:30 PM	Dr. Amit Kumar IIT Patna
Dinner		7:30 PM onwards	

Day-2 (16/12/2023)

Technical Session IV Chaired by Prof. H. Ila	IL10	9:00 to 9:30 AM	Prof. Jyotirmayee Dash IACS Kolkata
	IL11	9:30 to 10:00 AM	Prof. Alakesh Bisai IISER Kolkata
	IL12	10:00 to 10:30 AM	Prof. Parthasarathi Das IIT (ISM) Dhanbad
Tea		10:30 to 10:45 AM	
Technical Session V Chaired by Prof. K. K. Upadhyay	IL13	10:45 to 11:15 AM	Prof. Prasenjit Ghosh IIT Bombay
	IL14	11:15 to 11:45 AM	Dr. Uttam Manna IIT Guwahati
	IL15	11:45 to 12:15 PM	Dr. Dipankar Koley CDRI-Lucknow
	IL16	12:15 to 12:45 PM	Dr. Surya Prakash Singh CSIR IICT Hyderabad
Lunch & Poster Presentation		12:45 to 2:15 PM	
Technical Session VI Chaired by Prof. R. Venkatesh	IL17	2:15 to 2:45 PM	Dr. Amrendra K. Singh IIT Indore
	FP2	2:45 to 3:15 PM	Dr. Kamlesh Kumar Banaras Hindu University
	FP3	3:15 to 3:45 PM	Dr. Debanjan Guin Banaras Hindu University
	FP4	3:45 to 4:15 PM	Dr. Sailaja Sunkari Banaras Hindu University
Valedictory Function		4:15 to 5:00 PM	
Closing Tea		5:00 PM onwards	

Index

Talks

KEYNOTE SPEAKER

Prof. H. Ila

Organic Synthetic Laboratory

New Chemistry Unit (NCU)

Jawaharlal Nehru Centre for Advanced Scientific Research (JNCASR)

Jakkur P.O., Bengaluru 560064, Karnataka, India

EDUCATION

M.Sc (1962-1964), DAV College, Kanpur

Ph.D (1964-1968) IIT Kanpur

Postdoctoral research (1969), Purdue University; Alexander von Humboldt fellow 1984-1985

Research Area

'Small molecule heterocycles' play important role in both drug discovery and material science research providing one of the richest source of diversity, besides serving as rigid scaffolds for further display of a range of functionalities. Prof. Ila has been engaged in design and development of new efficient methodologies for a wide range of substituted and fused five and six membered heterocycles utilizing organosulfur synthons such as polarized ketene dithioacetals and the corresponding N, S- acetals derived from them, as versatile building blocks. She has recently developed and synthesized new class of organosulfur synthons and utilized them for designing new reactions for diverse class molecular entities. Some of our recent results on these new synthetic methods derived from easily accessible organosulfur building blocks involving organometallic methods, radical cyclizations, transition metal catalyzed intramolecular C-C, C-N, C-S and N-O bond formation, multicomponent reactions, dipolar cycloadditions of metalloisocyanides, domino reactions and simple condensation reactions will be presented in the lecture

Achievements and Honors

Fellow, Indian Academy of science Bangalore (FASc.), 1991

Fellow, Indian National Science Academy, New Delhi (FNA), 2002

Chemical research Society of India (CRSI), Life time Achievement award (gold medal), 2019

INVITED LECTURES

IL 1-17

Dr. Santosh J. Gharpure
Professor In-Charge, SINE &
Rasiklal Hemani Fragrance and Flavour Chair Professor
Department of Chemistry
Indian Institute of Technology Bombay
Powai, Mumbai - 400076, INDIA
Email: sjgharpure@chem.iitb.ac.in

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

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

IL-1

Alkyne-based approaches to the heterocycle synthesis

Santosh J. Gharpure*
Department of Chemistry
Indian Institute of Technology Bombay, Powai, Mumbai – 400076
(Email: sjgharpure@chem.iitb.ac.in)

Metal catalyzed transformations of alkynes have gained prominence for the synthesis of oxa- and aza-cycles. However, their utility under metal free conditions is still under explored. In this context, we have demonstrated that the oxonium and iminium ion intermediates generated from vinylogous carbonates and carbamates in the presence of Lewis acids can be trapped with alkynes to get access to 2,3-disubstituted dihydrobenzofurans and indoline derivatives. Over the years, these studies were extended to divergent synthesis of heterocycles such as indoles, quinolines, cyclic ethers and amines and cyclic acetals under not only Lewis acidic conditions but also under radical conditions (Figure 1). The talk will focus on some of the recent developments on using alkynes for the synthesis of heterocycles and their application in total synthesis from our laboratory.

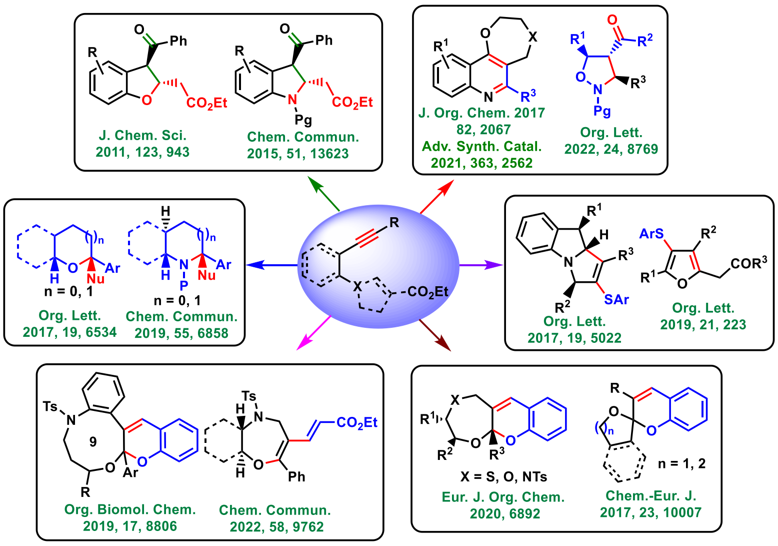


Fig. 1: Alkynes in the synthesis of heterocycles

References and Notes:

1. Gharpure, S. J.; Vishwakarma, D. S.; Patel, R. K. Chem. Commun., 2019, 55, 6858.
2. Gharpure, S. J.; Padmaja; Prasath, V.; Shelke, Y. G. Org. Lett., 2019, 21, 223.
3. Gharpure, S. J.; Fartade, D. J.; Gupta, K. S.; Patel, R. K. Chem. Commun., 2022, 58, 9762.
4. Gharpure, S. J.; Pal, J.; Pansuriya, K. C. Org. Lett., 2022, 24, 8769.
5. Gharpure, S. J.; Vishwakarma, D. S.; Hajam, S. A. Org. Lett. 2023, 25, 2525.
6. Gharpure, S. J.; Fartade, D. J.; Nanda, S. K.; Somani, S. Org. Lett. 2023, 25, 6155.
7. Gharpure, S. J.; Patel, R. K.; Gupta, K. S.; Org. Lett. 2023, 25, 5850.

Dr. Akhila K. Sahoo, PhD
Professor
School of Chemistry, University of Hyderabad, Hyderabad
Contact Number: 9908221898
e-mail: akhilchemistry12@gmail.com
akssc@uohyd.ac.in

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

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

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

Research topics:
-Development of novel synthetic methods for organic synthesis.
-Functionalizations of sp2 and sp3 C-H bonds. Stereoselective C-H functionalizations.
-Gold and silver-catalyzed organic transformations.
-Synthesis of fused-π-conjugated heterocycles.
-Synthesis of nitro and nitrogen-rich insensitive high energetic materials.

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

Supervision and Guidance: -PhD completed-19, -Currently supervising-09 -Total Citations 4723
[h-Index = 42; i10 Index = 79; Google Scholar as on 03/12/2023]

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

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

Contribution to National /International Forum

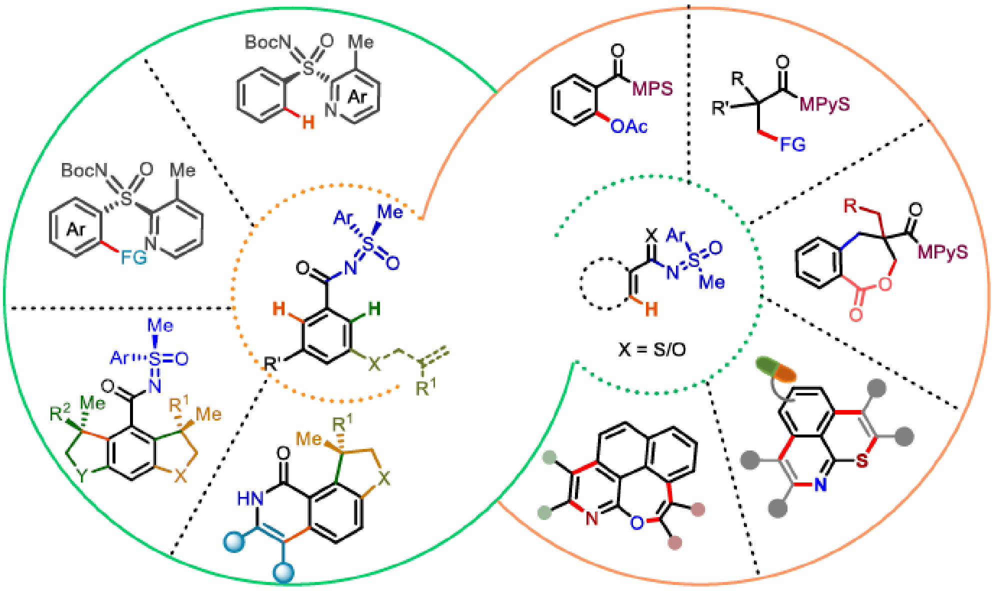
- Prof. Angela Marinetti, CNRS-ICSN, GIIF-sur-Yvette, Paris under CEFIPRA.
- Member of School Board of Chemistry: Central University of Rajasthan, BHU
- Council Member of the National Organic Symposium Trust (NOST; 2019-2021; 2022-2025).
- Treasurer of CRSI-India; Member of the RSC, Member of the ACS-USA

IL-2

Sulfoximine Directed C-H Functionalizations

Akhila K. Sahoo
Professor
School of Chemistry
University of Hyderabad, Hyderabad, India
(Email: akhilchemistry12@gmail.com / akssc@uohyd.ac.in)

Presented here is the discovery of a sulfoximine directed C□H functionalization. A monodentate methyl phenyl sulfoximine (MPS) directing group (DG) has been used for the C(sp^2)□H functionalization, while C(sp^3)□H functionalizations are realized in the presence of a bidentate pyridyl methyl sulfoximine (MPyS) DG. A bifunctional reagent 2-iodobenzoic acidhas been used for stitching two □-C(sp^3)□H bonds making unusual caprolactones. Multiple C□H annulations have also been probed under MPS-DG. Chiral sulfoximine auxiliaries have also influenced for the asymmetric two-fold C□H annulations. Kinetic resolution of sulfoximines is another notable outcome. The sulfoximine DG can be easily cleaved and reused, transformed, and also behave as a transient-DG.



asymmetric C–H functionalization

diverse C–H functionalizations/annulations

1. *Org. Lett.* ***2012,*** *14, 3724*
2. *Org. Lett.* ***2014,*** *16, 5258*
3. *JOC.* ***2014,*** *79, 6163*
4. *Angew. Chem. Int. Ed.* ***2016,*** *55, 7821*
5. *Chem. Sci.*, ***2020***, *11, 10770*
6. *Chem. Sci.*, ***2021***, *12, 6393*
7. *Chem. Sci.*, ***2021***, *12, 14863*
8. *Org. Lett.* ***2022***, *51, 9508*
9. *ACS Catal.* ***2023,*** *13, 7627*

Dr. S. S. V. Ramasastry
Associate Professor
Department of Chemical Sciences
Indian Institute of Science Education and Research (IISER) Mohali
Sector 81, S.A.S. Nagar, Punjab 140 306, INDIA
E-mail: ramsastry@iisermohali.ac.in
Webpage: https://web.iisermohali.ac.in/faculty/sastry

Ramasastry obtained Ph.D. in Chemical Sciences in 2005 from the Department of Organic Chemistry, Indian Institute of Science, Bangalore (India), under the supervision of Prof. A. Srikrishna. He then pursued postdoctoral studies with Prof. Carlos F. Barbas, III at The Scripps Research Institute, San Diego (USA). After briefly working in the industry, he became Assistant Professor in 2011 and then Associate Professor in 2017 at the Department of Chemical Sciences, IISER Mohali.

His research interests include the development of sustainable and atom economic reactions via organophosphine catalysis, palladium-catalyzed allylic alkylation reactions, one-pot cascade transformations employing sulfur ylides, and applying these strategies in the synthesis of bioactive natural products and pharmaceutically important compounds.

He was a recipient of the CDRI Award for Excellence in Drug Research 2022, ‘RSC Research Fund’ grant in 2020, DST-Swarnajayanti Fellowship 2018, CRSI Bronze Medal 2018, AVRA Young Scientist award 2018, OPPI Young Scientist award 2018, and Thieme Chemistry Journals award in 2017. He has been invited to become the ‘Fellow of the Royal Society of Chemistry (FRSC)’ under 'Leaders in the Field (LITF)' scheme. He served as an Editorial Advisory Board member of the RSC journal, Organic & Biomolecular Chemistry (OBC), during 2017-22. Since 2022, he has been an Editorial Board member of OBC. He was invited to become a council member of the NOST for 2023-26.

II -3

The Discovery and the Development of an Interrupted Corey-Chaykovsky Reaction

S. S. V. Ramasastry
Department of Chemical Sciences, IISER Mohali, Sector 81, SAS Nagar, Punjab 140306
(E-mail: ramsastry@iisermohali.ac.in)

Abstract:

Cyclopropanes are crucial structural units in several bioactive natural products and pharmaceutically relevant compounds, including a few marketed drugs.[1] The enhanced metabolic stability and conformational rigidity of cyclopropanes are critical during drug design and development.

The Corey-Chaykovsky reagent [dimethyloxosulfonium methylide (DOSM)] is typically employed for the preparation of cyclopropanes from electron-deficient olefins. However, we utilized DOSM as a nucleophilic trigger to induce cascade transformations to access several new classes of fused- and spirocyclopropanes with multiple stereocenters (Figure 1).[2-5] Since all these reactions involve unusual rearrangements associated with multiple proton shifts, we devoted significant efforts to elucidate the intriguing mechanistic details. Further, the cyclopropanoids were elaborated to various privileged structures with distinctive substitution patterns.

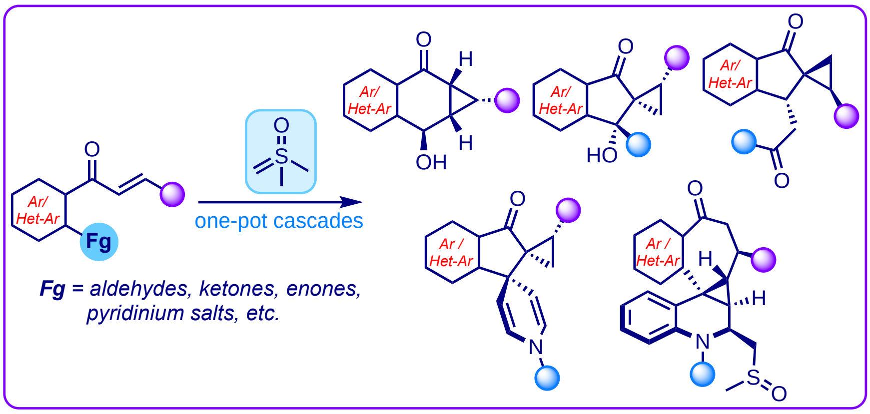


Figure 1: Summary of our work on the interrupted Corey-Chaykovsky reaction

References and Notes:

1. Selected reviews: (a) Chen, D. Y.-K.; Pouwer, R. H.; Richard, J.-A. Chem. Soc. Rev. 2012, 41, 4631. (b) Chawner, S. J.; Cases-Thomas, M. J.; Bull, J. A. Eur. J. Org. Chem. 2017, 5015.
2. Mishra, U. K.; Patel, K.; Ramasastry, S. S. V. Org. Lett. 2019, 21, 175.
3. Patel, K.; Mishra, U. K.; Mukhopadhyay, D.; Ramasastry, S. S. V. Chem. Asian J. 2019, 14, 4568 [Invited for a special issue on the 20th anniversary of CRSI]
4. Mishra, U. K.; Patel, K.; Ramasastry, S. S. V. Org. Lett. 2020, 22, 3815.
5. Singh, B.; Ansari, A. J.; Malik, N.; Ramasastry, S. S. V. Chem. Sci. 2023, 14, 6963.

Dr. Nandita Madhavan
Professor
Department of Chemistry
Indian Institute of Technology Bombay
E-Mail: nanditam@chem.iitb.ac.in
Homepage:https://www.chem.iitb.ac.in/facultyuserview/nandita-madhavan

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

Cyclic Peptide Drugs: Minimalistic Scaffolds and Sustainable Synthesis?

Nandita Madhavan
Department of Chemistry, Indian Institute of Technology Bombay
Email: nanditam@chem.iitb.ac.in

Abstract: A majority of the naturally occurring biologically active peptide drugs are cyclic with disulfide linkages. The method of choice for synthesizing medium-sized peptide drugs is solid phase peptide synthesis (SPPS)[1] as isolation of growing peptides is easy and quick. Excess coupling reagents and amino acids are added to improve reaction efficiency on the insoluble support. Liquid phase peptide synthesis (LPPS) utilizes supports that are soluble in the reaction medium to reduce reagent requirement.[2] The differential solubility of these supports in various solvents is exploited for peptide isolation via precipitation or extraction. Our group has developed polynorbornene supports with solubilizing groups that retain their solubility up to hexadecapeptide synthesis.[3] These polymers have an added advantage of being in an uncoiled form in the "pro/good solvent" that solubilizes them. This conformational preference facilitates on-support cyclization to access cyclic peptide drugs such as octreotide with an overall yield of 69% yield with high purity. These supports can also be recycled for peptide synthesis

Cyclic peptides with anion-binding domains are also promising targets for treatment of cystic fibrosis and cancer. Our group has developed one-pot macrocyclization strategies to access macrocyclic amides/peptides as transmembrane anion-transporters.[4]

References and notes:

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

Dr. Ravindar Kontham
Principal Scientist-CSIR
Associate Professor-AcSIR
Organic Chemistry Division
CSIR-National Chemical Laboratory
Pune, INDIA
E-Mail: k.ravindar@ncl.res.in

Homepage: https://konthamravindar.wixsite.com/my-site

Dr. Ravindar Kontham was born and raised in Warangal, which is situated 120 kilometers away from Hyderabad City. He earned his Bachelor of Science (BSc) degree from Kakatiya University, Warangal, and later completed his Master of Science (MSc) degree from Osmania University in Hyderabad, India. His journey in the field of chemistry commenced with a 9-month tenure at Dr. Reddys Laboratories, Hyderabad. In 2003, he joined the CSIR-Indian Institute of Chemical Technology (CSIR-IICT), Hyderabad, as a CSIR-JRF, culminating in the successful completion of his Ph.D. in Organic Synthesis under the mentorship of Dr. J. S. Yadav, the former Director of CSIR-IICT.

Subsequently, he served as an NSERC post-doctoral fellow with Prof. Pierre Deslongchamps at Université de Sherbrooke for two years and at Université Laval in Québec, Canada for three years. Following a short-term stint of nine months at the premier Contract Research Organization, Toronto Research Chemicals (TRC) in Toronto, Canada, as a Senior Research Scientist, he returned to India. In 2014, he assumed the role of a Senior Scientist in the Organic Chemistry Division at CSIR-NCL, Pune, India. Presently, he holds the position of Principal Scientist in the Organic Chemistry Division at CSIR-NCL, Pune.

His research interests include the development of novel cascade/domino reactions involving main group and transition metal catalysis and their application in the stereoselective total synthesis of bioactive natural products, the design and synthesis of new chemical entities for drug discovery applications, as well as chemical process development for Active Pharmaceutical Ingredients (APIs) and API intermediate.

He is the author of 47-reseach publications and holds 4-patents. Under his supervision, 6-students have been awarded Ph. D. degrees. 2-Post-doctoral students completed their work. He has also supervised 16-Master’s students for their dissertation. Presently, 8-Research Fellows are working toward their Ph. D., and 6-Project Associates are engaged in various CSIR and SERB projects.

IL-5

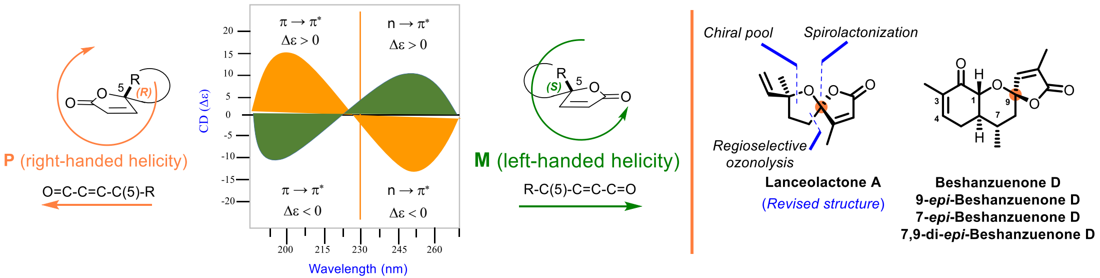
Total Synthesis of Oxaspiro Butenolide-Derived Natural Products: Unlocking the Absolute Configuration through Electronic Circular Dichroism (ECD)

Ravindar Kontham*
Organic Chemistry Division
CSIR-National Chemical Laboratory, Pune, India
(E-mail: k.ravindar@ncl.res.in)

Abstract:

Terpenoids represent a highly diverse and widespread class of natural products with a wide array of applications. Extensive in vitro, preclinical, and clinical drug discovery studies have affirmed the various pharmacological properties of this compound class, leading to their registration as marketable drugs. In recent years, several terpenoids featuring an oxaspirolactone moiety, particularly [5,5]- and [6,5]-oxaspirolactone (butenolide-derived compounds) have been isolated from diverse sources, revealing intriguing biological profiles.[1] This talk will spotlight the recent achievements of our research group in the context of the stereoselective total synthesis of bioactive natural products, including beshanzuenone-D[2] and its epimers, as well as lanceolactone A,[3] all of which are derived from oxaspiro-butenolides. Moreover, this talk will also showcase our research into the development of Electronic Circular Dichroism (ECD) as a versatile tool for determining the absolute stereochemistry of this class of natural products.[3]

Figure 1:



Sign of **Cotton effect** correlates with the configuration of the more polarizable bond at the **Spiro-carbon**

References and Notes:

1. Thorat, S. S.; Kontham, R. Org. Biomol. Chem., 2019, 17, 7270-7292 (Review Article).
2. Borade, B. R.; Dixit, R.; Kontham, R. Org. Lett., 2020, 22, 8561 – 8565.
3. Borade, B. R.; Kontham. R. J. Org. Chem., 2022, 87, 12867-12876.

Dr. Sudipta Raha Roy
Indian Institute of Technology Delhi

Dr. Sudipta Raha Roy earned his PhD from NIPER-Mohali under the supervision of Prof. Asit K. Chakraborti. Dr. Raha Roy joined the group of Prof. Ilan Marek at Technion, Israel as a PBC postdoctoral fellow. He further continued his postdoctoral studies with Prof. Paolo Melchiorre at ICIQ, Spain as a Marie Curie postdoctoral fellow. In November 2018, Dr. Raha Roy joined the Indian Institute of Technology Delhi as an Assistant Professor in the Department of Chemistry and subsequently promoted to Associate Professor in March 2023. His current research interests concern the discovery and development of sustainable catalysis for small molecule activation.

IL-6

Utilizing Renewable Energy to Functionalize C(sp^2)-H Bond for the Synthesis of Value-Added Compounds

Sudipta Raha Roy
Associate Professor
Indian Institute of Technology Delhi
New Delhi
Email: srr@chemisry.iitd.ac.in

Functionalization of C-H bonds owing to the large kinetic barrier associated with its bond cleavage has always been most dynamic topics to synthetic chemists.[1] Tremendous advancements have been done in the field of metal catalyzed C-H bond functionalization to achieve diverse functionalities.[2] These viable strategies offer great opportunities for the synthesis of pharmaceutically relevant molecules, agrochemicals, natural products and complex molecular scaffolds.[3] The classical methods mainly rely on utilization of pre-activated precursors for both reactivity as well as selectivity. However, the requirement for installation of an activating group prior to transformation adds cost to the synthetic route and lead to production of unwanted byproducts. Therefore, development of more atom and step-economical methodologies for direct C-H functionalization without any pre-activation of starting material is highly desirable.

As a part of our ongoing interest on the functionalization of C-H bonds[4], how the readily available and cost-effective building-blocks can be utilized to functionalize C(sp^2)-H bond in the presence of light and electricity will be discussed in this lecture.

References:

[1] D. Morton, Huw M. L. Davies, J. Org. Chem. 2016, 81, 343–350.

[2] L. Revathi, L. Ravindar, W.-Y. Fang, K. P. Rakesh, H.-L. Qin, Adv. Synth. Catal. 2018, 360, 4652–4698.

[3] D. J. Abrams, P. A. Provencher, E. J. Sorensen, Chem. Soc. Rev. 2018, 47, 8925–8967.

[4] Partha Pratim Sen, Rashmi Prakash, Sudipta Raha Roy, Org. Lett., 2022, 24, 4530-4535; Swati Singh, Neha Dagar, Sudipta Raha Roy, Chem. Commun., 2022, 58, 3831-3834; Swati Singh, Gopal Chakrabortty, Sudipta Raha Roy, Chem. Sci., 2023,14, 12541-12547.

Dr. Gnanamani Elumalai
Assistant Professor
Department of Chemistry
Indian Institute of Technology Roorkee
Roorkee, Uttarakhand – 247667.
Contact Number: +911332-284940
e-Mail: gnanam@cy.iitr.ac.in

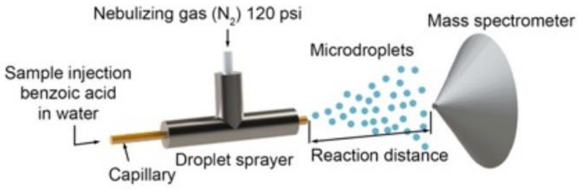
Web page: https://gnanam8.wixsite.com/gnanamlab
Dr. E. Gnanamani is currently an assistant professor of Organic Chemistry at IIT-Roorkee. He obtained his Ph.D. from Pondicherry University with Prof. C. R. Ramanathan in April 2013. In June 2013, he began a postdoctoral appointment at the ICCAS, where he researched asymmetric organocatalysis with Profs. Luo Sanzhong and Jin-Pei Cheng. In November 2014, he was awarded a Fulbright Fellowship to pursue further postdoctoral studies at Stanford University. At Stanford, he worked in Prof. B. M. Trost's group from January 2015 to March 2020 on a variety of different transition metal-catalyzed reactions. While at Stanford, Dr. E. Gnanamani also worked with Prof. R. N. Zare to develop methods of accelerating organic reactions in microdroplets. Dr. E. Gnanamani, a recipient of developing country international award and Fulbright award. Also, Dr. E. Gnanamani serving as associate editor of Current Indian Science: Organic Synthesis Journal. He has published research papers in high impact journals such as JACS, Nat. Cat., Angew. Chem. Int. Ed., PNAS etc.

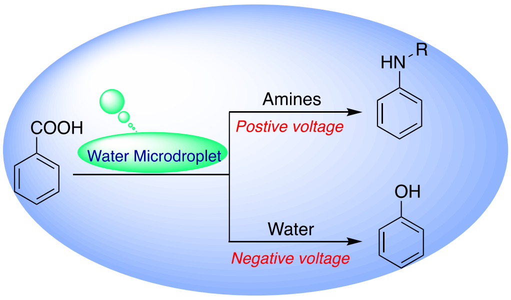
IL-7

Direct C-N and C-O Bond Formation Reactions in Water Microdroplets

Gnanamani Elumalai*
Department of Chemistry, Indian Institute of Technology Roorkee, Roorkee 247667, India.
Email : gnanam@cy.iitr.ac.in

Water microdroplets exhibit unusual reaction properties that are not observed in bulk water or other organic solvents.[1-3] Due to the advantages of hydrogen peroxide formation at the water-gas interface under the strong electric field, we and others utilized the hydroxyl radical to carry out various organic reactions.[4-5] Nitrogen and oxygen containing organic compounds play a major role in synthesis of biologically active targets, natural products synthesis and pharmaceuticals. Several methods were available for the synthesis of nitrogen and oxygen, containing organic molecules via C-N or C-O bond formation. The existing methods requires rather harsh reaction conditions, such as use of a metal catalyst, long reaction times, irradiation at different wavelengths, and high temperatures. More economical and green methods to rapidly form C–N or C-O bonds at room temperature are still under investigation. In this talk, I will briefly discuss the direct C–N and C-O bond formation reaction in water microdroplets. The C-N and C-O bond formation products were obtained in single step at room temperature without metal catalyst in water.[5-7]





References:

1. E. Gnanamani, X. Yan, R. N. Zare, Angew. Chem. Int. Ed. 2020, 59, 3069.
2. P. Basuri, L. E. Gonzalez, N. M. Morato, T. Pradeep, R. G. Cooks, Chem. Sci. 2020, 11, 12686.
3. A. Kumar, S. Mondal, Sandeep, P. Venugopalan, A. Kumar, S. Banerjee, J. Am. Chem. Soc. 2022, 144, 3347.
4. L. Xue, B. Zheng, J. Sun, ACS Sustain. Chem. Eng. 2023, 11, 12780.
5. Y. Meng, E. Gnanamani, R. N. Zare, J. Am. Chem. Soc. 2022, 144, 19709.
6. Y. Meng, E. Gnanamani, R. N. Zare, J. Am. Chem. Soc. 2023, 145, 32.
7. Y. Meng, R. N. Zare, E. Gnanamani, J. Am. Chem. Soc. 2023, 145, 19202.

Dr. Mahipal Ganji
Department of Biochemistry

IISc Bangalore

Assistant Professor (Oct 2020 onwards)

Postdoc: MPI Biochemistry, Germany, 2018-20

Postdoc: TU Delft, The Netherlands, 2016-18

PhD: TU Delft, The Netherlands, 2012-16

email: ganji@iisc.ac.in

IL8

Single molecule analysis of DNA base-stacking energies and their applications

Mahipal Ganji

IISc Bangalore

DNA double helix structure is stabilized by the base-pairing and the base-stacking interactions. Base-stacking interactions originating from hydrophobic interactions between the nucleobases predominantly contribute to the duplex stability. A comprehensive understanding of dinucleotide base-stacking interactions is lacking owing to the unavailability of sensitive techniques that can measure these weak interactions. Earlier studies attempting to address this question only managed to estimate the base-pair stacking interactions, however, disentangling individual base-stacking interactions was enigmatic. We implemented single molecule imaging in combination with DNA nanotechnology for multiplexed DNA-PAINT super-resolution imaging and experimentally measured the free energy of dinucleotide base-stacking. Multiplexed imaging enabled us to extract binding kinetics of an imager strand with and without additional dinucleotide stacking interactions in a single imaging experiment, abolishing any effects of experimental variations. The DNA-PAINT data showed that a single additional dinucleotide base-stacking results in as much as 250-fold stabilization of the imager strand binding. We found that the dinucleotide base-stacking energies vary from -1.18 ± 0.17 kcal/mol to -3.57 ± 0.08 kcal/mol for C|T and A|C base-stackings, respectively. We demonstrate the application of base-stacking energetics in designing DNA-PAINT probes for multiplexed super-resolution imaging. Our results reveal that the base-stacking energies are highly dependent on the DNA backbone sequence and will aid in designing functional DNA nanostructures, DNA and RNA aptamers, and facilitate better predictions of the local DNA structure.

Dr. Amit Kumar
Associate Professor
Department of Chemistry
Indian Institute of Technology Patna
Cell Number: +91-7761897841
E-Mail: amitkt@iitp.ac.in
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 ACIT 2023-2026
- Life-member- CRSI, India
- Life-member-ISCB, India
- Life-member, ACIIT, India

AK research group is primarily involved in the design and development of cost and atom-economical strategies for the 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

Decoding the Chemistry of Primary Amide/Imidates for Functionalization Reactions

Amit Kumar*
Department of Chemistry
Indian Institute of Technology Patna, Bihar, India
(E-mail: amitkt@iitp.ac.in)

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] However, major challenges lies with these methods regio- and chemo-selective functionalization of C-H bonds. To overcome these issues, the concept of a directing group was introduced, which offers chemoselective transformations.

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 primary amide/imidates functionality, has been rarely utilized as a DGs owing to its least reactive nature and makes an unattractive and challenging synthon. Considering the high abundance and challenges, we became interested in exploring the chemistry of primary amide/Imidates as optimal directing groups 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.

Dr Jyotirmayee Dash
Professor
Indian Association for the Cultivation of Science, Kolkata
School of Chemical Sciences, Jadavpur, 700032
E-mail: ocjd@iacs.res.in
Homepage:
http://iacs.res.in/athusers/index.php?navid=0&userid=IACS0034

Professor Jyotirmayee Dash obtained her Ph.D. in Organic Chemistry from IIT Kanpur, India. She was awarded Alexander von Humboldt fellowship at Freie University, Berlin, a postdoctoral fellowship at ESPCI-Paris, and Marie Curie fellowship at University of Cambridge, UK. She first joined IISER, Kolkata as an Assistant Professor in 2009 and is currently working as a Senior Professor at IACS-Kolkata. She has been serving as an advisory board member of journals like ACS Bioconjugate Chemistry, ACS Omega, Asian JOC, Chemical Communications, and Sectional editor (Organic and Biomolecular Chemistry) of Journal of the Indian Chemical Society.
Research Interests:
Her research interests include new organic transformations, supramolecular chemistry and structure and function of nucleic acids.

Awards and Honors:

1 Received DST Swarnajayanti (2015-2016) Fellowship
2 DBT Wellcome Trust (2020) Fellowship
3 Shanti Swarup Bhatnagar Prize (2020)
4 Bronze Medal, Chemical Research Society of India (CRSI) (2020)
5 Elected Fellow of the Indian Academy of Sciences (IASc), Bangalore, 2021

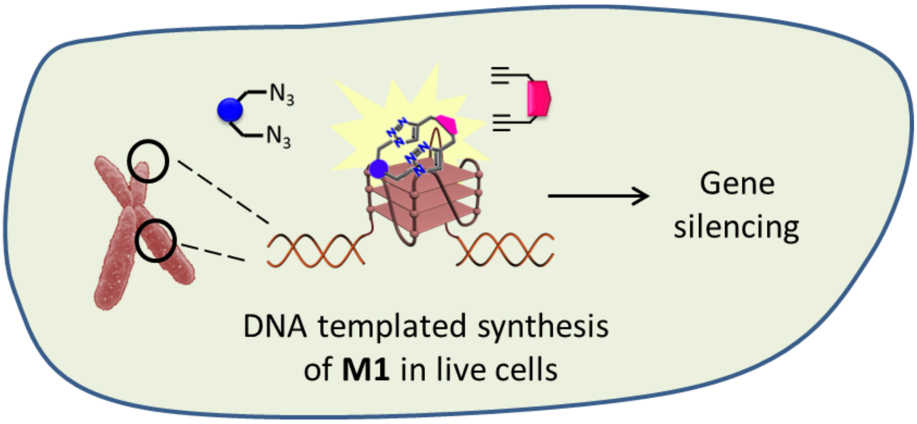
IL-10

Bioorthogonal synthesis using nucleic acid templates.

Jyotirmayee Dash*
ocjd@iacs.res.in
Indian Association for the Cultivation of Science, Kolkata, School of Chemical Sciences,
Jadavpur, 700032, India

Abstract:

Biorthogonal reactions are a class of reactions that rapidly join molecules under ambient or biological conditions. In this talk, bioorthogonal synthesis using nucleic acids as the template to synthesize small molecule binders will be described. DNA and RNA secondary structures have been used as templates to promote alkyne and azide cycloaddition in the absence of any metal catalysts. Non B-DNA structures like the four stranded G-quadruplexes and i-motifs have been used to synthesize with promising anticancer properties. The in situ synthesis of ligands in cellular system is a potential approach to directly achieve bioactive small molecules by combining synthesis and screening steps.



References

1. P. Saha, D. Panda, J. Dash, Chem. Soc. Rev., 2023, 52, 4248-4291.
2. R. Chaudhuri, P.Thumpati, J. Dash, Angew. Chem.Int. Ed. 2023, 62, e2022152 (front cover, appeared in Hot Topic: Bioorthogonal Chemistry).

Dr. Alakesh Bisai
Convener, PGAC & Professor
(& Former Professor, IISER Bhopal)
Department of Chemical Sciences
IISER Kolkata, India
Homepage: https://www.iiserkol.ac.in/~alakesh/

PhD Guided: 21 Current PhD Students: 15 BS-MS Guided: 18 Project Assistant: ~65
Extramural Funding: 14 Extramural Fundings (11 completed & 3 ongoing)

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

Representative Publications:
Chem. Sci. (2023, 14, 8047); ACS Catal. (2023, 13, 2118); Chem. Sci. (2022, 13, 11666); Chem. Commun. (2022, 58, 3929; Org. Lett. (2018, 20, 4421); Chem. Eur. J. (2017, 23, 11234)

Position held:

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

Awards & Recognitions:

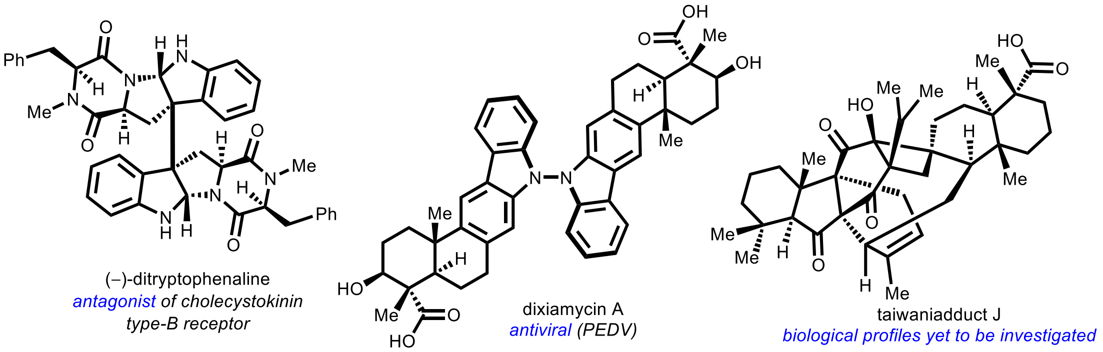
- Fellow, Royal Society of Chemistry (FRSC), (March 2023)
- STARS-MoE 2023 Grant
- Prof. A. Srikrishna Memorial Lecture 2023 (UoH)
- 'CDRI Award' 2022 for Excellence in Drug Research (2022)
- SERB Special Call on 'Reagentless Chemistry' 2022
- Prof. Dhananjay Nasipuri Memorial Award 2021 (ICS)
- Silver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

IL-11

Total Synthesis of Natural Products of Biological Relevance

Alakesh Bisai*
Department of Chemical Sciences, IISER Kolkata, Mohanpur, WB
e-mail: alakesh@iiserkol.ac.in

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.



(−)-ditryptophenaline
antagonist of cholecystokinin type-B receptor

dixiamycin A
antiviral (PEDV)

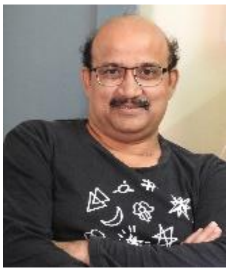
taiwaniadduct J
biological profiles yet to be investigated

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.
5. (a) N. Kumar, A. Maity, V. R. Gavit, A. Bisai, Chem. Commun. 2018, 54, 9083. (b) S. Sharma, S. Shaheeda, K. Shaw, A. Bisai, and A. Paul, ACS Catal. 2023, 13, 2118.

Dr. Parthasarathi Das
Professor and Head of Department
Department of Chemistry and Chemical Biology
Indian Institute of Technology (ISM) Dhanbad
Dhanbad 826004, INDIA
E-mail: partha@iitism.ac.in
Homepage: https://partha66.wixsite.com/medchem



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

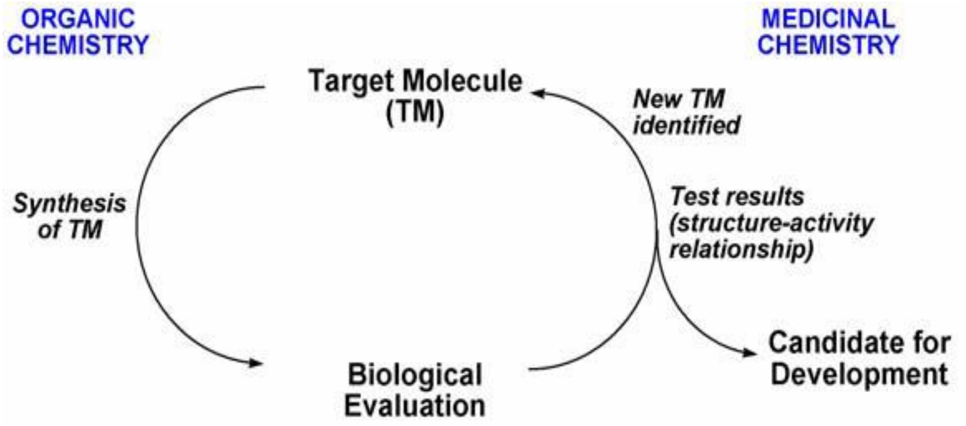
IL-12

Expanding the Medicinal Chemistry Toolbox: From Method Development to Delivery of Drug Like Molecules

Parthasarathi Das
Department of Chemistry and Chemical Biology
Indian Institute of Technology (ISM) Dhanbad
Dhanbad-826004, INDIA
Email: partha@iitism.ac.in

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]



References:

1. (a) K. Mondal, N. Mukhopadhyay, S. Patra, T. Roy and P. Das ACS Catal. 2023, 13, 11977; (b) A. Iqubal, P. Halder and P. Das J. Org. Chem. 2023, https://doi.org/10.1021/acs.joc.3c01959; (c) K. Mondal, S. Patra, P. Halder, N. Mukhopadhyay and P. Das Org. Lett. 2023, 25, 1235; (d) T. Roy, K. Mondal, A. Sengupta and P. Das J. Org. Chem. 2023, 88, 6058; (e) K. Mondal, N. Mukhopadhyay, A. Sengupta, T. Roy and P. Das Chem. Eur. J. 2023, e202203718; (f) P. Halder, A. Iqubal, K. Mondal, N. Mukhopadhyay and P. Das J. Org. Chem. 2023, 88, 15218; (g) P. Halder, V. Talukdar, A. Iqubal and P. Das J. Org. Chem. 2022, 87, 13965; (h) P. Halder, T. Roy and P. Das Chem. Commun. 2021, 57, 5235.

Dr. Prasenjit Ghosh

Room 363B, Chemistry Bldg.
pghosh@chem.iitb.ac.in
+91 22 25767178
Educational Background:
Ph.D., Columbia University, USA

M.Phil., Columbia University, USA
M.Sc., IIT Kanpur
B.Sc., Calcutta University, Kolkata

Professional Experience:
Post-doc, Brookhaven National Laboratory, USA

Post-doc, University of California Santa Barbara, USA

Assistant Professor, IIT Bombay (2003)

Associate Professor, IIT Bombay (2007)

Professor, IIT Bombay (2012)

IL 13

Late Transition Metal Heteroatom Stabilized Singlet Carbene Complexes in Single to Multi-Cycle Catalyses

Prasenjit Ghosh* pghosh@chem.iitb.ac.in, Indian Institute of Technology Bombay,

India One-pot multi-component tandem reaction promises a time-efficient step economic solution to many an intriguing synthetic target. The transition metal plays a crucial role in meeting the challenges by catalyzing these reactions. The talk will highlight our foray into the late transition metal-mediated one-pot multi-component tandem reactions through iterative mechanistic understandings in an effort towards accessing a large number of high-value synthetic targets of biological and industrial interests. Our journey across single-cycle catalyses like the alkyne hydroamination, and hydrohydrazination, to across various multi-component multi-cycle catalyses, namely, three-component amine-aldehyde-acetylene (A3), and azide−isocyanide couplings and the hydrazone-isocyanide-amine (HIA) coupling, will be narrated in keeping with the core theme of our research. Building superior catalysts through enhanced understanding of the catalyst mode of action lies at the heart of our endeavor.

Keywords:
Hydroamination; hydrohydrazination, amine-aldehyde-acetylene (A3) coupling; azide−isocyanide coupling; hydrazone-isocyanide-amine (HIA) coupling

Dr. Uttam Manna

Associate Professor
Department of Chemistry & Centre for Nanotechnology
Indian Institute of Technology-Guwahati
Assam-781039, India
Email: umanna@iitg.ac.in; su.uttam@gmail.com

Education/Professional Experience
Sep, 2019 - Present: Associate Professor, Department of chemistry, IIT- Guwahati
Jun, 2015 - Aug, 2019: Assistant Professor, Department of chemistry, IIT- Guwahati
2013 - 2015: Assistant Scientist (Prof. David M. Lynn)
Chemical & Biological Engineering Dept., University of Wisconsin-Madison, Madison, Wisconsin, USA.
2011- 2012: Post-Doctoral Research (Prof. David M. Lynn)
Chemical & Biological Engineering Dept., University of Wisconsin-Madison, Madison, Wisconsin, USA.
2009 - 2011 : Ph. D. (Prof. Satish A. Patil)
Solid State and Structural Chemistry Unit (SSCU), Indian Institute of Science (IISc), Bangalore, Karnataka
2006 - 2009 : M.S. (Prof. Satish A. Patil)
Solid State and Structural Chemistry Unit (SSCU), Indian Institute of Science (IISc), Bangalore,

Recognition/Awards/Fellowships
21. Pioneering Investigator in Chemical Communication, 2023.
20. CRSI Bronze Medal for the year 2023.
19. Editorial Advisory Board Member of ACS Applied Engineering Materials, ACS (2022 onwards).
18. Emerging Investigator in Chemical Society Reviews, 2022.
17. Elected as a Life Fellow of Indian Chemical Society in Feb, 2021.
16. Emerging Investigator in Nanoscale, 2021.
15. Editorial Advisory Board Member of Materials Horizons, RSC (2021 onwards)
14. Awarded the Humboldt Research Fellowship for Experienced Researchers. (2021-2023)
13. Invited Fellow of the Royal Society of Chemistry (FRSC) in Oct 2020.
12. Emerging Investigator in Chemical Communication, 2020.
11. Recipient of Merck Young Scientist Award (Runner-up), 2019 in Chemical Science
10. INSA-Young Scientist Award, 2019
9. Bilateral Exchange of Academics Award-2019 from DAAD, Germany
8. Emerging Investigator in Journal of Materials Chemistry A, 2018
7. NASI-Young Scientist Platinum Jubilee Award, 2018
6. Associate of the IAS (Indian Academy of Science), 2018
5. DAE-Young Scientist Research Award, 2017
4. DST Young Scientist, 2015.
3. Toulouse Medal: Best thesis award from SSCU, Indian Institute of Science (IISc), 2013.
2. Post Doctoral Fellowship: University of Wisconsin-Madison, USA, 2011.
1. CSIR (Council of Scientific & Industrial Research) Junior Research Fellowship, 2008.

Facile Chemical Approaches for Associating Bio-inspired Wettability

Uttam Manna*
Department of Chemistry,
Centre for Nanotechnology and Jyoti and Bhupat Mehta School of Health Science and
Technology Indian Institute of Technology Guwahati, Guwahati, Assam-781039 Email:
umanna@iitg.ac.in

ABSTRACT: The nature-inspired wettabilities that either extremely repelled or allowed effortless sliding of different liquids (oil/water) in air or underwater are with immense potential for various prospective applications. In common practice, essential chemistry and appropriate topography that conferred the special liquid wettabilities were mostly and generally achieved by associating delicate chemistry. Eventually, the synthesized materials suffered from poor durability issues. In the literature, very few designs are capable of providing durable bio-inspired wettability—but fabrication processes remain generally complex. Moreover, the integration of various other relevant physical properties with such durable liquid wettability is highly challenging to achieve. Hence, design of robust bio-inspired liquid wettability following a simple fabrication process that would allow to integrate different and relevant physical properties is utmost important for various fundamental and applied contexts. Related to this, recently, our research group has extended 1,4 conjugate addition reactions between amine and acrylates at ambient conditions to develop tolerant and functional liquid wettability. 1-10 The controlled tailoring of different bioinspired liquid wettability from the porous and chemically reactive interfaces—following strategic post modulation of the chemically reactive interfaces will be discussed in this invited lecture. A strategic association of adequate crosslinkers can provide a highly tolerant and hard superhydrophobic coating on geometrically complex and soft materials. Such a simple chemical approach also allowed to reveal important fundamental aspects related to different bio-inspired wettability. Taking advantage of the durable bio-inspired wettability, the synthesized nature inspired interfaces were successfully applied to demonstrate some practically relevant applications—including controlled release of small molecules, oil/water separation, water harvesting, sensing, anticounterfeiting etc.

References

1. Jaysri Das, Subhankar Mandal, Angana Borbora, Sonam Rani, Mizuki Tenjimbayashi* and Uttam Manna* Adv. Funct. Mater., 2023, 2311648.
2. Angana Borbora, Yang Xu, Souradeep Dey, Xin Wang, Yuxing Yao, Biman B. Mandal*, Xiaoguang Wang * and Uttam Manna* "Lubricated Interfaces Enabling Simultaneous Pulsatile and Continuous Chemical Release Modes" Advanced Materials, 2023,35, 2302264.
3. Borbora, A.; Dhar, M.; Shome, A.; Barman, N.; Roy, S.; Manna, U.* Adv. Funct. Mater. 2023, 33, 2302569.
4. Barman, N.; Shome, A.; Kumar, S.; Mondal, P.; Jain, K.; Tenjimbayashi, M.; Manna, U.* Adv. Funct. Mater. 2023, 2214840.
5. Shome, A.; Das, A. Borbora, A.; Dhar, M.; Manna, U.* Chemical Society Reviews, 2022, 51, 5452– 5497.
6. Dhar, M.; Das, A.; Parbat, D.; Manna, U.* Angewandte Chemie International Edition, 2022, 61, e20211676.

Dr. Dipankar Koley
Principal Scientist,
Medicinal and Process Chemistry Division,
CSIR-Central Drug Research Institute,
Lucknow, 226031, India

Dr. Dipankar Koley received his B. Sc and M. Sc. in chemistry from Burdwan University. He obtained his Ph.D. in organic chemistry from the Indian Institute of Chemical Technology, Hyderabad, in 2007. After completing his post-doc training from the Purdue University, Indiana, USA, in 2009, Dr. Koley joined CSIR-CDRI, Lucknow as as scientist. Dr. Koley was promoted to the Senior scientist in 2013. Since 2017, he is serving as a principal scientist in the Medicinal and Process Chemistry, CSIR-CDRI.

His research interest includes C-H functionalization, asymmetric catalysis, total synthesis and medicinal chemistry. He has published many peer reviewed organic Chemistry journals such as Angew Chem Int Edn, Organic Letters, Chem Comm. Adv Syn Cat etc. He has guided 9 Ph. D. students and 6 Ph. D. students are on course.

IL-15

S-016-1348: A preclinical SMAC mimetic candidate as apoptosis inducing agent against solid tumor

Dipankar Koley*
Principal Scientist, Medicinal and Process Chemistry Division, CSIR-Central Drug Research Institute, Lucknow, 226031, India

A small molecule smac mimetic as an apoptosis inducing agent has been developed against solid tumors. A de novo design, library synthesis, structural activity relationship along with pharmacokinetic studies furnished the lead compound S-016-1348. Various in-vivo studies, and other PK/PD studies suggested that the developed compound is superior than the currently available clinical candidates. Further the result of the efficacy and the pre-clinical toxicological studies are found to be very encouraging to take it to the next level of the drug-discovery pipeline. In this presentation, we shall discuss the hypothesis, design, bioactivity and toxicity studies of the aforementioned preclinical candidate.

Dr. Surya Prakash Singh

Polymers and Functional Materials Department,

CSIR-Indian Institute of Chemical Technology

Uppal road, Tarnaka, Hyderabad, 500007

E-mail: spsingh@iict.res.in

Dr. Surya Prakash Singh is a Principal Scientist at Polymer and Functional Material Deportment, CSIR-Indian Institute of Chemical Technology, Hyderabad. He studied chemistry at the University of Allahabad, India, and obtained his Ph.D. degree in 2005. Later, he joined CSIR-Indian Institute of Chemical Technology, Hyderabad as Research associate. After working at Nagoya Institute of Technology, Japan, as a postdoctoral fellow (2006-2008), he joined Osaka University, in 2008 as an Assistant Professor. He worked as a researcher at Photovoltaic Material Unit, National Institute for Materials Science (NIMS), Tsukuba, Japan (2012-2011). Recently, he worked as BASE fellow at University of California, Santa Barbara with Prof. Bazan's research group. He has been involved in design and synthesis of functional H-conjugated molecules for photonic applications and published over 180 papers, reviews in peer-reviewed journals and patents, edited two books and author of one book chapter.

Synthesis of Diketopyrrolopyrrole Based Photoactive Materials via Photoredox C-H Activation

Vinay Kumar,[a] B. Yadagiri,[a] and **Surya Prakash Singh***[a,]

[a]Polymers and Functional Materials Department, CSIR-Indian Institute of Chemical Technology
Uppal road, Tarnaka, Hyderabad, 500007
E-mail: spsingh@iict.res.in

Abstract: Diketopyrrolopyrrole (DPP) derivatives have been widely explored in a variety of applications. Mostly, the synthesis of DPP derivatives followed the well-known conventional cross coupling methods such as Suzuki, Stille, Sonogashira, and Negishi cross-coupling reactions. However, these methods required unfavorable reaction conditions, organometallic precursors, and high temperature. Therefore, synthesis of DPP based derivatives by using simple and efficient methods are most necessary. The thiophene-diketopyrrolopyrrole (TDPP) is considered as an ideal unit for direct C-H alkyl/arylation with a variety of coupling partners in organic chemistry due to more electron rich behavior beneficial for formation of stable intermediates and highly selective reaction at the 2/5 positions. In this work, we have synthesized a series of TDPP based π-conjugated molecules consisting of diverse alkyl/aryl substituents *via* Pd-catalyzed photoredox methodology with moderate to good yields. A wide variety of TDPP based semiconducting materials were synthesized with this novel methodology by using different kinds of N-hydroxyphthalimide (NHP) coupling partners and studied its optical and electrochemical properties. To the best of our knowledge, this is the first report on synthesis of TDPP based π-conjugated materials via photoredox method. The synthetic pathways were subsequently improved by novel synthetic methods and studied its application towards technological and scientific importance. Foremost, DPP pigments have been widely used in inks, paints, and plastic industry. Recently, DPP based conjugated small molecules and polymer materials have been broadly explored in the application of optoelectronics due to its broad and tunable optical absorption from visible to NIR-region, high hole, and electron mobilities and their exceptional stability

Dr. Amrendra K. Singh
Associate Professor
Department of Chemistry
Indian Institute of Technology Indore
Contact Number: +91 731 660 3185
e-Mail: aks@iiti.ac.in
Homepage: https://people.iiti.ac.in/~aks/

Career Profile and representative publications

Amrendra K. Singh grew up in Gorakhpur, Uttar Pradesh and completed his bachelor's and master's degrees from DDU Gorakhpur University. He was a recipient of Shyama Prasad Mukherjee Fellowship from CSIR for his doctoral studies and obtained Ph.D. (2009) from IIT Bombay under the supervision of Prof. Pradeep Mathur. He spent two years (2010-2012) at Lund University, Sweden as a postdoctoral fellow in Prof. Ebbe Nordlander's lab. Then he moved to Michigan State University, USA, for another postdoctoral position in Prof. Aaron Odom's lab. He joined IIT Indore as Assistant Professor in 2016 and was promoted to Associate Professor in 2022. The research activities in AKS group fall under the broad domain of inorganic/organometallic chemistry and catalysis. Designing new pincer and N-heterocyclic carbene ligands and their transition metal complexes capable of small molecule activations and investigation of fundamental aspects of their reactivities and mechanisms are carried out for the potential application in the development of renewable energy and sustainable chemical processes.

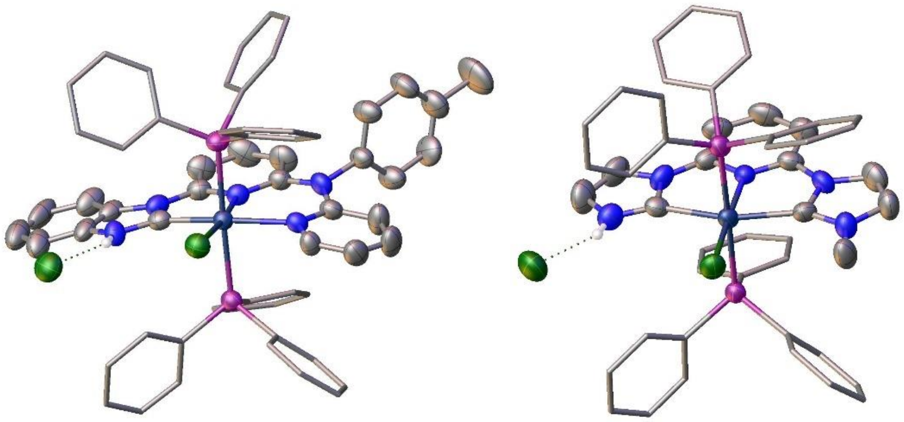
- Nath, S.; Yadav, E.; Raghuvanshi, A.; Singh, A. K. Mechanistic Insights and Comparative Analysis of Ru(II)-NNC Pincer Complexes with Anionic-, Protic-, and Classical-NHCs for Transfer Hydrogenation of Ketones. Catal. Sci. Technol., 2023, DOI: 10.1039/D3CY01383A.
- Singh, R. K.; Yadav, D.; Singh, A. K. Cationic Ruthenium(II)-CNC Pincer Complexes as Phosphine-free Catalysts for Nitrile Hydration to Amides in Aqueous Medium. Molecular Catalysis, 2023 549, 113523.
- Nath, S.; Yadav, E.; Raghuvanshi, A.; Singh, A. K. Ru(II) Complexes with Protic- and Anionic-Naked-NHC Ligands for Cooperative Activation of Small Molecules. Chem. Eur. J., 2023, e202301971.
- Shahid, N.; Singh, R. K.; Srivastava, N.; Singh, A. K. Base-Free Synthesis of Benchtop Stable Ru(III)-NHC Complexes from $RuCl_3 \cdot 3H_2O$ and Their Use as Precursors for Ru(II)-NHC Complexes. Dalton Trans., 2023, 52, 4176.

IL-17

Protic-NHC Complexes for Cooperative Small Molecule Activations and Catalytic Applications

Amrendra K. Singh
Department of Chemistry
Indian Institute of Technology Indore
(Email: aks@iiti.ac.in)

N-heterocyclic carbenes (NHCs) serve as excellent spectator ligands that influence the properties of metal complexes or catalysis through a combination of electronic and steric effects. However, the NR,NR-NHC ligands (classical NHCs) do not directly interact with substrates. In contrast to classical NHCs, the NH group of protic-NHCs (NH,NR- or NH,NH-NHC) may allow H-bonding interactions, β-deprotonations, and nucleophilic additions, demonstrating the protic-NHCs' potential to behave as "mutually supportive" or "non-innocent" ligands. We have designed two different types of Ru-pincer complexes (Figure 1) based on a new $NNC^{R/H}$ ligand and a $C^{R}NC^{H}$ ligand which allows the preparation and comparison of structure, properties and reactivities of Ru(II)-pincer complexes with protic or classical NHCs. A set of ruthenium(II)-protic-N-heterocyclic carbene complexes and their deprotonated analogues are prepared in our group and shown to activate H−H bond of hydrogen, $C(sp^3)$-I bond of iodomethane, and C(sp)-H bond of phenylacetylene.[1,2] The activation of small molecules and catalytic applications of these complexes will be discussed.



1 2

Figure 1: Molecular structures of protic-NHC complexes. Hydrogen atoms, except N-H groups, are omitted, and phenyl rings of the PPh_3 ligands are drawn as tubes for clarity.

References:

1. Nath, S.; Yadav, E.; Raghuvanshi, A.; Singh, A. K. Catal. Sci. Technol., 2023, DOI: 10.1039/D3CY01383A.
2. Nath, S.; Yadav, E.; Raghuvanshi, A.; Singh, A. K. Chem. Eur. J., 2023, e202301971.

FACULTY PRESENTATIONS
FP 1-4

Prof. M. S. Singh (FNA, FASc, FNASc)
JC Bose Fellow & CNR Rao Chair Professor

Department of Chemistry, Institute of Science
Banaras Hindu University, Varanasi- 211005
Email: *mssingh@bhu.ac.in*

Maya Shankar Singh received his M. Sc. degree in Organic Chemistry from Banaras Hindu University, Varanasi, India in 1981, where he also earned his Ph. D. degree in 1986 working under the tutelage of (Late) Professor K. N. Mehrotra. After postdoctoral work, he joined Vikram University Ujjain in 1990 as Assistant Professor in Organic Chemistry, and moved to Gorakhpur University as Associate Professor in 1998, then to Banaras Hindu University in 2004, where he is currently Senior Professor in Organic Chemistry since 2018. During his sabbatical, he has visited University of Arizona, Tucson and Michigan State University, East Lansing, Michigan, USA; Nagoya Institute of Technology, Nagoya, Japan; Loughborough University and University of Leicester, UK; RMIT University, Melbourne, Australia; University of Hohenheim, Stuttgart and RWTH Aachen University, Aachen, Germany. He has successfully guided 27 Ph. D. students, which have resulted over 195 publications and 8 reviews in peer reviewed journals. Additionally, Prof. Singh has authored five textbooks in organic chemistry from Pearson-Education and Wiley-VCH, Weinheim, Germany.

Research Interests:
His research interests are centered on Synthetic Organic Chemistry with special emphasis towards the development of efficient, eco-compatible one-pot synthetic methods engaging β-ketodithioesters/thioamides and their derivatives as an antecedent in chemical synthesis. Center of attention of his research group is design and development of sustainable diversity oriented synthetic (SDOS) methods for foremost biologically molecules/drug intermediates via domino/tandem/cascade reactions.

Awards and Honours:

He received some awards and recognitions, which include: T. R. Seshadri Memorial Lecture Award, JC Bose National Fellowship, CNR Rao Chair Professor, Fellow of all the three Indian Science Academies (i.e. FNA, FASc, FNASc), CRSI Bronze and Silver Medals, UGC-BSR Mid Carrier Award & One-Time-Grant, Vice-Chancellor's (BHU) award for Excellence in Research, and most productive researcher award, Institute of Science, BHU.

FP-1

Adventures in Dithioesters & Thioamides Chemistry
Chemical Psychology of Heterocycles

Maya Shankar Singh

Department of Chemistry, Institute of Science
Banaras Hindu University, Varanasi- 211005
E-mail: *mssingh@bhu.ac.in*

Abstract:

The reactivity of β-keto-/α-enolic dithioester (a sulfur analogue of β-ketoester) and thioamides has been exploited for the construction of numerous useful bioactive scaffolds with substituent and skeletal diversity. The polyfunctional simple dithioester/thioamide molecule bearing several nucleophilic/electrophilic reactive sites furnished the desired molecules in a highly selective manner upon treatment with different catalysts/reagents under varying conditions. The salient features of these domino strategies are methodical simplicity, structural diversity, short reaction times, sustainability, and formation of multiple C–C and C–heteroatom bonds in a single operation, making these novel protocols highly useful in diversity oriented synthesis (DOS).[1-4] The details of the recent accomplishments towards this endeavour will be presented during the talk.

References and Notes:

1. (a) Anup Kumar Yadav, Vipin Kumar, Pragya Pali, Subhasish Ray, Abhineet Verma and Maya Shankar Singh, *Adv. Synth. Catal.* **2023**, *365*, 2943-2948. (b) Pragya Pali, and Maya Shankar Singh, *Org. Lett.* **2023**, *25*, 2258-2263. (c) Shahnawaz Khan, Monish Arbaz Ansari, and Maya Shankar Singh, *Org. Lett.* **2023**, *25*, 642-646.

2. (a) Gaurav Shukla, Keshav Raghuvanshi, and Maya Shankar Singh, *J. Org. Chem.* **2022**, *87*, 13935-13944. (b) Subhasish Ray, Saurabh Singh, Ganesh Kumar, Gaurav Shukla, and Maya Shankar Singh, *Adv. Synth. Catal.* **2022**, *364*, 3204-3210. (c) Pragya Pali, Dhananjay Yadav, Subash C. Sahoo, and Maya Shankar Singh, *J. Org. Chem.* **2022**, *87*, 12342-12351. (d) Sonam Soni, Gaurav Shukla, and Maya Shankar Singh, *Org. Biomol. Chem.* **2022**, *20*, 6784-6798. (e) Monish Arbaz Ansari, Shahnawaz Khan, Subhasish Ray, Gaurav Shukla and Maya Shankar Singh, *Org. Lett.* **2022**, *24*, 6078-6082. (f) Gaurav Shukla, Dhananjay Yadav, Saurabh Singh, and Maya Shankar Singh, *Adv. Synth. Catal.* **2022**, *364*, 1982-1988. (g) Monish Arbaz Ansari, Ganesh Kumar, and Maya Shankar Singh, *Org. Lett.* **2022**, *24*, 2815-2820.

3. (a) aurav Shukla, Priya Saha, Pragya Pali, Keshav Raghuvanshi, and Maya Shankar Singh, *J. Org. Chem.* **2021**, *86*, 18004-18016. (b) Pragya Pali, Gaurav Shukla, Priya Saha, and Maya Shankar Singh, *Org. Lett.* **2021**, *23*, 3809-3813. (c) Dhananjay Yadav, Abhijeet Srivastava, Monish Arbaz Ansari, and Maya Shankar Singh, *J. Org. Chem.* **2021**, *86*, 5908-5921.

4. (a) Monish Arbaz Ansari, Dhananjay Yadav, and Maya Shankar Singh, *J. Org. Chem.* **2020**, *85*, 8320-8329. (b) Sonam Soni, Pragya Pali, Monish Arbaz Ansari, and Maya Shankar Singh, *J. Org. Chem.* **2020**, *85*, 10098-10109. (c) Monish Arbaz Ansari, Dhananjay Yadav, and Maya Shankar Singh, *Chem. Eur. J.* **2020**, *26*, 8083-8089

Dr. Kamlesh Kumar
Assistant Professor
Address: Department of Chemistry, Institute of science
Phone: 9453481027
Email: kamlesh.kumar@bhu.ac.in
ORCID Id: https://orcid.org/0000-0001-7374-5941
Personal Website: https://sites.google.com/view/kamlesh-research-group/home

Educational Qualification

- **Ph.D. (2007–2012):** Department of Chemistry, IIT Kanpur, India (*Thesis Advisor*: Prof. B. D. Gupta and Prof. G. Anantharaman)
- **M. Sc. (2006)**: D. D. U. Gorakhpur University, Gorakhpur, India, 1st Division (70%)
- **B. Sc. (2004)**: D. D. U. Gorakhpur University, Gorakhpur, India, 1st Division (74%)

Postdoctoral Research

- Postdoctoral Research Fellow, University of Johannesburg (2013-2017)
- European Union Erasmus Mundus Postdoctoral Fellow, Lund University Sweden (2012-2013)
- Postdoctoral Research Fellow, Schulich Faculty of Chemistry, Technion-IIT, Israel (2012)

Teaching Experience

- Assistant Professor, Department of Chemistry, Institute of science, B.H.U. Varanasi (2018-present)
- Assistant Professor, Department of Chemistry, J. P. University, Chapra, Bihar (2017).

Research Interest

- Inorganic and Organometallic Chemistry
- Catalysis
- Therapeutic applications of Organometallic compounds

Research Projects as PI and Co-PI

- BHU-IoE Startup Grant (12 Lakhs)
- UGC BSR Startup Grant (10 lakhs)
- DST-SERB (47 Lakhs) Co-PI

PhD//MSc student Supervision

PhD Scholars: 04 (on going)
M.Sc. Project Students: 13
Research Publications: 23
Book Chapters: 05
Book edited: 01 (Publisher SPRINGER, Year 2021)
Invited Talks: 05

FP-2

Coordination Chemistry and Catalytic Applications of Metal Complexes containing Thiolato Ligands

Dr. Kamlesh Kumar

Department of Chemistry, Institute of Science, Banaras Hindu University, Varanasi-221005

Mobile: 9453481027 ; E-mail: kamlesh.kumar@bhu.ac.in

Keywords: Thiolato Lignds; Metal Complexes; Coordination Chemistry; Catalysis

Sulphur containing ligands have already proved to be extremely versatile ligands for metal directed self-assembly and supramolecular structures. Starting from the primarily synthetic exploratory stage the field has now grown up to a more advanced stage covering molecular architectures and varied functional properties. Metal complexes of thiolato ligands continue to attract the attention of chemists because of their multifaceted chemistry, chemical reactivity, catalysis, magnetic, conducting and optical properties as well as sensitizing activities.

The Knoevenagel reaction, a well-known synthetic methodology for C–C bond formation by condensation of aldehydes and active methylene compounds have been extensively applied for the synthesis of important chemicals and pharmaceutical products. Also, the products of Knoevenagel condensation are key intermediates in many one-pot multicomponent organic transformation reactions including the synthesis of 2-amino-4*H*-chromene and imidazopyrimidine derivatives. We have developed several transition metal complexes of functionalized thiolato ligands that afford systematically designed ordered architectures. Further, these complexes have been utilised as catalysts in the C-C bond formation through Knoevenagel and one-pot multicomponent reactions and also water splitting reactions.

***Reference**:*

1. S. K. Pal; B. Singh; J. K. Yadav; C. L. Yadav; M. G. B. Drew; N. Singh; A. Indra; K. Kumar, **Dalton Trans**., 2022, 51, 13003.
2. Anamika, C. L. Yadav; M. G. B. Drew; K. Kumar; N. Singh, **Inorganic Chemistry,** 2021, 60, 6446
3. C. L. Yadav; Anamika; G. Rajput; **K. Kumar;** M. G. B. Drew; N. Singh, **Inorganic Chemistry,** 2020, 59, 11417
4. Anamika; D. K. Yadav; K. K. Manar; C. L. Yadav**; K. Kumar;** V. Ganesan; M. G. B. Drew; N. Singh, **Dalton Trans.**, 2020, 49, 3592

Dr. Debanjan Guin
Assistant Professor,
Department of Chemistry, Institute of Science,
Banaras Hindu University, Varanasi 221005 INDIA
Tel: (91) 9982289330, (91) 990304475
E.Mails: debanjan.guin@gmail.com, debanjan.chem@bhu.ac.in
Website: http://debanjanguin.wixsite.com/debanjanguin

Research Interests

- Target-oriented synthesis of functional nanoparticles.
- Naked eye/ photoluminescence detection of biomolecules (glucose, cholesterol), and water pollutants (toxic ions).
- Development of electrochemical sensor for glucose, bilirubin.
- Asymmetric catalysis using nanoparticles as catalyst.
- Development of nanoparticles for detection of cancer cells, separation and purification of proteins.
- Development of materials for super-capacitor, solar cell and LED applications.
- Synthesis of functional superparamagnetic nanomaterials for water purification.

Research and work experience

- Nov 2017-till date: Assistant Professor, Department of Chemistry, Institute of Science, Banaras Hindu University (BHU) Varanasi, India
- Jan 2014- Nov 2017: UGC-Assistant Professor under UGC-FRP Department of Chemistry, University of Rajasthan, India
- Aug 2012-Jan 2014: DST Fast Track Fellow, Biochemistry Division, National Chemical Laboratory (NCL), Pune, India
- Sept 2010-Aug 2011: Postdoctoral Research Associate, Department of Chemistry, Cologne University, Germany
- Jan 2010-Sept 2010: Postdoctoral Research Associate, Department of Organic and Macromolecular Chemistry, Heinrich-Heine University, Dusseldorf, Germany
- June 2008-Oct 2009: Postdoctoral Research Associate. Department of Chemistry, University of Arizona, Tucson, Arizona, USA
- April2003-April 2008: PhD in Chemistry Indian Institute of Chemical Technology (IICT), Hyderabad, India Education
- 2000-2002: M.Sc. in Chemistry (Physical Chemistry Special) Kalyani University, West Bengal, India
- 1998-2000: B.Sc. in Chemistry Hons. Burdwan University, West Bengal, India

FP-3

Investigating the Potential Applications of Surface-functionalized Metal Nanoparticles

Debanjan Guin
Quest Research Laboratory
Department of Chemistry
Institute of Science, Banaras Hindu University (BHU)

Target-oriented synthesis of noble metal nanoparticles is a vibrant area of ongoing research. For that purpose, it is necessary to tune the surface properties of nanoparticles by introducing diverse surface-modifying agents. This presentation centres on the synthesis of surface-functionalized noble metals, predominantly silver nanoparticles (Ag NPs), and customize their surfaces to suit specific applications. We stabilized and modified the surface property of Ag nanoparticles on different substrates and used them as 'dip catalysts' for important organic transformation reactions and removal of water pollutants. Surface functional Ag nanoparticles are used as optical, electrochemical, photoluminescence, and SERS-based sensors for the detection of different biomolecules and water pollutants. Composite incorporating Ag nanoparticles serves as a draw solution to develop a forward osmosis-based water purification system. This discussion encompasses the catalyst/sensor development, highlighting their limitations and detailing subsequent modifications to enhance their applicability, durability, and user-friendliness, with a focus on practical application perspectives.

Dr. Sailaja S. Sunkari
Associate Professor,
Mahila Mahavidyalaya,
Banaras Hindu University

Dr. Sailaja S. Sunkari obtained her Ph.D. from the University of Hyderabad in 2003. She was a JSPS postdoctoral fellow (2003-2005) and JSPS Bridge fellow (2016) at the Department of Chemistry, University of Tokyo, Japan. Before joining Mahila Maha Vidyalaya in 2008, she was a DST Women Scientist at the Department of Chemistry, Banaras Hindu University. Since 2008, she's teaching Inorganic Chemistry to undergraduates at Mahila Maha Vidyalaya and pursuing research in the field of hybrid functional materials, with a focus on understanding the structural dependence of functional properties especially, molecule based magnetism and luminescence of supramolecular assemblies. She has supervised four doctoral theses and has about 30 research publications for her credit.

FP-4

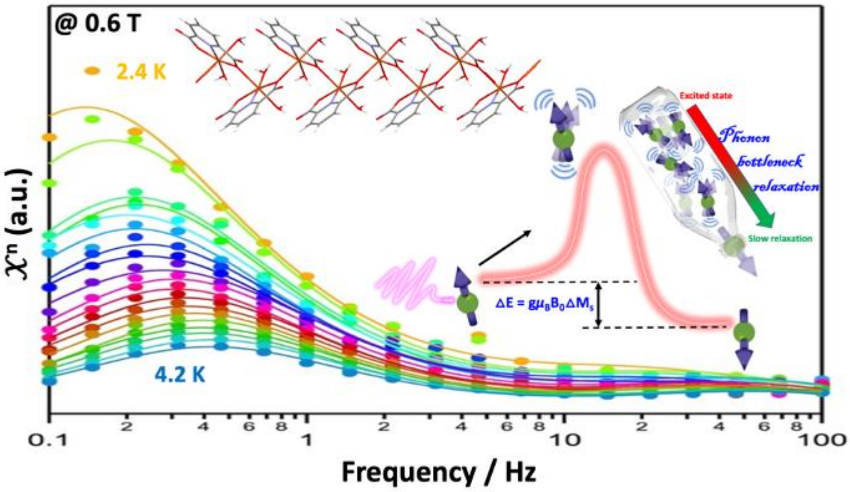
Slow Magnetic Relaxation in a Ferromagnetically Coupled Cu(II) Polymer Chain with Pyridine-2,6-dicarboxylic acid

Sailaja S. Sunkari*

Department of Chemistry, Mahila Mahavidyalaya, Banaras Hindu University, Varanasi, India.

sailaja.sunkari1@bhu.ac.in; sunkari.s7@gmail.com

Slow magnetic relaxation is an exciting phenomenon, that's crucial for realising the potential of molecules to behave as ***molecule based magnets***, for their anticipated applications in quantum computation, spintronics, high density information storage etc. Such investigations provided a comprehensive understanding of the key features that lead to slow magnetic relaxation, thereby helping realise several single molecule/ single chain/ and single ion magnets. In all such studies, synthetic strategies though not highlighted, but play a key role as in obtaining solids exhibiting desired properties amid several structure directing forces, and a basic challenge to overcome. Such challenges become manifold, especially when the ligands are flexible in their coordination capabilities, providing excellent opportunities for a synthetic coordination chemist to customize their skills. A systematic fine tuning of synthetic conditions promises isolation of diverse solids with vast structural changes that may have potential for molecular magnetism studies. Exploring such opportunities in a Jahn-Teller active Cu(II) with highly flexible pyridine-2,6-dicarboxylic acid, we present our findings of four structurally close Cu(II) complexes, of which ferromagnetically coupled chain $[Cu(dipic)(OH_2)_2]_n$, exhibits slow magnetic relaxation induced by the phonon bottleneck effect under a magnetic field of 0.6 T, with a relaxation time of 2.2 s at 2.8 K, a first of its kind.



1. O. Kahn, Molecular Magnetism, Wiley-VCH, New York, 1993.
2. D. Gatteschi, R. Sessoli and J. Villain, Molecular Nanomagnets, Oxford University Press, Oxford, U.K., 2006.
3. R. Winpenny, Single-molecule magnets and related phenomena, Struct. Bonding, 2006, 122, 1.
4. M. Yamashita, Next generation of multifunctional nano-science on advanced metal complexes with quantum effects and nonlinearity, Bull. Chem. Soc. Jpn., 2021, 94, 209.

POSTER PRESENTATIONS

PP-1

Exploring the Synergistic Power of Layered Au and Pt Bi-metallic Nanoparticles for Efficient Methanol Oxidation

*Raman Kumar and Shanmugam Manivannan**
Nanomaterial and Electrochemistry Laboratory (NEL), Department of Chemistry, Institute of Science,
Banaras Hindu University, 221005, Varanasi, INDIA.

The quest for highly effective and durable catalysts for methanol oxidation remains a contemporary research endeavor in the domain of fuel cells and direct methanol fuel cells (DMFC). The present investigation delves into the synergistic potential inherent in switching the layered gold (Au) and platinum (Pt) nanostructures of the bimetallic system for the boosting of methanol oxidation efficiency. Hence a simple strategy of switching the nanostructured layers between Au and Pt and electrodepositing both Au and Pt precursors together was adopted for fabricating the AuPt electrocatalyst through the electrodeposition method. Three unique AuPt electrocatalysts were characterized by morphological, physiological, and electrochemical characterization tools. Interestingly the AuPt catalyst has exhibited remarkable performance and long-term durability in facilitating the methanol oxidation reaction as methanol is known to adsorb directly on the Pt surface and Au has a great potential in assisting the transformation of CO-likes into CO_2, thus positioning it as a promising candidate for DMFC. Besides, the silicate sol-gel matrix as a solid support facilitates the embedment of the first layer of Au nanostructures, through such safe guard Au can renew the outer exposed Pt surface for the long term, all together synergistic catalyst efficiency is noted.

PP-2

Multifunctional Core@Shell Structured Gold Nanodendrites@Gold Nanoclusters: An Efficient Catalytic and Sensor Domain for Environmental Remediation Applications

*Ritesh Tolani and Shanmugam Manivannan**
Nanomaterial and Electrochemistry Laboratory (NEL), Department of Chemistry, Institute of Science,
Banaras Hindu University, 221005, Varanasi, INDIA.

The rapid progression of industrialization and globalization, occurring at the expense of over-exploitation of natural resources, is leading to a multifold increment in pollutant levels. Industrial effluents containing various pollutants such as heavy metals (Mercury, Lead, Arsenic, Chromium, etc.), organic dyes (Methylene Blue, Rhodamine B, etc.), POPs (Nitrophenols, pesticides, PCBs, etc.) are constantly drained into the environment. The discovery of a multifunctional catalyst provides the propitious solution for the eradication of toxic environmental pollutants. The intriguing properties of nanomaterials facilitate their employment for environmental applications. As a result of this, this work reports a facile one-step inverted synthesis of multifunctional core@shell–structured Au nanodendrites@Au nanocluster (Au ND@Au NC) using methionine. The synthesis procedure yields monodisperse nanoclusters with varied sizes depending on the concentration of Au. The synthesis procedure eliminates the employment of any harmful surfactants, polymers, or seed-based strategy. The synthesized Au ND@Au NC performs the dual functioning of being catalytically active material performing degradation of nitroaromatic compounds and organic dyes as well as an excellent colorimetric sensor for Cd^{2+} ions with LOD of 2.5μM. The dual functionality of the synthesized nanocluster is attributed to the methionine functionalization.

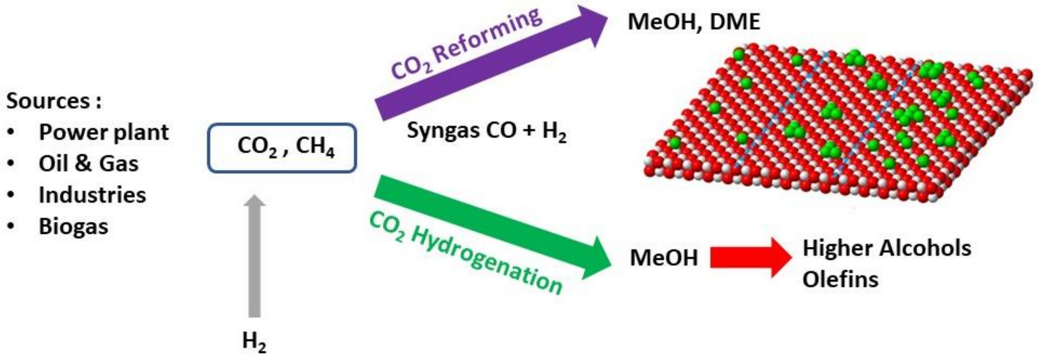
PP-3

Single Atom Heterogeneous Catalysts for Carbon Dioxide Hydrogenation Reaction

Satyam Verma[1]& Kanak Roy[1]*

[1]Department of Chemistry, Banaras Hindu University, Varanasi, Uttar Pradesh - 221005, INDIA

** corresponding email: kanak.roy@bhu.ac.in*



One promising direction in the search for long-term solutions to the world's problems caused by climate change and depleting fossil fuel resources is the creation of effective catalysts for carbon dioxide (CO_2) capture and utilization. Single atom catalysts (SACs) are one such advancement in the field of heterogeneous catalysis research. These catalysts consist of individual atoms spatially isolated and anchored onto nanostructured support materials. Metal oxides, metals (single atom alloys), metal hydroxides, zeolites, and metal organic frameworks (MOFs) are common supports for SACs. In this report, copper and indium based bimetallic catalysts (Cu-In/SiO_2 and Cu-In/TiO_2) of low metal dispersion, featuring copper (Cu) and indium (In) particles supported on a silica (SiO_2) substrate have been studied for CO_2 hydrogenation. Using conventional incipient wetness impregnation method, high metal dispersion and low nuclearity were achieved. The catalytic activity has been tested in a fixed-bed high pressure reactor and the products were analyzed with an online gas chromatograph equipped with a thermal conductivity detector (TCD).

PP4

Infiltration of Gold Ions in Partially Porous Prussian blue-Fe_2O_3 mixed Microstructure to Obtain 3-D Nano-catalytic Networks via Electroless Deposition for Environmental Remediation Applications

*Sachin Kumar and Shanmugam Manivannan**
Nanomaterial and Electrochemistry Laboratory (NEL), Department of Chemistry, Institute of Science,
Banaras Hindu University, 221005, Varanasi, INDIA.

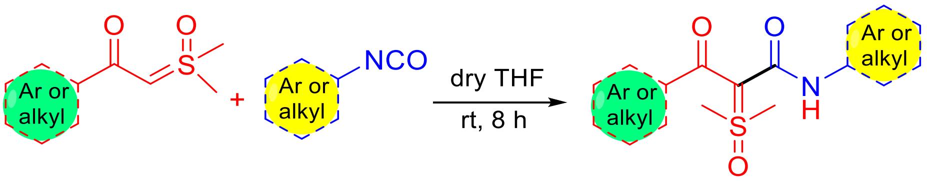
Metal and metal oxide nanocomposites are promising candidates for heterogeneous catalytic applications. However, most of the metal oxide volume remains as a dead volume of not participating in the catalysis. Only the metal/metal oxide hetero-junctions available at catalyst surfaces are involved in the catalysis. Besides, narrow interlayer spacing, inferior intrinsic electronic conductivity, and poor structural stability of the metal oxides still limit its practical applications. Herein, we report a two-step strategy to infiltrate the gold nanoparticles into the 3D-porous Prussian blue/Fe_2O_3 microstructures (PPFM-Au) boosted as a heterogeneous catalyst for environmental remediation applications. The porosity of the Prussian blue microstructures is thermally tuned to infiltrate the gold ion precursor to facilitate the galvanic displacement reaction between Fe and Au. Of note, Au ions could replace the Fe ions via electro-less deposition to enlarge the lattice spell and form Au nanoparticles 3D-networks compared with the only surface attached Au/Fe_2O_3 composite (PPFM-Au), the structural stability and electron transfer kinetics of the PPFM-Au are enhanced. As expected, the obtained PPFM-Au catalyst exhibits remarkable catalytic efficiency for Rhodamine-B dye degradation and p-nitrophenol reduction remediations.

PP-5

Synthesis of α-Carbonyl-α'-amide Sulfoxonium Ylides from Isocyanates with Complete Atom Economy

*Ajay Kant Gola, Ajay Sharma, and Satyendra Kumar Pandey**
Department of Chemistry, Banaras Hindu University, Varanasi 221005, India
Corresponding author Email: skpandey.chem@bhu.ac.in
Presenting author Email: ajaykant9927@gmail.com

A catalyst- and additive-free method was developed for the efficient synthesis of α-carbonyl-α-amide sulfoxonium ylides from isocyanates and β-ketosulfoxonium ylides, ensuring complete atom economy. The reaction demonstrated broad functional group tolerance, yielding α-carbonyl-α-amide sulfoxonium ylide derivatives in moderate to high yields. Scalability was confirmed through large-scale reactions, and the synthesized ylides were successfully transformed into valuable compounds, highlighting the practicality and versatility of this synthetic approach.[1] The specifics of the findings will be shared at the poster presentation session.



- Mild conditions
- C-C bond formation
- Metal- and additive-free
- Broad substrate scope
- 32 examples up to 95% yield

References:

1. Gola, A. K.; Sharma, A.; Pandey, S. K. Org. Lett. 2023, *25*, 1214–1217.

PP-6

Multifunctional Pyrazine Based Donor-Acceptor Molecules with Donor Directed Light Harvesting Application

Ankit Kumar Srivastava, Surendra Kumar, Roop Shikha Singh and Daya Shankar Pandey**
Department of Chemistry, Institute of Science
Banaras Hindu University, Varanasi-221005
Email id: roopshikha22singh@gmail.com

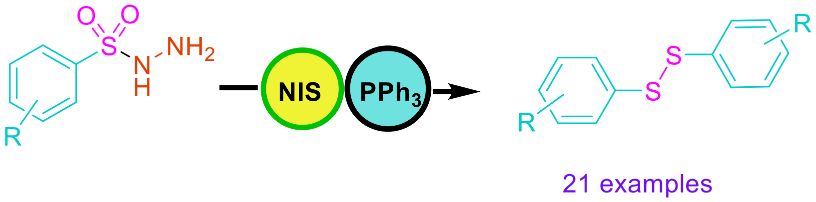
Organic materials exhibiting solid-state emission that reacts to external stimuli hold considerable importance across a spectrum of applications in materials, biomedical sciences, and optoelectronics. Incorporating organic molecules with diverse donor-acceptor structures, coupled with aggregation-induced emission (AIE) fluorophores, has played a pivotal role in crafting mechanofluorochromic (MFC) materials. Our study focuses on the design and synthesis of derivatives rooted in triphenylamine for above mentioned purposes. In this work we designed compounds **A1**, **A2** and **A3** by varying donor moieties. The compounds **A1**, **A2** and **A3** manifest AIE, solvatochromic, TICT, RIR and mechanochromic behaviour. In this work a comprehensive comparison of the photophysical properties (Solvatochromism, AIE, RIR, TICT) and mechanofluorochromic properties of the derivatives has been studied by varying donor moiety. In which **A1** has shown considerably better photophysical and mechanochromic properties. On the basis of above properties compounds **A1**, **A2** and **A3** can be used as a potential real time fluorescent material in development of latent fingerprint.

PP-7

Synthesis of Symmetrical Disulfides *via* NIS-PPh_3-Mediated Reductive Self-coupling of Sulfonyl Hydrazide

*Ashvani Yadav, Amrit Gond, Rohit Kumar and Virendra Prasad**
Department of Chemistry, Institute of Science,
Banaras Hindu University, Varanasi, UP, 221005, INDIA
****E-mail:*** *vprasadbhu@gmail.com*

The present study discloses an NIS/PPh_3-mediated reductive self-coupling of arylsulfonyl hydrazides to prepare symmetric diaryl disulfides. This methodology has a broad functional-group tolerance and a high scalability. This strategy permits the introduction of sulfonyl hydrazides into the synthesis of symmetrical organic disulfides without the use of a catalyst or base, and symmetrical aromatic disulfides can be prepared in moderate to excellent isolated yields from inexpensive and readily available starting materials.



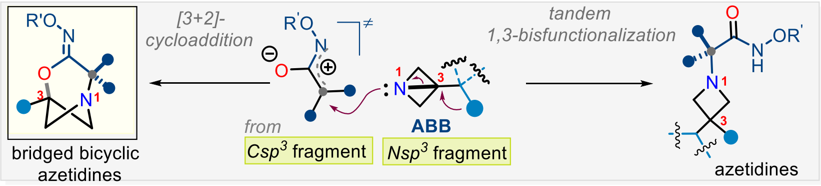
- Metal-free/base-free
- Broad substrate scope
- Yields up to 95 %
- Simple to handle
- Inexpensive chemicals
- R = H, EDG, EWG

PP-8

TITLE

Bandana Singh, *Vinod. P. Singh and Jaideep Saha*
Email:sbandana766@gmail.com, jdsaha2000@gmail.com
Division of Molecular Synthesis & Drug Discovery, Centre of Biomedical Research (CBMR),
SGPGIMS Campus. Raebareli Road, Lucknow 226014, Uttar Pradesh, India.

It is very desirable to have access to 1,3-functionalized azetidines using a diversity-oriented approach in order to find novel uses for them in drug discovery. The functionalization of azabicyclo[1.1.0]-butane (ABB) using strain-release has attracted a lot of interest in order to achieve this goal. C3-substituted ABBs are demonstrated to produce tandem N/C3-functionalization/rearrangement through suitable N-activation, providing azetidines; nevertheless, the specific mechanisms of this N-activation in relation to N-functionalization are still restricted to a particular group of electrophiles. The current work presents a flexible cation-driven ABB activation method. Utilizing Csp3-precursors that may produce reactive (aza)oxyallyl cations in situ is the key to this method. In this case, effective C3 activation is mandated by N-activation, which results in the formation of a crowded C-N bond. The concept can be further extended to formal [3+2]-annulation involving azaoxyallyl cation and ABB, leading to bridged bicyclic-azetidines.



References:

a) A. Fawcett, A. Murtaza, C. H. U. Gregson, V. K. Aggarwal, *J. Am.Chem. Soc.* **2019**, *141*, 4573;-
b) c) J. L. Tyler, A. Noble, V. K. Aggarwal, *Angew. Chem. Int. Ed.* **2021**, *60*, 11824;

PP-9

High fidelity detection of Picric acid by a novel binuclear Zn^{II}-metallacycle following proton prompted fluorescence quenching mechanism

*Prem Chand, Amit Pandey, and Ashish Kumar**
[a]Department of Chemistry, Institute of Science, Banaras Hindu University, Varanasi – 221 005
Email: akumar.chem@bhu.ac.in

A novel highly fluorescent binuclear Zn^{II} metallacycle **1** **[(ZnL)$_2$]** based on 2,7-dimethylacridine-3,6-diyl-bis(azaneylylidene)-bis(methaneylylidene)-bis(3-diethylaminophenol) (**H$_2$L**) has been synthesized under optimized laboratory conditions. These were characterized by various spectral (FT-IR, ^{1}H-NMR and HRMS) analyses followed by structural authentication of **1** by single crystal X-ray diffraction analysis. Complex **1** is strategically equipped with four -N(C_2H_5)$_2$ groups for being useful in detection towards picric acid which is one of the most exploited molecule in forensic applications and a toxic pollutant.[1] According to UV-vis, fluorescence and ^{1}H-NMR studies, **1** displays excellent selectivity and sensitivity towards PA among other nitro aromatic compounds in 50% aqueous medium. Mechanism of detection has been followed by UV-vis, fluorescence and ^{1}H-NMR titration studies which substantiated a static quenching mechanism.[2] The spectral observations were well supported through DFT along with demonstration of naked eye detection of PA in solid, liquid and vapour phases.[3]

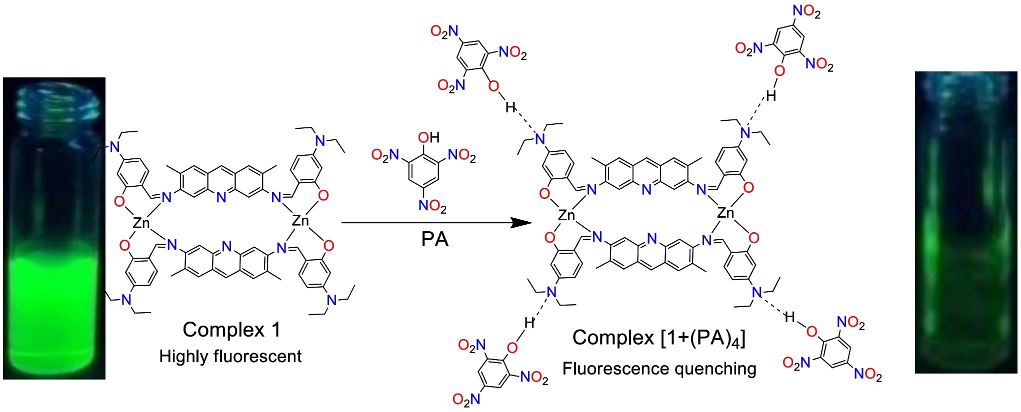


Fig. 1 Synthesis of fluorophores sensor from **1** under optimized laboratory conditions.

Keyword: Detection of PA**;** Zn^{II} metallacycle**;** Chemosensor**;** Fluorescence quenching.

References:

(1) A. Kumar, A. Kumar and D. S. Pandey, *Dalton Trans*., 2016, **45**, 8475–8484.
(2) P. Chand and A. Kumar, *New J. Chem*., 2023, **47**, 6135–6143.
(3) G. Radha, T. Leelasre, D. M. kumar, R. S. Pillai and H. Aggarwal, *New J. Chem*., 2021, **45**, 12931-12937; (b) Y. Xiao, Y. Wang, Z.-X. You, Q.-L. Guan, Y.-H. Xing, F.-Y. Bai, and Li-X. Sun, *Cryst. Growth Des.,* 2022, **12**, 6967–6976.

PP-10

Aggregation-Induced Emission in Quinolone–Quinazoline Conjugates Facilitated by Intermolecular Hydrogen Bonding, with Potential Application in Acidochromism

*Irshad Ali, Bhupendra Kumar Dwivedi, Vishwa Deepak Singh, and Daya Shankar Pandey**
Department of Chemistry, Institute of Science, Banaras Hindu University, Varanasi-221005, India

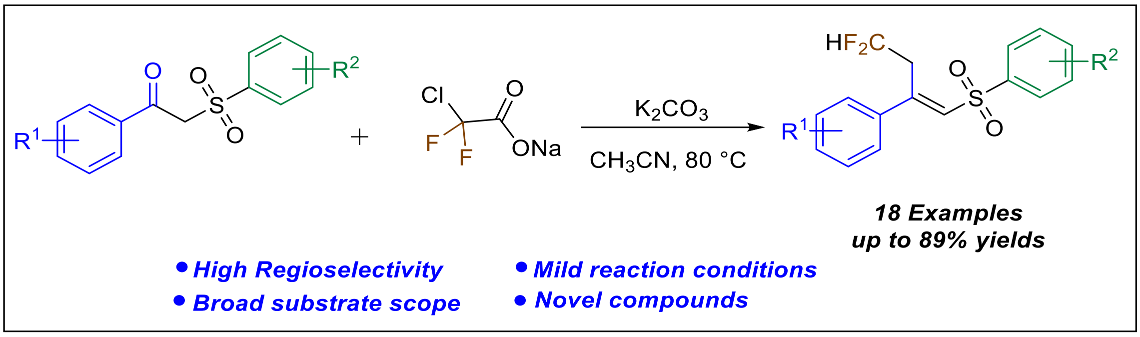
The impact of intermolecular hydrogen bonding on the aggregation behavior of quinolone–quinazoline based donor–acceptor systems (Q1–Q3) is discussed. These compounds were deliberately designed, synthesized, and thoroughly characterized through various spectral techniques. The inclusion of electron-donating groups in Q1–Q3 leads to solvent-dependent emission, suggesting a polarized excited state and enhanced intramolecular charge transfer. Aggregation-induced emission (AIE) in Q1–Q3 is attributed to restricted intramolecular rotation and vibrations via intermolecular hydrogen bonding. The influence of solvent and substituents on the photophysical behavior and morphology of Q1–Q3 was explored through various measurements. Additionally, electron-donating substituents (-CH3 in Q2 and -OCH3 in Q3) were found to lower the energy gap between HOMO and LUMO, as supported by DFT studies. Moreover, Q1–Q3 exhibit reversible acid/base-induced "ON–OFF–ON" type signaling, and their acidochromic behavior has been validated through various studies.

PP-11

A simple regioselective synthesis of β-difluoromethoxy vinyl sulfones via *O*-difluoromethylation of β-ketosulfones using sodium chlorodifluoroacetate

*Km Ishu, and Krishna Nand Singh,**
Department of Chemistry, Institute of Science, Banaras Hindu University,
Varanasi- 221005, India
Email: ishuyadaviitb@gmail.com

A practical synthesis of new β-difluoromethoxy vinyl sulfones has been explored by *O*-difluoromethylation of β-ketosulfones using inexpensive and easily workable sodium chlorodifluoroacetate as a difluorocarbene precursor. The strategy is convenient, regioselective, and is endowed with adequate substrate scope and functional group tolerance.



18 Examples
up to 89% yields

- ***High Regioselectivity***
- ***Broad substrate scope***
- ***Mild reaction conditions***
- ***Novel compounds***

K, Ishu, N.S. Prabhakar, K.N Singh**,** ***Org. Biomol. Chem.*****,** 2023, **21**, 6588-6594.

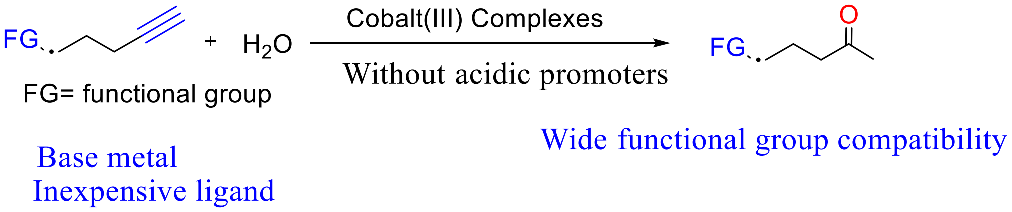
PP-12

Chemoselective hydration of terminal alkynes catalysed by bis(dimethylglyoximato)cobalt(III) complexes

*Ujala Maddheshiya, Jitendra Kumar Yadav and Kamlesh Kumar**
Department of Chemistry, Institute of Science, Banaras Hindu University
Varanasi, Uttar Pradesh-221005, India
Email:kamlesh.kumar@bhu.ac.in

The mild reaction condition with inexpensive features and easy availability of the cobaloxime complexes well address the current challenges in the field of alkynes hydration. These complexes are bench stable and could be easily prepared in large quantities in laboratory. Cobaloxime complexes emerge as a crucial catalyst for the conversion of alkynes to carbonyl compounds with numerous industrial applications.

Because of increasing interest in cobalt transition metal complexes, bis(dimethylglyoximato)cobalt(III) complexes have been synthesized and characterized by ^{1}H NMR, ^{13}C{^{1}H} NMR and FT-IR spectral studies. The synthesized complexes are investigated as hydration catalyst for a wide range of terminal alkynes to corresponding methyl ketones. Cobaloximes exhibits high activity to afford desired products in good to excellent yields methyl ketones without adding any external acidic promoters.



Reference:

(1) Hou, S.; Yang, H.; Cheng, B.; Zhai, H.; Li, Y. Cobaloxime-catalyzed hydration of terminal alkynes without acidic promoters. *Chem. Commun.* **2017,** *53*, 6926.

(2) Kang, S.-M.; Han, S.-S.; Zhu, Y.-Y.; Wu, Z.-Q. Cobalt (III) Porphyrin-Decorated Stereoregular Polyisocyanides Enable Highly Effective Cooperative Catalysis for Hydration of Alkynes. *ACS Catal.* **2021,** *11*, 13838.

(3) Ötvös, S. n. B.; Szécsényi, Z.; Fülöp, F. Bismuth (III)-catalyzed hydration of terminal alkynes: sustainable synthesis of methyl ketones in batch and flow. *ACS Sustain. Chem. Eng.* **2019,** *7*, 13286.

(4) Salvio, R.; Bassetti, M. Sustainable hydration of alkynes promoted by first row transition metal complexes. Background, highlights and perspectives. *Inorganica Chim. Acta* **2021,** *522*, 120288.

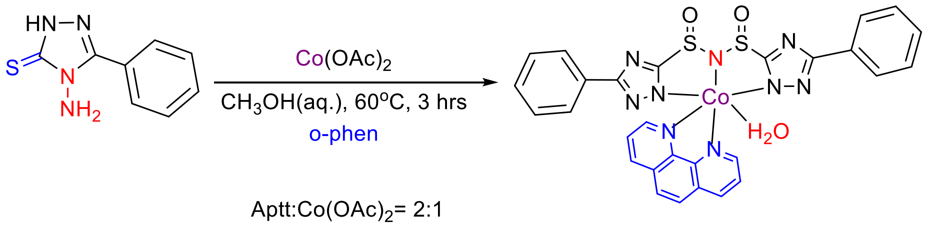
PP-13

Antiproliferative activity of Co(III) complexes stabilized by *in situ* generated *bis*(5-phenyl-1,2,4-triazole)-3-sulfinamide

*S. K. Pandey[a], S. P. Sonkar[b], S. Yadav[b], Alok Shukla,[c], A. Acharya[c], Manoj K. Bharty[a]**

[a]Department of Chemistry, Banaras Hindu University, Varanasi-221005, India
[a]Department of Chemistry, Banaras Hindu University, Varanasi-221005, India
[c]Department of zoology, Banaras Hindu University, Varanasi-221005, India

Abstract: A cobalt (III) complex [Co(ptsm)(*o*-phen)]·H_2O {ptsm = *bis* (5-phenyl-1,2,4-triazole)-3-sulfinamide} were synthesized and characterized by various spectroscopic and X-ray crystallography techniques. The crystal structure is stabilized by various types of hydrogen bonding. Complex was tested for its cytotoxicity against Dalton's lymphoma (DL) cells employing MTT assay which discloses IC_{50} value as 30 Mm. The remarkable IC_{50} value for Complex **1** shows that it can be utilized as a potential anticancer agent against DL cells.



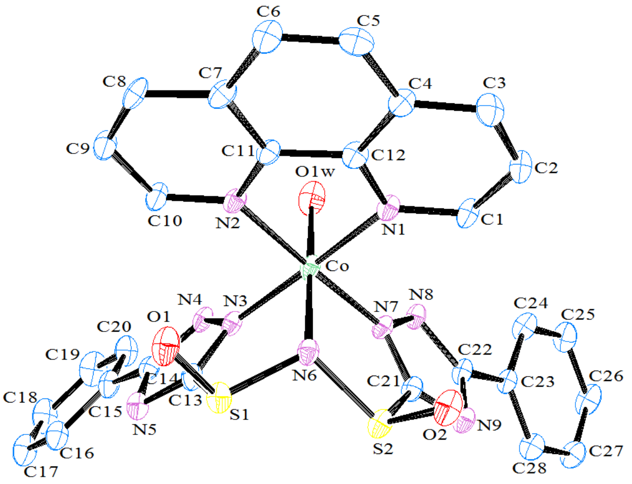


Fig. ORTEP diagram of [Co(ptsm)(*o*-phen)]·H_2O

References:

1. K. S. Sandhya, G. S. Remya, C. H. Suresh, *Inorg. Chem*. **2015**, *54*, 11150.
2. N. Armaroli, V. Balzan, *Chem. Eur. J.* **2016**, *22*, 32–57.
3. J. D. Blakemore, R. H. Crabtree, G. W. Brudvig, *Chem. Rev*. **2015**, *115*, 12974–13005.
4. S. Komeda, A. Casini, Next-Generation Anticancer Metallodrugs, *Curr Top Med Chem*. **2012**, *12*, 219-235.

PP-14

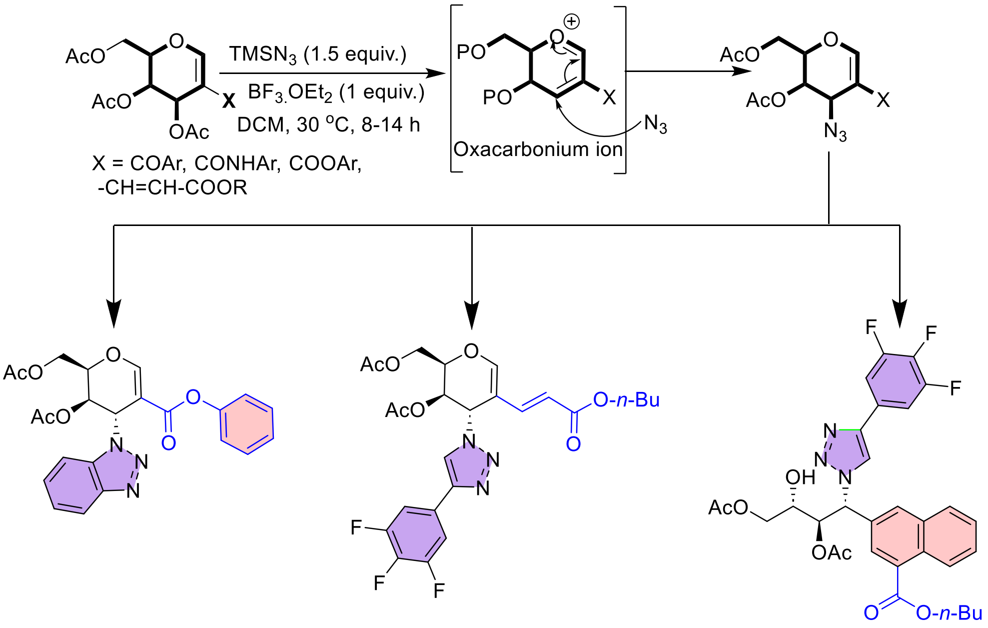
Site- Selective chiral azidation of Glycals: access to C-3 branched Glycoconjugates and *α*- triazolo chiral Naphthalene scaffold

Ram Pratap Pandey and *Nazar Hussain*

Department of Medicinal Chemistry, Institute of Medical Sciences, Banaras Hindu University-Varanasi- 221005

Glycals are sugar enol-ethers having endocyclic double bond between carbon 1 and 2. The reactivity of both the unsaturated centers is quite different due to the presence of oxygen atom inside the ring. In the presence of different reactive centers in a complex molecule it is challenging to synthesize highly regio- and stereoselective compounds. Organic azides are versatile inter- mediates in synthetic chemistry and the importance of such moieties is well-established in chemical biology, medicinal chemistry, and the material sciences. The versatility of organic azides is well recognized due to their importance in the synthesis of amines, amides, and some privileged heterocyclic.

Herein we designed a strategy for the synthesis of regio- and stereoselective displacement of the C3- acetate group by azide moiety at the C3- position of various C2- substituted glycals. The reactivity of various C2-substituted glycals reveals that electron-withdrawing groups are necessary for the regioselective introduction of the azide group at the C3 position. The newly launched azido group was used as a handle for the click, Staudinger, and Diels-Alder reaction for the synthesis of various C3 glycoconjugates and α- chiral aromatic building blocks.



PP-15

A simple TICT/ICT based molecular probe exhibiting ratiometric fluorescence Turn-On response in selective detection of Cu^{2+}

*Ravisen Rai[a], Rimpi Bhandari[a], Mohammed Kaleem[a], Nilesh Rai[b], Vibhav Gautam[b] and Arvind Misra[a]**
[a] Department of Chemistry, Institute of Science, Banaras Hindu University, Varanasi–221005 UP INDIA
[b] Centre of Experimental Medicine and Surgery, Institute of Medical Sciences, Banaras Hindu University, Varanasi–221005, UP INDIA
Corresponding author: amisra@bhu.ac.in; arvindmisra2003@yahoo.com

The work reported herein describes photophysical behavior of a new fluorescent probe **APDA.** The probe exhibited sensitivity for Cu^{2+} ion in 80% aqueous acetonitrile medium. Probe shows dual emission due to TICT and ICT states and upon interaction with different metal ions Cu^{2+} induces hydrolysis of imine bond to rejuvenate aldehyde derivative with ratiometric "turn–On" fluorescence response, through ICT state while emission due to TICT state get diminished. Similarly, the synthesized model compound ADA under similar experimental condition supported hydrolysis of imine bond in the presence of copper. Jobs plot analysis, based on emission titration data suggested a 1:1 binding stoichiometry between probe **APDA** and Cu^{2+} ion. The limit of detection (LOD) was found to be 4.4×10^{-8} M (44 nM). The probe has been applied on test paper strip to detect Cu^{2+} ion with naked-eye sensitive response. Also, the cell imaging studies revealed the potential applicability of probe to detect Cu^{2+} ion in live cells. The mechanism of sensing was confirmed by ^{1}H, ^{13}C NMR, FTIR and mass spectrometry data analysis.

References:

[1] A. W. Czarnik, Fluorescent Chemosensors for Ion and Molecule Recognition, J. Am. Chem. Soc. Washington, DC. (1993).

[2] A. Prasanna De Silva, H.Q. Nimal Gunaratne, T. Gunnlaugsson, A.J.M. Huxley, C.P. Mccoy, J.T. Rademacher, T.E. Rice, Signaling Recognition Events with Fluorescent Sensors and Switches, Chem. Rev .97 (1997) 1515-1566.

PP-16

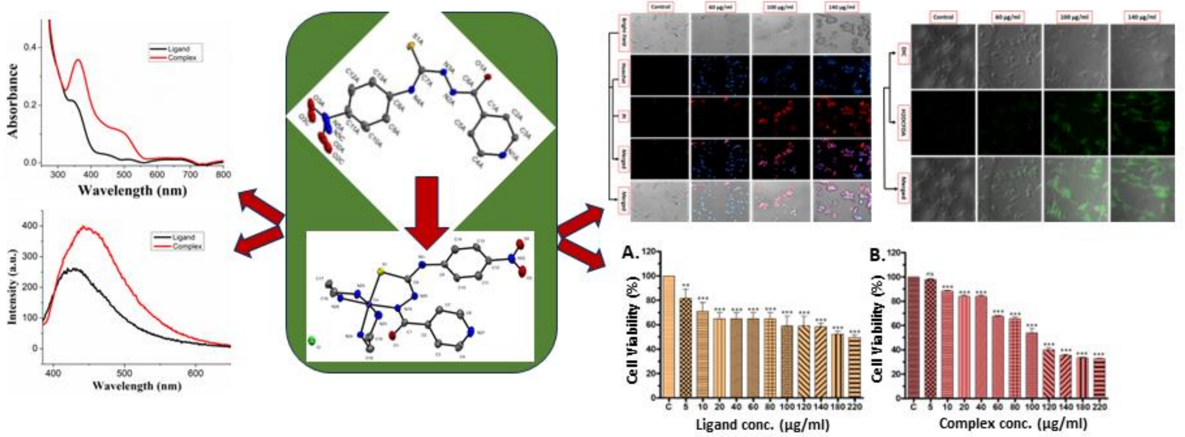
Synthesis, structural characterization and photophysical studies of Co(III) complex of 1-isonicotinoyl-4-(4-nitrophenyl)-3-thiosemicarbazide and its Anticancer activity

Riya Kumari[a], Ram Nayan Gautam[a], Alok Shukla[b], Arbind Acharya[b], M. K. Bharty[a]

[a] Department of Chemistry, [b]Department of Zoology, Banaras Hindu University, Varanasi-221005, India

**Corresponding author E-Mail: mkbharty@bhu.ac.in*

A new complex [Co((intph)(en)$_2$] derived from 1-isonicotinoyl-4-(4-nitrophenyl)-3-thiosemicarbazide (H$_2$intph) has been reported. The synthesized complex has been characterized by infrared, UV-vis. spectrometry and single-crystal X-ray data. The anticancer effect of a cobalt complex of thiosemicarbazide was investigated against glioblastoma cell lines (U87). Our results reveal a significant reduction in cell viability following treatment with the cobalt complex. Therefore, the treatment induced both apoptotic and necrotic modes of cell death in glioblastoma cells. We also observed an increase in reactive oxygen species (ROS) production, suggesting a potential involvement of oxidative stress in the anticancer activity of the cobalt complex. These findings highlight the promising anticancer activity of non-platinum metal complexes, specifically cobalt thiosemicarbazide, in combating glioblastoma, a highly malignant and aggressive form of brain cancer. Further, exploration of the molecular mechanisms underlying this cytotoxicity may open some ways for the development of effective anticancer strategies.



References:

[1] P. Jyothi, V. Sumalatha, D. Rajitha, Inorganic Chemistry Communications. 145 (2022) 110029

[2] B. Garcia, J. Garcia-Tojal, R. Ruiz, R. Gil-Garcia, S. Ibeas, B. Donnadieu, J.M. Leal, J. Inorg. Biochem. 102 (2008) 1892-1900.

[3] M.K. Bharty, R.K. Dani, P. Nath, A. Bharti, N.K. Singh, Om Prakash, Ranjan K. Singh R.J. Butcher, Polyhedron 98 (2015) 84-95.

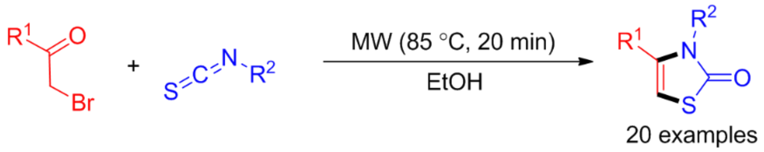
[4] S. Jaiswal, S.K. Pandey, J. Prajapati, S. Chandra, M.K. Gond, M.K. Bharty, I. Tiwari, R.J. Butcher, Appl. Organomet. Chem. 37 (2023) 7085.

PP-17

Microwave-Assisted Diversity-Oriented Synthesis of Thiazol-2(3H)-ones and Its Interaction with Biomacromolecules

*Mahesh Kumar, and Krishna Nand Singh**
Deparment of Chemistry, Institute of Science, Banaras Hindu University,
Varanasi-221005
Email: maheshdubey9936@gmail.com

An expeditious catalyst-free heteroannulation reaction has been developed to access functionalized thiazol-2(*3H*)-ones by using isothiocyanates and 2-bromoketones in EtOH under controlled microwave irradiation. The synthetic strategy is simple, straightforward, and offers two points of structural diversity to expand the product versatility.



- Catalyst/additive-free
- Eco-safe
- Broad-substrate scope
- C-N and C-S bond formation
- Evaluation of potent AChE inhibitors

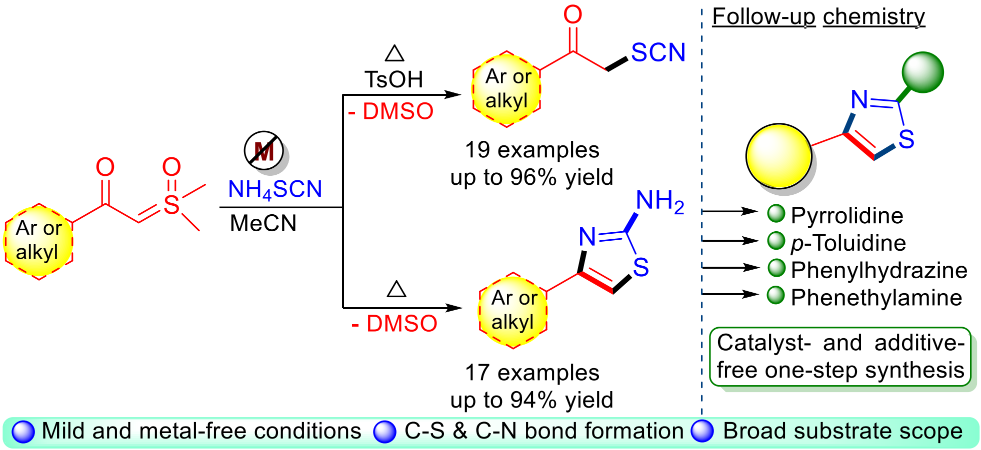
Preeti[+], M. Kumar[+], A. Jaiswal, K. N. Singh, Asian J. Org. Chem. **2022**, *11*, e202100389.

PP-18

Straightforward Access to α-Thiocyanoketones and Thiazoles from Sulfoxonium Ylides

*Ajay Sharma, Ajay Kant Gola, and Satyendra Kumar Pandey**
Department of Chemistry, Institute of Science, Banaras Hindu University, Varanasi 221 005, India
Corresponding Author Email: skpandey.chem@bhu.ac.in
Presenting Author Email: avbaragi@gmail.com

Efficient, versatile, and metal-free synthetic strategies for synthesizing α-thiocyanoketones and thiazoles from β-ketosulfoxonium ylides and NH_4SCN have been described. Due to its simplicity, benign reaction conditions, excellent chemoselectivity, and high yield, this method represents a unique approach for divergent synthesis. Finally, the potential value of the developed methods is demonstrated *via* large-scale reactions and synthesizing other valuable compounds in one-step *via* α-thiocyanoketone as an intermediate along with the synthesis of Fanetizole, an anti-inflammatory drug.[1] The specifics of the findings will be shared at the poster presentation session.



Reference:

1. **Sharma, A.**; Gola, A. K.; Pandey, S. K. ***Chem. Commun.*** **2023,** *59*, 10247.

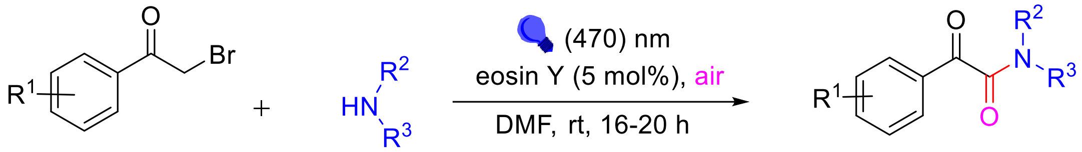
PP-19

Visible-Light-Mediated Synthesis of α-Ketoamides via Oxidative Amination of 2-Bromoacetophenones Using Eosin Y as a Photoredox Catalyst

*Kaushal Kishor, Neha Sharma Prabhakar, and Krishna Nand Singh**
Department of Chemistry, Institute of Science, Banaras Hindu University,
Varanasi-221005

Email: kaushal20121999@gmail.com

An oxidative amination of 2-bromoacetophenones has been accomplished to provide *α*-ketoamides by using photoredox catalysis with air as oxidant. The reactants are readily accessible, and the method is endowed with broad substrate scope and good functional group tolerance (**Scheme 1**). The practicality of the approach is also demonstrated by a gram-scale reaction.



21 Examples
upto 86% yield

- ***Photoredox reaction***
- ***C-N/C-O Bond creation***
- ***Metal-free***
- ***Air as oxidant***

Scheme 1 Synthesis of α-Ketoamides.

Reference: K. Kishor, N. S. Prabhakar, and K. N. Singh, *Chem Asian J.* **2023**, *18*, e202300669.

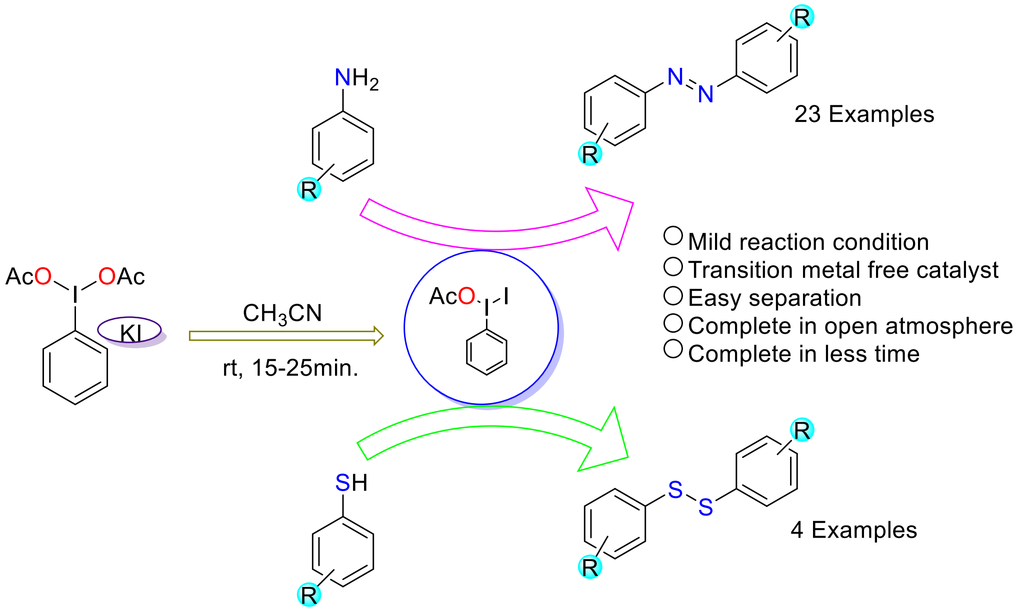
PP-20

Transition Metal-Free Catalyzed Oxidative Coupling of Anilines to Azo Compounds and Thiophenols to Disulfides

*Vikas Yadav, Ram Singh Kuri, Mitushree Ghosh and Virendra Prasad,**

Department of Chemistry, Institute of Science, Banaras Hindu University (BHU), Varanasi, 221005, India.
****Email:*** *vprasadbhu@gmail.com*

Herein we are reporting the efficient oxidative transformations of aryl amines to azoarenes and aryl thiols to the corresponding disulfides using diacetoxyiodobenzene and potassium iodide as transition metal-free catalysts in acetonitrile at room temperature. The developed protocols are highly efficient and employ readily accessible, inexpensive, and environmentally friendly starting.



References:

1. *Current Organic Chemistry, 2023, 27, 435-443*

Assessing the structural dependent optical properties of Eu^{3+} doped in La/YPO_4 nano phosphors for anticounter fitting applications

Prince Kumar[1], Pradeep Kumar Vishwakarma[1], Amresh Bahadur[1], Shyam Bahadur Rai[1]*
[1]Laser and Spectroscopy Laboratory, Department of Physics, Institute of Science,
Banaras Hindu University, Varanasi 221005, India
Email - princepearl531@gmail.com

Exploring the advantageous optical features of Eu^{3+} ion in a composite La/YPO_4 nanophosphors host is particularly appealing for anti-counterfeiting applications. REs ions (Eu^{3+}) doped La/YPO_4 inorganic nano phosphor have been synthesized by wet chemical route i.e., hydrothermal method (200°C), which is further calcined at 300°C and 500°C to improve its structural and optical properties. Rietveld refinement of XRD patterns has confirmed the formation of individual phases of $LaPO_4$ and YPO_4 as a composite matrix, with monoclinic and tetragonal phases respectively however the discrepancy in particle sizes corresponding to both phases as observed from SEM & TEM images. XPS analysis has confirmed the presence of each constituent element. In Downshifting optical properties of Eu^{3+}, the intense magnetic dipole transition is observed in less asymmetrical hosts as in orthophosphate (PO^{4-}).[1] The emission peak intensity of the Eu^{3+} (λ_{Exi}=395 nm) is 5 times more intense than excitation with CTB (λ_{Exi}=266 nm). A slight tunable emission was observed under the excitation by 266nm (CTB Eu^{3+}- O^{2-}) and 395nm (4f-4f transitions) due to the presence of two different doping sites. Herin,[2] the Eu^{3+} has two sites Ln^{3+}(La^{3+} and Y^{3+}) where at La^{3+} sites, CTB emission dominates nearly two-fold intense ${}^5D_0 \rightarrow {}^7F_1$ emission as compared to ${}^5D_0 \rightarrow {}^7F_2$ emission and at Y^{3+} sites overall 4f-4f emission is too intense along with both the transitions ${}^5D_0 \rightarrow {}^7F_1$ and ${}^5D_0 \rightarrow {}^7F_2$ are equally probable. Apart from that a broad emission in the range of 300-550 nm with significant intensity is observed only when the nano-phosphor samples are excited with 266nm which may be due to oxygen vacancy which is confirmed by XPS O1s peak fitting so that oxygen vacancies induce the formation of intermediate/mid-gap bands in host structure[3]. On raising the calcination temperature from 300°C to 500°C, the emission intensity increased by more than 30% and their lifetime also increased slightly which is mainly due to an increase in crystallinity. Examining the properties of this phosphor material such as nano-particles, with sharp transition, high color purity, and slight tunability with highly intense orange emission shows strong temptation in multiple fields such as anticounter fitting, security ink etc.

References:

[1] K. Binnemans, "Interpretation of europium(III) spectra," Coordination Chemistry Reviews, vol. 295, pp. 1-45, 1 July 2015.

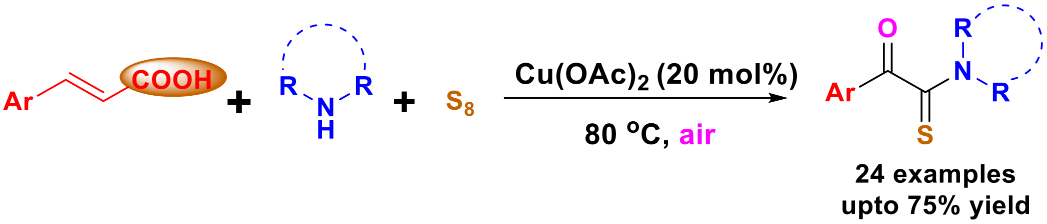
[2] G. H. Dieke, Spectra and Energy Levels of Rare Earth Ions in Crystals, H. C. H. M. Crosswhite, Ed., New York: Jons Wiley & Sons, 1968.

[3] A. K. Parchur, "Observation of intermediate bands in Eu3+ doped YPO4 host: Li+ ion effect and blue to pink light emitter," AIP ADVANCES 2, 2012

Copper-Catalyzed Decarboxylative Synthesis of α-Ketothioamides using α,β-Unsaturated Arylcarboxylic acids, Alicyclic Secondary Amines and Elemental Sulfur

*Anjali Jaiswal and Krishna Nand Singh**
Department of Chemistry, Institute of Science, Banaras Hindu University, Varanasi-221005
Email: anjalijaiswal354979@gmail.com

α-Ketothioamides have been especially exploited for their terminating property in Sanger-DNA sequencing reaction,[1, 2] and are used as *in vitro* PHGDH inhibitors which selectively abrogates the proliferation of cancer cells.[3] An efficient and straightforward synthesis of α-ketothioamides has been accomplished via *in situ* decarboxylative oxidative thioamidation using α,β-unsaturated arylcarboxylic acids, alicyclic secondary amines and elemental sulfur under solvent-free aerobic conditions.



A. Jaiswal, A. K. Sharma, Preeti and K. N. Singh, *Asian J. Org. Chem.* **2021**, *10*, 1748–1751.

References:

1. (a) P. Q. Huang, *Acta Chim. Sinica.* **2018,** *76,* 357–365. (b) J. Matysiak, A. Niewiadomy, G. Macik-Niewiadomy, T. Kornillowicz, *Eur. J. Med. Chem.* **2000**, *35*, 393.
2. K. Schwarzer, C. Wojczewski, J. W. Engels, *Nucleosides Nucleotides Nucleic Acids.* **2001**, *20*, 879.
3. R. Séverine, C. Cyril, S. Quentin, D. Alice, D. R. Anita, M. Edouard, C. C. Lewis, F. Olivier, F. Raphaël, *J Med Chem*. **2017**, *60*, 1591–1597.

PP-23

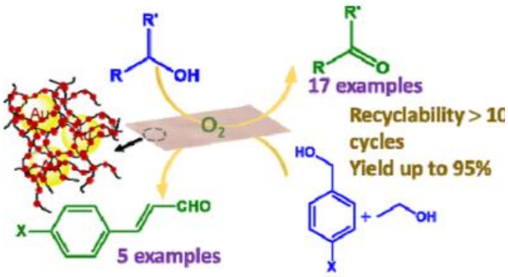
UV Cross-Linked Polymer Stabilized Gold Nanoparticles as a Reusable Dip-Catalyst for Aerobic Oxidation of Alcohols and Cross Aldol Reaction

Anshuman, Biplab K Kuila

Department of Chemistry, Institute of Science, Banaras Hindu University, Varanasi, U.P., India, 221005

Email: bkkuila.chem@bhu.ac.in

Among the precious metal nanoparticles, gold nanoparticle (AuNP) based catalysts have become a hot research topic in recent years due to their variety of reactions like oxidation, reduction, dye degradation, coupling reactions, etc[1-3]. To prevent their aggregation, AuNPs have been immobilized on suitable supports like alumina, silica spheres, zeolites, graphenes, different polymers, etc. In all cases, one of the major challenges is separating the catalyst from the reaction mixture after the completion of the reaction. Such as filtration, precipitation, and centrifugation are adopted to remove such catalysts, and the reusability of these catalysts sometimes becomes difficult in the next cycle. Here, we have demonstrated a novel strategy to develop a gold nanoparticle (AuNP)-embedded composite polymer membrane for dip-catalysis, the composite membrane was fabricated by simply depositing the PVP-AuNP on the membrane followed by UV cross-linking and utilized as a dip-catalyst for the aerobic oxidation of alcohols to carbonyl compounds under oxygen and clean reaction conditions. The catalyst was further tested for performing cross-aldol reactions. The dip-catalysts are highly stable under the reaction conditions without significant leaching of Au into the solution. The dip-catalyst demonstrates outstanding reusability, easily recovered by simply pulling it out from the reaction mixture once the reaction is complete.



References

1) Candu, N.; Simion, A.; Coman, S. M.; Primo, A.; Esteve-Adell, I.; Parvulescu, V. I.; Garcia, H. Graphene Film-Supported Oriented 1.1.1 Gold(0) Versus 2.0.0 Copper(I) Nanoplatelets as Very Efficient Catalysts for Coupling Reactions. Top. Catal. 2018, 61 (14), 1449– 1457.
2) Guo, S.; Fang, Q.; Li, Z.; Zhang, J.; Zhang, J.; Li, G. Efficient Base-Free Direct Oxidation of Glucose to Gluconic Acid over TiO2- Supported Gold Clusters. Nanoscale 2019, 11 (3), 1326–1334.
3) Fang, Q.; Qin, Z.; Shi, Y.; Liu, F.; Barkaoui, S.; Abroshan, H.; Li, G. Au/NiO Composite: A Catalyst for One-Pot Cascade Conversion of Furfural. ACS Appl. Energy Mater. 2019, 2 (4), 2654–2661.

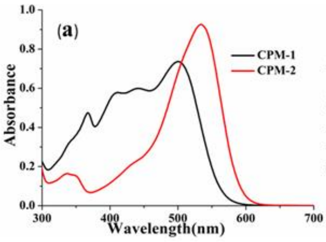
PP-24

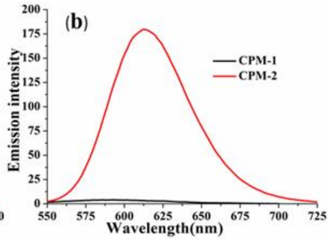
Lysosome Targeting Solid State NIR Emissive Donor-Acceptor Molecules: A Study on Photophysical Modulation through Architectural Distinction

*Ashish Kumar Kushwaha, Anjani Kumar and Roop Shikha Singh**
Department of Chemistry, Institute of Science
Banaras Hindu University, Varanasi-221005
Email id: roopshikha22singh@gmail.com

The prevalence of D–A strategy in achieving red-shifted emission has been established through designing of symmetric and asymmetric D–A molecules of D–A–D and A–D–Aconstruct. Architectural control over such D–A systems integrates solid state NIR emission with lysosome tracking and sets a multifarious goal of photophysical modulation in a comprehensive way. In particular two compounds, **CPM–1** (D–A–D) and **CPM–2** (A–D–A) have been synthesized introducing carbazole based donors and difluoroboron acceptors. Lysosome targeting and imaging has been achieved through incorporation of morpholine unit which ultimately imparts viscosity sensitivity to the construct. The fluorophores exhibited significant emission in solution along with distinctive solvatochromism, viscochromism and TICT. A comparative account of these competitive photophysical properties revealed the superior charge transfer properties of asymmetric D–A construct (**CPM–2**) while symmetric D–A molecule (**CPM–1**) was found to be a better molecular rotor with marked viscochromism. Owing to its excellent viscochromic behvaiour **CPM–1** has been successfully utilized in lysosome targeting in wild-type *Drosophila* flies (Oregon R$^+$ strain) through co-localization.

.





PP-25

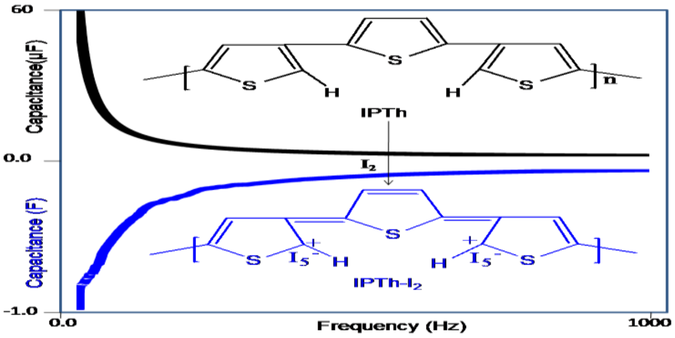
Isomeric Polythiophene: Promising Material for Low Voltage Electronic Devices

Devendra Kumar, *S. Krishnamoorthi*[*]

Department of Chemistry, Institute of Science, Banaras Hindu University, Varanasi, India

Email: devendrabhu53@gmail.com, skmoorthi@bhu.ac.in

In this investigation, we present empirical observations detailing the manifestation of substantial negative capacitance (NC), reaching up to -1F, within iodine-doped isomeric polythiophene (IPTh-I_2). NC observed in our case is not transient but stable enough to be measured for as long as the optimum concentration of iodine dopant is available. In contrast, undoped isomeric polythiophene (IPTh) manifests a modest positive capacitance ranging from 30 to 60 μF. Concatenation of IPTh-I_2 and IPTh in series results in an augmentation of the total capacitance of the system (~170 μF), exemplifying a characteristic feature of NC. Conversely, a bilayer configuration consisting of IPTh:IPTh exhibits a reduction in total capacitance by 38%. A notable amplification in the dielectric constant, escalating from 30 in IPTh to approximately 2000 in IPTh-I_2, signifies extensive conformational and structural alterations arising from interactions between the doped polymer chain and various iodide species, attributing to the emergence of NC. Furthermore, we document a single-sided p-n junction diode with a low knee voltage (below 0.5V) as a model device, illustrating the potential of IPTh as a promising material for the design and development of negative capacitance-based field-effect transistors. This research offers avenues for the scientific community to conceive low knee voltage-operating diodes, transistors, supercapacitors, and various other electronic devices based on all-organic semiconductors.



PP-26

Cationic Heteroleptic Ni(II) Dithiocarbamate Complexes: Synthesis, Characterization, and Electrocatalytic Oxygen Evolution Reaction

*Sarvesh Kumar Pal, Anjali Mishra***,** *Kamlesh Kumar**
Department of Chemistry, Institute of Science, Banaras Hindu University,
Varanasi, Uttar Pradesh-221005, India
Email: kamlesh.kumar@bhu.ac.in

Four new cationic heteroleptic Ni(II) dithiocarbamate complexes of the formula **$[Ni(LL')_2]PF_6]$ (1-4)** L = N-benzyl-N-benzyl methyl dithiocarbamate, (L1) and N-benzyl-N-3-pyridyl methyl dithiocarbamate (L2); L' = 1,2 bis(diphenylphosphino)ethane (dppe) and 1,1 bis(diphenyphosphino)ferrocene (dppf) have been synthesized and characterized by FT-IR, UV–Vis, ^1H, $^{13}C\{^1H\}$, $^{31}P\{^1H\}$, and $^{19}F\{^1H\}$ NMR spectroscopic techniques. All cationic complexes (**1-4**) have also been characterized by single-crystal X-ray crystallography. The molecular structures revealed distorted square planer geometry around the Ni(II) center with bidentate S^S dithiolate chelating ligands (**KL1** and **KL2**) and P^P chelating phosphine ligands. These complexes are immobilized on activated carbon cloth (CC) and their electrocatalytic activity for the oxygen evolution reaction (OER) have been investigated in aquation alkaline solution.

PP-27

Modulating Flexible Triarylmethanes into Rigid Xanthene Fluorophores

*Soumya Singh and Satyen Saha**

Organic fluorescent probes have revolutionized fluorescence imaging. Small probes, such as coumarins, naphthalimides, BODIPYs, and cyanines, offer non-gene expression-dependent exploration of biological phenomena. Xanthenes, including fluorescein and rhodamine derivatives, are widely used for bioimaging and as colorimetric probes. Xanthenes also serve as DNA labels, and chemical sensors, capable of detecting alterations in pH, metal ions, and other analytes, aiding in environmental monitoring and analytical chemistry. Fluorene fluorophores find applications in chemosensing, solar cells, and dye removal. Triarylmethanes have medicinal potential and are explored for their structure, photophysical properties, and applications. In our study, we investigate the photophysical behavior of a flexible triaryl methane and a conformationally rigid xanthene derivative. We also discuss their biological applications, including DNA interactions and cytotoxicity assays, which are essential in drug development. Our study provides valuable insights into the difference in the photophysical properties of flexible triaryl methane and conformationally rigid xanthene derivatives, shedding light on their potential use in various fields, including bioimaging and drug development. These findings contribute to the broader understanding of organic fluorescent probes and their diverse applications in scientific and technological domains.

PP-28

Green Synthesis of Titanium Dioxide Nanoparticles and its Integration into Dye-Sensitized Solar Cells for Enhanced Photovoltaic Performance

*Nikhil Srivastav, Sakshi Singh, Himanshu Patel, Yoganand Singh, Pankaj Srivastava**
Department of Chemistry, Institute of Science, Banaras Hindu University
*Varanasi 221005, INDIA; *E-mail: pankaj@bhu.ac.in*

In recent years, the growing need to create safe and non-toxic compounds, low-cost methods, environmentally acceptable solvents, and renewable materials has drawn a lot of attention to the green synthesis of nanoparticles. During nanoparticle synthesis, one of the key areas of concern is the use of capping agents to control growth, aggregation, physical and chemical properties [1]. TiO_2 nanoparticles are considered the prominent photoanode materials for dye-sensitized solar cells (DSSCs) [2]. Papaya seeds have diverse compositions of antioxidant chemicals, such as flavonoids and phytosterols. Papaya seed extract (PSE) constituents have the potential to act as reducing agents in the synthesis of metallic nanoparticles (Au NPs) as well as having antibacterial and antioxidant activities [3]. In this work, titanium nanoparticles are synthesized by using ethanolic PSE, which serves as a green-capping agent. The structure, size, and optical properties of as-synthesized TiO_2 NPs were characterized by XRD and UV-visible measurements. The surface area and porosity were investigated by BET analysis. Electrochemical impedance spectroscopy (EIS) studies revealed electronic resistance and electron lifetime. The DSSC fabricated with optimized PS-2.5 TiO_2 photoanode exhibited greater light-to-current conversion efficiency, 0.96% compared to un-capped TiO_2 nanoparticles (bare) based cell, 0.68% as shown in **Fig.1**. The illustrated result showed that capped TiO_2 using PSE as a capping agent has a greater potential with an enhanced efficiency of DSSC.

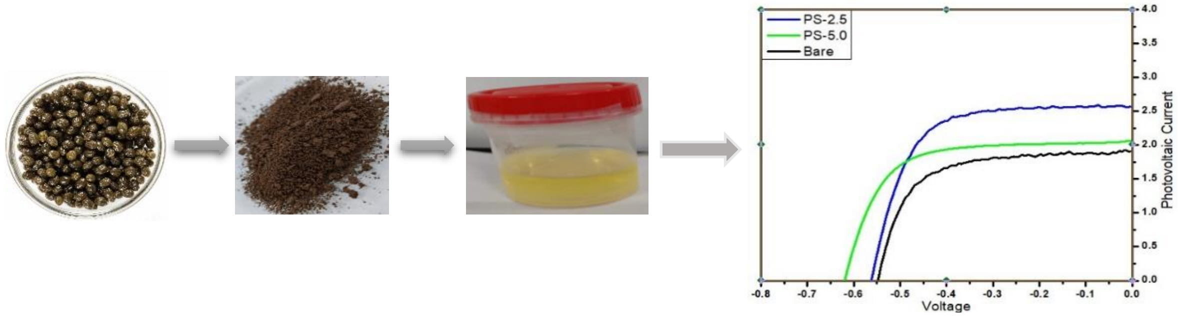


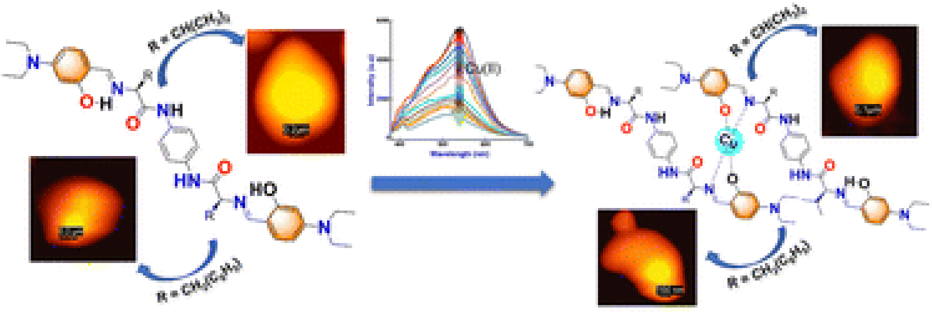
Fig. 1 J-V characteristics of cell fabricated with bare and PSE capped TiO_2

PP-29

Copper-guided tuning of supramolecular nano-assembly in pseudopeptide-based soft bioinspired materials

*Arpna Tamrakar, Tarkeshwar Maddeshiya, Surabhi Asthana, and Mrituanjay D. Pandey**
E-mail ID: mdpandey.chem@bhu.ac.in
**Department of Chemistry, Institute of Science, BHU.*

Pseudopeptide-based soft materials inspired by biology have emerged as cutting-edge components in the realm of recognition and supramolecular self-assembly. In our work, we've developed C2-symmetric pseudopeptidic soft materials using L-valine and L-phenylalanine. These materials demonstrate a remarkable ability for selective and sensitive detection of Cu(II) ions in an aqueous-organic medium, using the CHEQ mechanism. Additionally, they display the potential for Cu(II)-guided tuning of supramolecular nano-assembly, opening promising avenues for material nano-architectonics applications.



Keywords: pseudopeptide, sensing, supramolecular chemistry

References: -

(1) Tamrakar, A.; Nigam, K. K.; Pandey, M. D. Copper-guided tuning of supramolecular nano-assembly in pseudopeptide-based soft bioinspired materials. *New J. Chem*., **2023**,47, 20785-20792.

(2) Gao, R.; Ge, Q.; Cong, H.; Zhang, Y.; Zhao, J. Preparation and Biomedical Applications of Cucurbit [n] uril-Based Supramolecular Hydrogels. *Molecules*, **2023**, *28*(8), 3566.

(3) Marti-Centelles, V.; Pandey, M. D.; Burguete, M. I.; Luis, S. V. Macrocyclization reactions: The importance of conformational, configurational, and template-induced preorganization. *Chem. rev.*, **2015,** *115*(16), 8736-8834.

PP-30

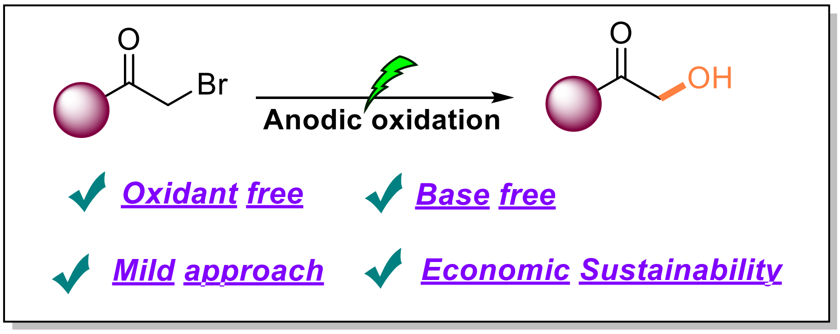
Electrochemical Hydroxylation of *α*-Bromoketones: Access to *α*-Hydroxy Ketones

Saurabh Singh[a], *Subhasish Ray*[a], *Gaurav Shukla*[a], *Malkeet Singh*[a] *and Maya Shankar Singh*[a]*

[a]*Department of Chemistry, Institute of Science, Banaras Hindu University, Varanasi 221005, India*
**Corresponding Author E-mail: mssingh@bhu.ac.in*

Herein, a new electrochemically divergent, effective, and eco-sustainable method has been developed for the synthesis of various hydroxy ketones via an electro-oxidation process. It involves electrocatalytic hydroxylation via debromination of C(sp^3)□Br bond. Here, simultaneous breaking of carbon-bromine (C□Br) bond and formation of a new carbon-oxygen (C□O) bond is achieved through electrolysis using DMSO. This method is very simple and appropriate because of its oxidant-free, base-free reaction conditions. The protocol features easy performance, mild conditions, and short reaction time.

Keywords: Electrochemical; Hydroxylation; Metal-free; Bromoketones.



PP-31

Synthesis, characterization and electrochemical biosensing behaviour of 25-Hydroxy vitamin-$D_3$by using FeO/MgO polypyrrole platform

*Sarita Shaktawat and Jay Singh**

[1]Department of Chemistry, Institute of Sciences, Banaras Hindu University Varanasi Utter Pradesh -221005
*(*E-mail- jaysingh.chem@bhu.ac.in)*

Vitamin D (Vit-D) is a metabolically active fat-soluble vitamin known to prevent serious human body disorders, including osteoporosis, chronic diseases, neurological conditions, infections, and cancers. In the scientific domain, efforts are continuously made to enhance human life while minimizing environmental impact on a global scale.In this study, a FeO/MgO polypyrrole (FeO/MgO-ppy) nanocomposite was synthesized using a hydrothermal method with leaf extract from the *Graptopetalum paraguyense* plant. The confirmation of the synthesized FeO/MgO-ppy nanocomposite was achieved through various characterizations such as Vis-UV, FTIR, XRD, XPS, AFM, SEM, EDX, TEM, and HRTEM.The synthesized FeO/MgO-ppy nanocomposite was employed for the electrochemical detection of 25-Hydroxy Vitamin D3 (25(OH)D3), an essential organic, fat-soluble micronutrient for proper metabolic regulation. The electrochemical detection utilized the fabrication of a bioelectrode, specifically ITO/FeO/MgO-polypyrrole/Antibody-25-OH vitamin D/BSA (ITO/FeO/MgO-ppy/((Anti-25-OH)D)/BSA) electrode.Electrochemical studies of 25(OH)D3 and its detection were performed through cyclic voltammetry (CV), differential pulse voltammetry (DPV), and electrochemical impedance spectroscopy (EIS) on the fabricated ITO/FeO/MgO-ppy/((Anti-25-OH)D)/BSA bioelectrode. The results of the fabricated electrochemical biosensor indicated profound stability, specificity, reproducibility, and high sensing performance.These findings confirm that the developed electrochemical biosensor, ITO/FeO/MgO-ppy/((Anti-25-OH)D)/BSA bioelectrode, presents a successful approach for the detection of 25(OH)D_3.

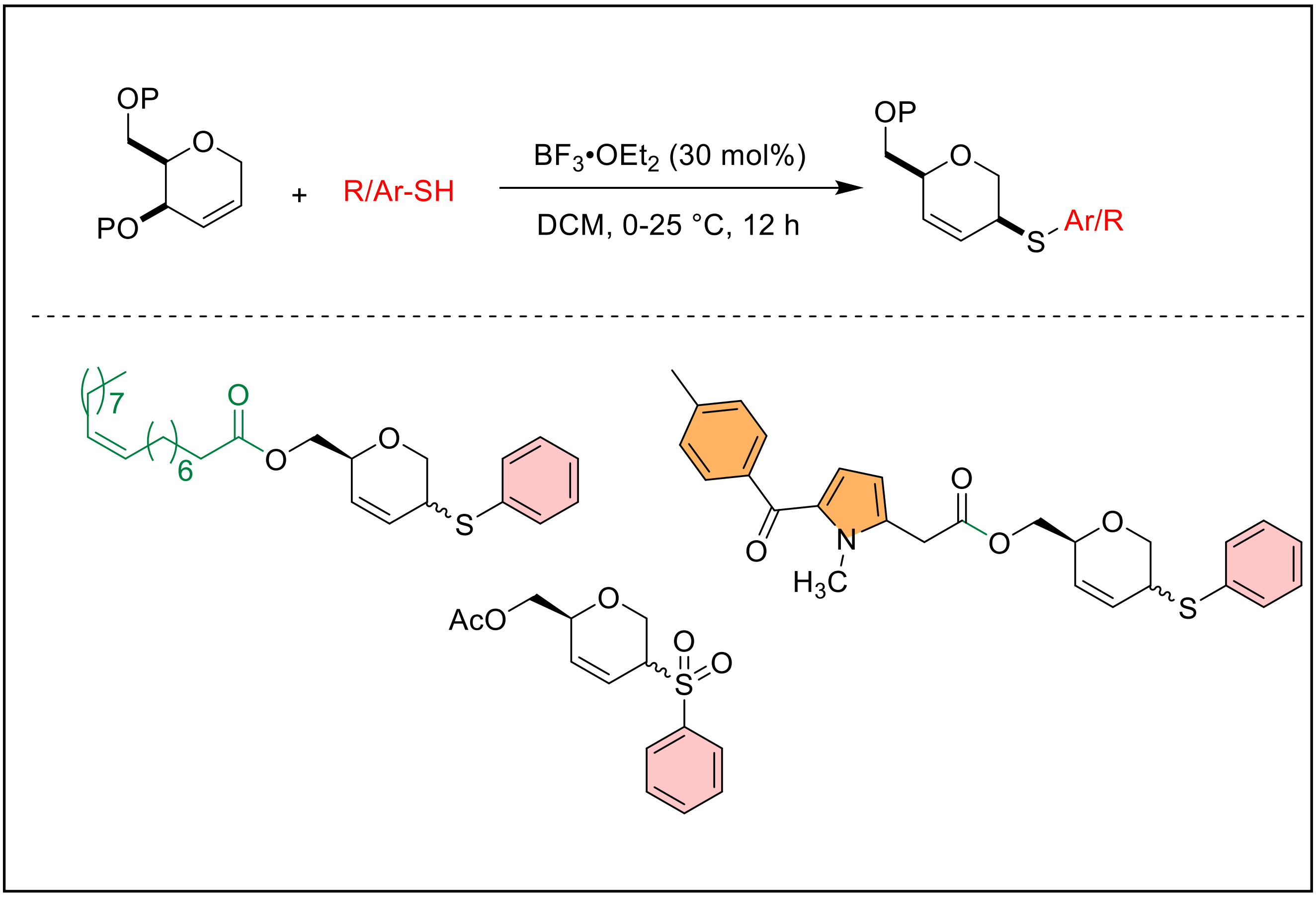
Keyword's: Vitamin D3, Biosensor, FeO/MgO nanocomposites

PP-32

Lewis acid mediated stereo- and regioselective Transformation of Pseudoglycals Towards the Synthesis of 2-thioaryl/alkyl Glycosides

<u>Bindu Tiwari</u> and Nazar Hussain
Department of Medicinal Chemistry, Institute of Medical Sciences, Banaras Hindu University-Varanasi, 221005, India.

Thioglycosides serve as a key building blocks for the construction of glycosidic bonds to generate different glycosides. Among all glycosides, thioglycosides seem more attractive to organic chemists because of their stability under various reaction conditions for the manipulations of protecting groups. To synthesize thioglycosides there are various routes available and among all the methods Lewis acid-mediated transformation of acetylated sugars was extensively studied. Herein, we disclosed a site-selective Lewis acid-mediated transformation of pseudoglycals with various thiols for the synthesis of C-2 thioaryl glycosides. The potential synthetic utility of the synthesized compounds was demonstrated to get C2-branched sulfone and sulfoxide. The late-stage modified drugs and pharmaceuticals linked with the glycal were also explored to afford the desired 2-thioaryl glycosides. Overall, a new entry to branched sugar that could have the potential in new drug discovery program.



PP-33

Fabrication of g-C_3N_4/WO_3 Nanocomposite for Enhanced Visible Light Photocatalytic Degradation of Rhodamine B

Richa Kumari[1,]*, *Debanjan Guin*[2] *and Chandra Shekhar Pati Tripathi*[1]
[1]*Department of Physics, Institute of Science, Banaras Hindu University, Varanasi*
[2]*Department of Chemistry, Institute of Science, Banaras Hindu University, Varanasi*
E-mail: singhricha.phy@gmail.com

Semiconductor photocatalysis is recognized as a highly effective and cost-efficient approach for the degradation of organic pollutants present in diverse water environments[1]. In this study, we employed a straightforward hydrothermal method to synthesize tungsten oxide (WO_3) nanorods and then formed its composite with sheet like graphitic carbon nitride (g-C_3N_4). These composites were then evaluated for their efficacy in degrading Rhodamine B dye, serving as a model pollutant. Various characterization techniques, including X-ray diffraction (XRD), scanning electron microscopy (SEM), transmission electron microscopy (TEM), fourier transform infrared spectroscopy (FTIR) were employed to examine the physicochemical properties of the particles. The investigation delved into the impact of parameters such as initial pH, catalyst loading, and initial pollutant concentration. The findings revealed that the composite with 3wt.% WO_3 content displayed superior photocatalytic efficiency in comparison to pure WO_3, unmodified g-C_3N_4, and other composites. Under these conditions, the catalyst exhibited an outstanding degradation efficiency of 95.9% after 90 minutes of visible light irradiation. This enhancement might be credited to the increased light absorption in visible-light region and enhanced charge separation efficiency. The composite's superior photocatalytic activity, long-term stability, and reusability make it a promising material for applications in wastewater treatment.

Keywords: Tungsten Oxide, graphitic carbon nitride, wastewater treatment

References:

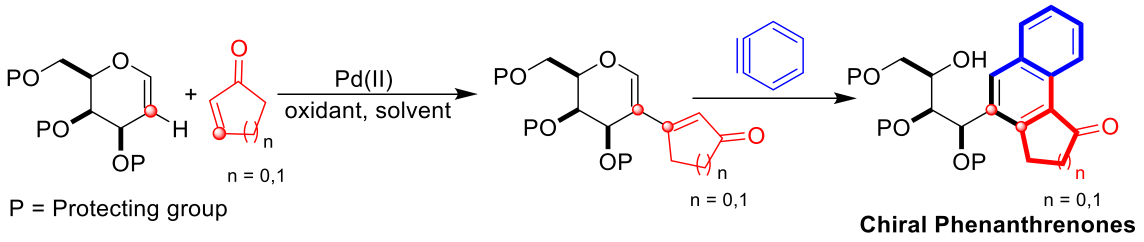
1. Wang, Y., Wang, Q., Zhan, X., Wang, F., Safdar, M., & He, J. (2013). Visible light driven type II heterostructures and their enhanced photocatalysis properties: a review. Nanoscale, 5(18), 8326-8339.

PP-34

Direct functionalization of glycals with cycloalkenones catalyzed by palladium acetate: Application to the Synthesis of Chiral Phenanthrenones

Mittali Maheshwari[a] *and Nazar Hussain**[a]
[†]*Department of Medicinal Chemistry, Institute of Medical Sciences, Banaras Hindu University,*
Varanasi-221005, India.
Email: mittali2212@bhu.ac.in

Glycals are important structural compounds used for the synthesis of glycosides and also act as a key synthon in the preparation of various biologically potent molecules. Glycosylation reactions using glycals have been well explored with different glycosyl acceptors for the synthesis of different glycosides such as C, O, N, and S glycosides. C-glycosides are the most significant and studied glycosides due to their enzymatic stability and presence in plenty of natural products and synthetic drugs. Pd-catalyzed reactions have been extensively studied and applied for the synthesis of C-glycosides by utilizing both the C-1 and C-2 positions of glycals. palladium-catalyzed direct C–H functionalization of glycals with cycloalkenones is described and a series of C-2 functionalized glycals were synthesized efficiently with cyclic enones. The direct C–H functionalization of glycals with Pd(II) and subsequent insertion of cyclic enones via b-hydride elimination is the key to the synthesis of 2C-branched glycals. The synthetic utility of this methodology for chiral phenanthrenones has also been demonstrated by coupling the synthesized 2C-branched glycals with arynes via 4+2 cycloaddition followed by concomitant pyran ring opening[1-7].



References

1. T. Bililign, B. R. Griffith and J. S. Thorson, *Nat. Prod. Rep.*,2005, 22, 742.
2. M. Hocek, *Chem. Rev.*, 2009, 109, 6729–6764.
3. D. Lee and M. He, *Curr. Top. Med. Chem.*, 2005, 5, 1333–1350.
4. Y. Du, R. J. Linhardt and I. R. Vlahov, *Tetrahedron*, 1998, 54, 9913–9959.
5. F. Nicotra, 1997, pp. 55–83.
6. J.-M. Beau and T. Gallagher, 1997, pp. 1–54.
7. S. S. Kulkarni and J. Gervay-Hague, *Org. Lett.*, 2006, 8, 5765–5768.

PP-35

Antiproliferative Activity of Bioactive on Mucosal Carcinoma

*Komal Kumari, Anant Kumar Singh, Dr. Surajit Rakshit**
Department of Chemistry, Institute of Science,
Banaras Hindu University, Varanasi
Uttar Pradesh-221005, India.

Mucosal melanoma is a rare kind of cancer, which starts from mucus's primary mucin-producing cells, where overexpression, aggregation of mucin was involved. Aberrant expression of mucins can aid in the loss of polarity in epithelial cells and encourage the Epithelial-Mesenchymal Transition (EMT), which increases cell motility and invasion potential, a crucial stage in the development of tumours. The aggregation can be inhibited in two ways:(i) by reducing the aggregate (ii) by influencing the initial step of aggregation i.e. phase separation. We depicted the integration of bioactive into both step of mucin aggregation. It has shown promising potential in various biomedical applications for novel treatments and interventions in a wide range of mucosal-related diseases and drug delivery applications.

Keywords: Mucosal carcinoma, Bio-actives.

PP-36

Synthesis of thermoresponsive homopolymers poly(*N*-ethyl)-*N*-(3-(isopropylamino)-3-oxopropyl) acrylamide and its copolymers with poly(ethylene glycol) methyl ether acrylate

*Sourov Mondal, Payal Gupta and Jaydeep Singh, Biswajit Ray**
Department of Chemistry, Institute of Science, Banaras Hindu University, Varanasi- 221005, India
Email: biswajitray2003@yahoo.co.in

A new monomer *N*-ethyl-*N*-(3-(isopropylamino)-3-oxopropyl)acrylamide (**M2**)-based different molecular weight homopolymers and copolymers of varying compositions with poly(ethylene glycol) methyl ether acrylate (PEGA) have successfully been synthesized *via* reversible addition-fragmentation chain-transfer (RAFT) polymerization using 1-phenylethyl phenyl dithioacetate (PEPD) as RAFT agent. The synthesized polymers are characterized by 1H NMR, GPC, UV-Vis, fluorescence, TGA, DSC, DLS and TEM techniques. The glass transition temperature (T_g) of homopolymers exhibits almost minimal reduction with decreasing molecular weight and remains constant at ~100°C, while the same of copolymers increases with decrease in PEGA content. The lower critical temperature (LCST) of the homopolymers shows no dependency on their molecular weight and has been found almost constant value at ~17°C, while those of the copolymers decrease with decrease in PEGA content within the range 42.6 – 78.4°C.

References:

Mondal S, Kumari A, Mitra K, Verma A, Saha S, Maiti B, Singh R, Manna P P, Maiti P, Watanabe H, Kamigaito M and Ray B , J. Mater. Chem. B, 2022,8462-8477

Mitra K, Maity S, Hajra A, Singh S, Mondal S., Singh J, Maiti P and Ray B, International Journal of Polymeric Materials and Polymeric Biomaterials, 2023, doi.org/10.1080/00914037.2023.2182780

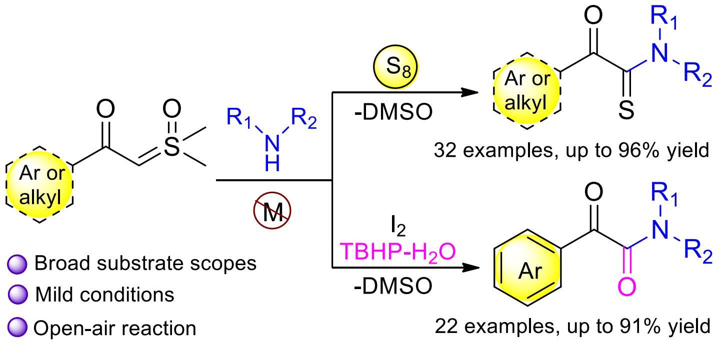
Kumari A, Vishwakarma S, Mitra K, Chen C, Cui S, Biswas CS., Maiti B, Mondal S, Maiti P, Stadler F J, Ray B Macromol. Chem. Phys. 2021;2100118

Metal-Free Syntheses of *α*-Ketothioamide and *α*-Ketoamide Derivatives from Sulfoxonium Ylides

*Paran Jyoti Borpatra and Satyendra Kumar Pandey**

Department of Chemistry, Institute of Science, Banaras Hindu University, Varanasi, Uttar Pradesh 221005, India, Email: paranjyoti89@gmail.com

An efficient base, additive, and metal free synthetic methods for *α*-ketothioamide and *α*-ketoamide derivatives from readily available sulfoxonium ylides have been described. Sulfoxonium ylides with primary or secondary amines afforded *α*-ketothioamides in the presence of elemental sulfur, whereas *α*-ketoamides when I_2 and TBHP were present. The reaction proceeded well at room temperature and generated the corresponding molecules in good to excellent yields. The reaction can be scaled-up and tolerated by a range of functional groups with simple operational procedures.[1] The specifics of the findings will be shared at the poster presentation session.



References:

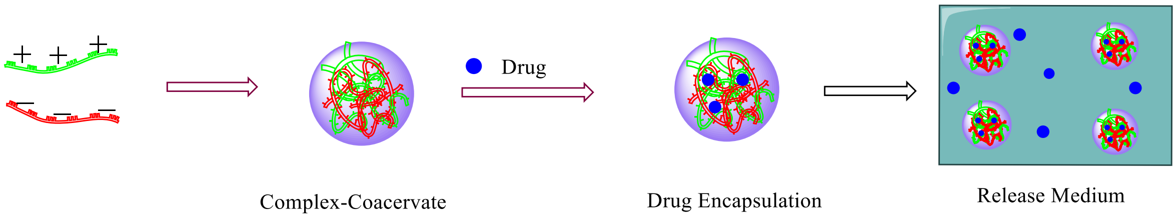
(1) Chaubey, T. N.; Borpatra, P. J.; Pandey, S. K. *Org. Lett.* **2023**, *24*, 8062-8066.

PP-38

Revealing the Promise of Complex Coacervate-Driven Drug Delivery Systems in the Biomedical Landscape

*Priyankar Mandal and Dr. Surajit Rakshit**
Department of Chemistry, Institute of Science, Banaras Hindu University, Varanasi, Uttar Pradesh-221005, India.
priyankarmandal7@gmail.com, srakshit.chem@bhu.ac.in

Complex coacervation is a phase separation phenomenon that arises from the electrostatic interactions between polyelectrolytes with opposite charges. This phenomenon has gained prominence as a versatile strategy in drug delivery applications. The reversible swelling and de-swelling behavior of complex coacervates, which respond to environmental cues like pH, temperature, or ionic strength, allow for precise control over the modulation of drug release profiles. Encasing drug molecules within these fluidic phases offers shielding from degradation and supports a prolonged, sustained release. The adjustability of complex coacervates, attained by thoughtfully choosing polymers conducive to coacervate formation and manipulating environmental factors, permits tailoring of release kinetics to fulfill distinct therapeutic needs. Moreover, the responsiveness of complex coacervates to environmental cues presents possibilities for precise drug delivery, guaranteeing the release of therapeutic payloads at the intended site of action. This summary underscores the potential of complex coacervation as a versatile and promising method for accomplishing controlled drug delivery across various biomedical applications.

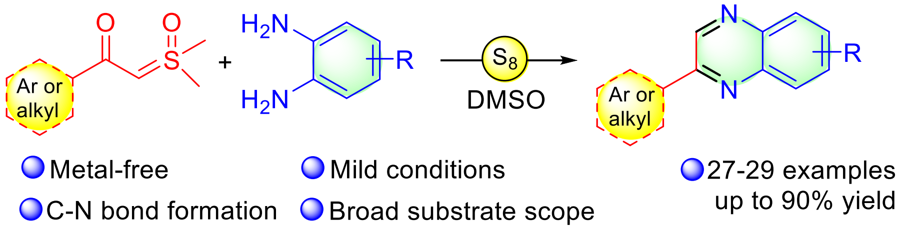


PP-39

Elemental Sulfur-Mediated Synthesis of Quinoxalines from Sulfoxonium Ylides

Trayambek Nath Chaubey, *Paran J. Borpatra and Satyendra Kumar Pandey**
Department of Chemistry, Banaras Hindu University, Varanasi 221005, India
Email: skpandey.chem@bhu.ac.in

A novel metal-free sulfur assisted synthetic protocol for the synthesis of Quinoxalines derivatives has been developed This protocol involves the reaction of *β*-ketosulfoxonium ylide and *o*-phenylenediamine at room temperature. The *o*-phenylenediamines and sulfoxonium ylides adorned with various functional groups provided moderate to high yields of quinoxaline derivatives and were well tolerated because of the straightforward and mild reaction conditions. Certain biologically active compound has also been synthesized by using the quinoxaline derivatives to investigate the potential applicability of our approach. Furthermore, certain pyrazine derivatives have also been synthesized with the same process.[1] The specifics of the findings will be shared at the poster presentation session.



References:

1. Chaubey, T. N.; Borpatra, P. J.; Pandey, S. K. *Org. Lett.* **2023**, *25*, 5329–5332.

PP-40

Synergistic WS_2@Chitosan Nanocomposites based Electrochemical Platform for Nonenzymatic Histamine Detection

*Diksha Singh and Jay Singh**

Department of Chemistry, Institute of Sciences, Banaras Hindu University Varanasi Utter Pradesh -221005

*(*E-mail- jaysingh.chem@bhu.ac.in)*

Histamine, a pivotal chemical within certain cells of the human body, is responsible for eliciting various allergic symptoms such as sneezing and a runny nose. In cases of allergies, where the immune system misidentifies typically harmless substances like certain foods or dust as harmful, the need for an efficient histamine sensor becomes imperative. This research introduces a novel sensing platform by employing a hybrid material comprising hydrothermally synthesized WS_2 nanoparticles and chitosan (CS) biopolymer on a screen-printed carbon electrode. The integration of WS_2 and CS components enhances conductivity and various sensor properties synergistically. The resulting WS_2/CS nanocomposites were subjected to thorough characterization, including phase identification, determination of crystalline size, and assessment of surface morphology. The WS_2/CS nanocomposites were drop-casted onto the screen-printed electrode (SPE), forming a modified WS_2/CS/SPE electrode for histamine detection using Differential Pulse Voltammetry (DPV). Histamine measurements were conducted within a linear range of 1-100 µM, with a detection limit of 0.0844 µM and sensitivity of 1.44×10^{-4} mA/µM cm^2. The developed sensor exhibited notable levels of sensitivity, selectivity, stability, and repeatability, along with an extended linear range. The findings recommend the utilization of electrochemical sensing on modified WS_2/CS/SPE electrodes for accurate histamine detection.

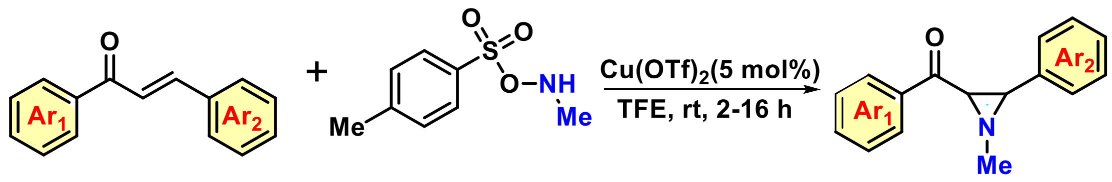
Keywords- CS, Histamine, SPE, WS_2.

PP-41

Direct N-Me Aziridination of Enones

Ashirwad Divedi, Dr. Jawahar L. Jat
Department of Chemistry, School of Physical and Decision Sciences
Babasaheb Bhimrao Ambedkar University (A Central University)
Lucknow, UP, India, 226025
Email-jawaharlj@bbau.ac.in, ashirwad515@gmail.com

Aziridines are often found as key intermediates in the synthesis of amine building blocks, chiral auxiliaries, industrially crucial monomers, and medicinally important compounds. N-H/N-Me aziridines containing molecules such as mitomycins, azicemicins, azinomycins, aziridonin, ficellomycin, and apoziquone shows anti-tumor activity. They are also used as reactive intermediates in organic synthesis for attaining sundry of nitrogen-containing products. Herein we report the first and direct N-Me aziridination of enones using TsONHMe (N-methyl-O-tosylhydroxylamine) as nitrogen source and $Cu(OTf)_2$ as catalyst in TFE solvent. This mild, one pot and operationally simple aziridination process provides a wide range of N-Me aziridines in good to excellent yields and diastereoselectivity. The reaction is supposed to proceed via Aza-MIRC (Aza-Michael Initiated Ring Closer) pathway.



- **First process for direct N-Me aziridination of enones**
- **Mild and operationally simple procedure.**
- **Broad substrates scope**
- **Good to excellent Yield.**

Keyword: Enones, Aziridine, TsONHMe, $Cu(OTf)_2$.

Reference: Jawahar L. Jat, Ajay K. Yadav, Chandra Bhan Pandey, Dinesh Chandra, Bhoopendra Tiwari. Direct N-Me Aziridination of Enones. *The Journal of Organic Chemistry* **2022**, *87* (5), 3751-3757

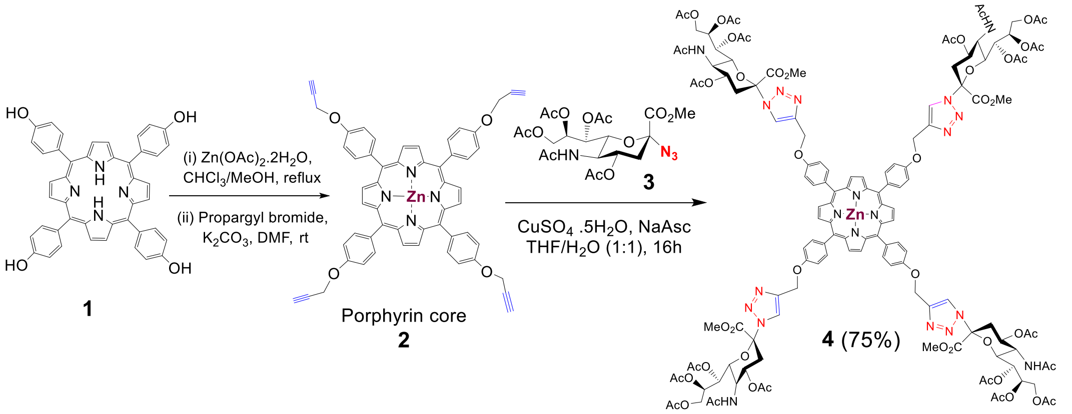
CuAAC 'Click' inspired Synthesis of Sialo-Dendrimer and its Biological Application

*Vinay K Pandey, Manoj K. Jaiswal and Vinod K Tiwari**

Department of Chemistry, Institute of Science, Banaras Hindu University, Varanasi, India

Email: vinaypandeyau@gmail.com

Sialic acids are a family of 9-carbon carboxylate saccharides involved in many important biological processes such as anticancer, antivirals, and antiulcers etc. [1] The SARS-CoV-2 gains its foothold to the host cell surface first via attachment factors (e.g., sialic acid, heparan sulphate, etc.) and then specific receptors (e.g., angiotensin-converting enzyme 2 (ACE2), neuropilin-1) through interactions with its spike viral glycoprotein (S protein). [2] Furthermore, CuAAC Click Chemistry has been well explored in glycol-science for various emergin application including glycol-dendrimer synthesis.[3] Toward this end, we introduce triazole at the C-2 position of sialic acid via introducing an azide group **3** high yielding step. Then, we coupled a porphyrin core **2** by treating it with azide **3** under CuAAC Click Condition to deliver sialo-dendrimer with 75 % yield **4** (**Scheme 1**). In recent year, the respiratory syndrome coronavirus-2 (SARS-CoV-2) is a significant threat to human health and societies across the globe. The effect of sialic acids on SARS-CoV-2 binding and suggests that effective inhibition of virus binding to its receptor can lead to a significant drop in infectivity [4]. The developed sialo-dendrimer **4** exhibited promising binding affinity against SARS-CoV-2.



Scheme 1. Click chemistry inspired synthesis of porphyrin cored sialo-dendrimer **4**.

Acknowledgment: This work was supported and grant awarded by the DST-SERB project, New Delhi for funding to laboratory and IoE BHU.

Reference:

1. (a) Carmi, C.; Cavazzoni, A.; Zuliani, V.; Lodola, A.; Zuliani, V.; Bordi, F.; Plazzi, P. V.; Alfieri, R. R.; Petronini, P. G.; Mor, M. Bioorg. Med. Chem. Lett. **2006**, *16*, 4021–4025.
2. (a) Allen, J. D.; Watanabe, Y.; Chawla, H. Newby, M. L. Crispin, M. J. Mol. Biol. **2021**,*433*, 166762.; (b) Yan, R. et al. Science., **2020**, *367*, 1444.
3. (a) Bose, P; Jaiswal, MK; Singh, SK; Singh, RK; Tiwari, VK Carbohydrate Res., **2023**, 108804; (b) VK Tiwari, et al., Chem Rev, **2021**, 7638-7956; (c) VK Tiwari, Chem. Rec., **2021**, 21, 3029-3048; (c) Kushwaha, D; Tiwari, VK. J. Org. Chem., **2013**, *78*, 8184.

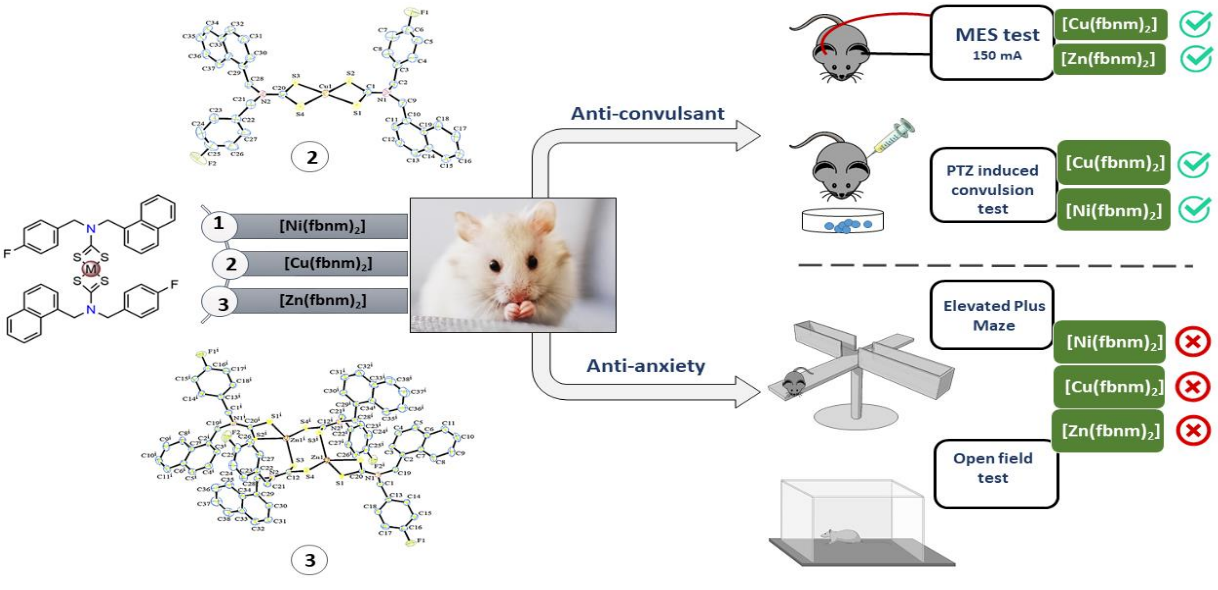
4. Simon, J. L.; Petitjean.; Ravikumar, Jimmidi.; Jinsung Yang.; Danahe, Mohammed.; Steeve, Boulant.; Stéphane P. Vincent and David Alsteens.;Nature Communications, **2022,***13*, 2564.

PP-43

Synthesis, crystal structure and screening for anticonvulsant and antianxiety activities of three new Ni(II), Cu(II), and Zn(II) dithiocarbamate complexes

Anupam Singh[a], *Lal Bahadur Prasad*[a]*
[a]*Department of Chemistry, Institute of Science, Banaras Hindu University, Varanasi 221005, India*
**Corresponding authors Email: lbprasad@bhu.ac.in*

A potassium N-(4-fluorobenzyl) N-(naphthalen-1-ylmethyl) dithiocarbamate ligand (fbnm) has been isolated in a basic medium and its Ni(II), Cu(II), and Zn(II) complexes 1-3 were synthesized. All new compounds have been characterized by elemental analyses, magnetic susceptibility, IR, NMR, and UV-Vis techniques. Complexes 2 and 3 have been further characterized by single-crystal X-ray diffraction data. Zn(II) complex adopts tetrahedral geometry whereas Ni(II) and Cu(II) complexes adopt square planer geometry around the metal ions. Complexes 2 and 3 are stabilized by intermolecular C-H⋯S, C-H⋯π and CH⋯F interactions. The thermal degradations of metal complexes 1-3 have been examined by TG-DTA data which designates that metal sulfide is formed as the final entity. The anticonvulsant activity of ligand fbnm and its Ni(II), Cu(II), and Zn(II) complexes have been tested through the MES test and PTZ-induced convulsion test and found that complex (2) may be used as an anticonvulsant compound in the future by further biochemical or neurotransmitter estimations to control the onset of generalized tonic-clonic seizures. The antianxiety activity has also been performed via Elevated plus maze and Open field test and observed that all synthesized compounds are non-significant for anti-anxiety effect[1].



Keywords: Dithiocarbamate**;** crystal structures; TGA; anticonvulsant & antianxiety activity.

Reference

1 A. Singh, R. Kumar, K. Shiv, S. K. Pandey, M. K. Bharty, R. J. Butcher and L. B. Prasad, *J Mol Struct*, 2024, **1298**, 137052.

PP-44

Facile Synthesis of 2D Magnesium Oxide Nanosheets for Non-Enzymatic, Selective and Sensitive Electrochemical Detection of Hydrogen Peroxide

Surbhi Sharma and Debanjan Guin
Department of Chemistry, Institute of Science, Banaras Hindu University, Varanasi, India
E-mail: surbhisharma1606@gmail.com

A breakthrough in sensor technology has led to the development of an enzyme-free sensor, designed on a glassy carbon electrode (GCE) platform, featuring 2-dimensional nanoporous magnesium oxide nanosheets (MgO-NSs). MgO-NSs were successfully synthesized through a single-step, non-hazardous, and cost-effective, sugar-blowing technique. The microstructure, porosity, thermal stability, and morphology of MgO-NSs were analyzed under XRD, FT-IR, FESEM, HR-TEM, TGA, and BET surface area. The electrochemical properties of the MgO-NSs/GCE were investigated for their sensing capabilities towards hydrogen peroxide (H_2O_2) using CV, DPV, EIS, and amperometry techniques at varying concentrations, different pH values and different scan rates. The fabricated electrode exhibited outstanding selectivity, high sensitivity, and a linear response to H_2O_2 in a wide concentration range (20 μM – 1000 μM) at neutral pH, with a low limit of detection (LOD) of 0.224 μM and a limit of quantification (LOQ) of 0.753 μM. The proposed electrochemical sensor based on MgO-NSs/GCE offers multiple advantages, including exceptional sensitivity, high selectivity, stability, reproducibility, and excellent performance towards the detection of hydrogen peroxide in real samples.

References

1. **Sharma, S.,** et al., *Fabrication of a non-enzymatic electrochemical sensor based on magnesium oxide nanosheets for selective and sensitive detection of hydrogen peroxide in food samples.* Journal of Applied Electrochemistry, 2023: p. 1-13.
2. Liu, S., et al., *Mesoporous magnesium oxide nanosheet electrocatalysts for the detection of Lead (II).* ACS Applied Nano Materials, 2019. **2**(5): p. 2606-2611.
3. Nguyen, H.V., et al., *Electrochemical sensing of etoposide using carbon quantum dot modified glassy carbon electrode.* Analyst, 2016. **141**(9): p. 2665-2675.
4. Salazar, P., et al., *One-step green synthesis of silver nanoparticle-modified reduced graphene oxide nanocomposite for H2O2 sensing applications.* Journal of Electroanalytical Chemistry, 2019. **855**: p. 113638.

PP-45

Determination of Critical Aggregation Concentration of Surfactants and Ionic Liquids by Probing Hydrogen-Bonded Water Structure using Raman and Hyper-Raman Spectroscopy

Krishanu Bandyopadhyay, Abhineet Verma, Surajit Maity, Satyen Saha
Department of Chemistry
Banaras Hindu University (BHU), Varanasi, India

Micelles, well-established supramolecular structures, contrast with the relatively recent exploration of micro-heterogeneity in Ionic Liquids (**ILs**), owing to the challenges in accurately estimating aggregation concentration. Several electrochemical and analytical methods, such as conductometry, potentiometry, UV-Visible, fluorescence, and NMR spectroscopy, have been employed for aggregation concentration determination. However, these methods may lack precision, leaving gaps in molecular-level insights. In this study, we introduce Raman spectroscopy as a novel analytical tool to determine the aggregation concentration of prominent surfactants (**CTAB**, **SDS**, **TX-100**) and imidazolium-based Ionic Liquids with varying chain lengths ($n = 4$ to 10) in a 20% ethanol-water (**EW**) solution. Our findings reveal that water in 20% **EW** forms a more stable hydrogen-bonded network structure. By examining the strongly hydrogen-bonded O-H stretching mode of water at different concentrations of surfactant/ionic liquid, a sudden drop in the O-H stretching mode intensity occurs at a specific concentration. This phenomenon is attributed to the disruption of the strongly hydrogen-bonded water structure due to micelle formation. Hyper-Raman spectroscopy, another non-linear spectroscopic method, strongly supports these results. Consequently, our study provides a molecular-level understanding of changes in water structure in the presence of surfactants/ionic liquid, enabling accurate measurement of Critical Aggregation Concentration (**CMC**) in a 20% **EW** solution.

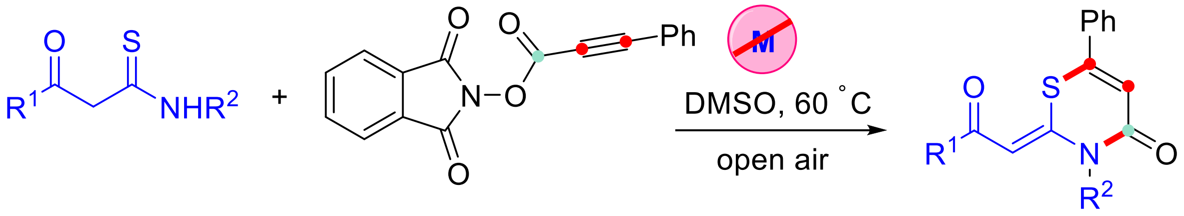
PP-46

Metal-free [3+3] heteroannulation of thioamides with alkynyl NHPI-esters to access 2*H*-1,3-thiazin-4(3*H*)-ones

*Ganesh Kumar, Monish Arbaz Ansari, and Maya Shankar Singh**

The first chemo- and regioselective one-pot convergent synthesis of 2*H*-1,3-thiazin-4(3*H*)-ones has been successfully realized employing □-ketothioamides and alkyne derivatives of N-hydroxyphthalimide (NHPI)-ester under mild conditions in good to excellent yields. The process is triggered by the *in-situ* generation of dienolate intermediate followed by intramolecular selective N-cyclization. Remarkably, metal- and additive-free conditions, an open atmosphere, non-hazardous reagents, and easy purification are added characteristics to this cascade [3+3] annulative strategy. This heteroannulative approach will not only provide an effective method to access various 1,3-thiazin-4-ones but also augment the research domain of thioamides.

[3+3] Heteroannulative cascade coupling *via* ester C-O bond cleavage



Operationally simple, C-S & C-N new bonds, 32 examples, yield up to 82%

Keywords: Heteroannulation; Thioamides; NHPI-esters; Metal-free; Thiazinones.

PP-47

FRET based Charge Transfer in PDY-132:F8T2 Polymer Blend for OLED

Dr Surendra K. Yadav*[1], *Dr Jay Singh*[1,]
[1]*Department of Chemistry, Institute of Science, Banaras Hindu University, Varanasi, 221005, UP, Bharat*
*Corresponding Author *Surendraky@gmail.com*

PDY-132 and its blend with different concentrations of Poly (9,9-dioctylfluorenyl-co-3 bithiophene) F8T2 employed as an emissive matrix for Organic Light-Emitting Devices (OLEDs). The Urbach energy lies well below 50 meV, reflecting the reduced energetic disorder signifies the efficient charge transfer in polymer blends. The photoluminescence time constants vary proportionally 0.89 ns - 0.35 ns as a function of acceptor concentration in FRET pairs, reflecting 2.5x faster charge transfer in blends than PDY-132. Förster radius 57 Å, decay time 0.89 ns, quenching constant 0.12 μM^{-1}, quenching rate constant 1.4×10^{8} $\mu M^{-1} * s^{-1}$, charge transfer lifetime 6.21 ns to 2.38 ns, and non-radiative transfer rate 4.0×10^{8} s^{-1} exhibit excellent parameters for efficient charge transfer within the blend resulted in lowering turn on voltage 67% from 6.5 V to 2 V. The current density 3 mA/cm^2 increases to 25 mA/cm^2, 8x with increasing the concentration of F8T2.

Keywords: OLED; Turn on voltage; FRET; lifetime; Urbach Energy.

References

1. Noriega, R.; Rivnay, J.; Vandewal, K.; Koch, F. P. V.; Stingelin, N.; Smith, P.; Toney, M. F.; Salleo, A., A general relationship between disorder, aggregation and charge transport in conjugated polymers. Nature Materials 2013, 12 (11), 1038-1044.
2. Heeger, A. J., Semiconducting and Metallic Polymers: The Fourth Generation of Polymeric Materials (Nobel Lecture). Angewandte Chemie International Edition 2001, 40 (14), 2591-2611.
3. Sirringhaus, H.; Tessler, N.; Friend, R. H., Integrated Optoelectronic Devices Based on Conjugated Polymers. Science 1998, 280 (5370), 1741-1744. 4.
4. Reineke, S.; Lindner, F.; Schwartz, G.; Seidler, N.; Walzer, K.; Lessem, B.; Leo, K., White organic light-emitting diodes with fluorescent tube efficiency. Nature 2009, 459 (7244), 234-238.

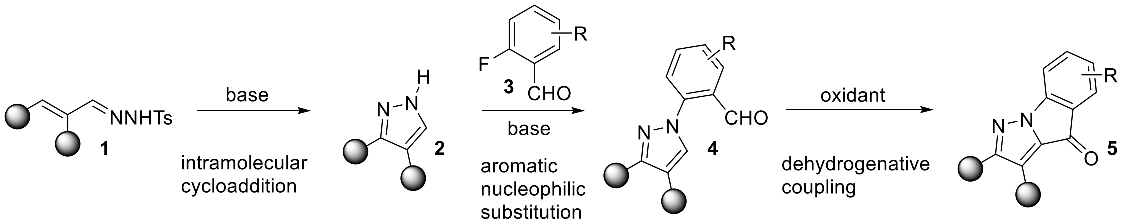
PP-48

One-pot Synthesis of Pyrazoloindolones via Base Promoted Intramolecular Oxidative Cyclization Under Aerobic Conditions

Harshita Singh Korawat, *Ashok K. Basak**

Department of Chemistry, Institute of Science, Banaras Hindu University, Varansi-221005

Pyrazole fused heterocyclic compounds have been evaluated to exhibit antileishmanial efficacy and act as inhibitors of phosphoinositide 3-Kinase γ (PI3Kγ).[1] They are also considered as potential candidates for the treatment of Alzheimer's and Parkinson's diseases.[2] This report describes the one-pot synthesis of novel pyrazoloindolones from *N*-sulfonylhydrazones for the first time. The synthesis relies upon base promoted intramolecular [3+2]-cycloaddition, intermolecular C-N coupling with 2-fluorobenzaldehydes and crucial intramolecular oxidative cyclization reaction under aerobic conditions. Our method provides access to wide variety of novel pyrazoloindolones which might be useful in medicinal chemistry research. We have also demonstrated that synthesized pyrazoloindolones can be further functionalized under standard reaction conditions.



References:

(1) (a) de Mello, H.; Echevarria, A.; Bernardino, A. M.; Canto-Cavalheiro, M.; Leon, L. L. Antileishmanial Pyrazolopyridine Derivatives: Synthesis and Structure−Activity Relationship Analysis. *J. Med. Chem*. **2004**, *47*, 5427–5432. (b) Sekikawa, I.; Nishie, J.; Tono-oka, S.; Tanaka, Y.; Kakimoto, S. Antituberculous compounds. XXVIII. Synthesis of pyrazolopyridines. *J. Heterocyclic Chem*. **1973**, *10*, 931–932.

(2) Tucker, T. J.; Sisko, J. T.; Tynebor, R. M.; Williams, T. M.; Felock,P. J.; Flynn, J. A.; Lai, M.-T.; Liang, Y.; McGaughey, G.; Liu, M.; Miller, M.; Moyer, G.; Munshi, V.; Perlow-Poehnelt, R.; Prasad, S.; Reid, J. C.; Sanchez, R.; Torrent, M.; Vacca, J. P.; Wan, B.-L.; Yan, Y. Discovery of 3-{5-[(6-Amino-1*H*-pyrazolo[3,4-*b*]pyridine-3-yl)methoxy]-2-chloro phenoxy}-5-chlorobenzonitrile (MK-4965): A Potent, Orally Bioavailable HIV-1 Non-Nucleoside Reverse Transcriptase Inhibitor with Improved Potency against Key Mutant Viruses. *J. Med. Chem*. **2008**, *51*, 6503–6511.

Synthesis and crystal structure of new transition metal complexes of ferrocene functionalized dithiocarbamate-dipyrromethene ligands.

Dr. Santosh K. Singh *

Department of Chemistry, Hari Prasad Sah College
Nirmali, Supaul-847452
Bihar
Email: *singhsantosh39@gmail.com, sksinghhps@gmail.com*

The transition metal complexes of dithiocarbamate ligands have been extensively studied because of their diverse coordination chemistry, conducting, magnetic and optical properties and industrial applications. Heteroleptic transition metal complexes [M(Fcdpm)(Fcdtc)] (M=Ni **1**, Pd **2**; Fcdpm = 5-Ferrocenyl dipyrromethene Fcdtc = N-ferrocenylmethyl-N-furfuryl dithiocarbamate) have been prepared and characterized by elemental analysis, IR, 1H and 13C NMR and UV–vis. spectroscopy. Their structures have been elucidated by X-ray crystallography.

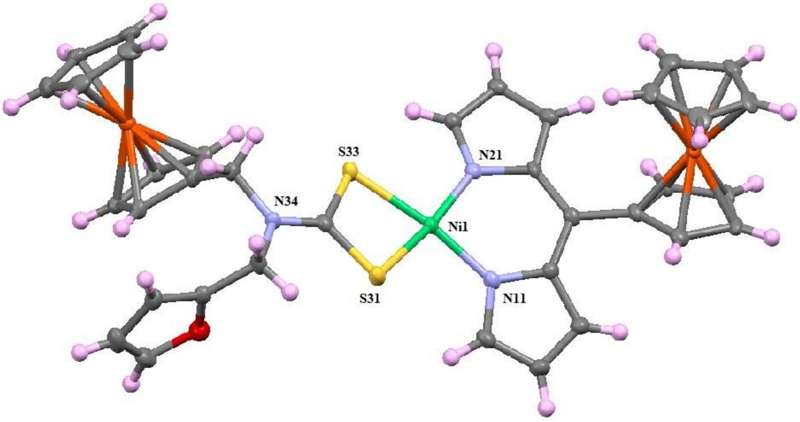


Fig. Structure of complex **1**.

Reference:

1. D. Coucouvanis, *Prog. Inorg. Chem.*, 1979, **26**, 301..
2. Santosh K. Singh, Vinod Kumar, Michael G.B. Drew, Nanhai Singh, *Inorg. Chem. Commun.,* **2013**, 37, 151.
3. Kiran Diwan, Bandana Singh, Santosh K. Singh, Michael G. B. Drew and Nanhai Singh, *Dalton Trans.*, **2012**, 41, 367.
4. B. Singh, M.G. B. Drew, G. K. Kohn, K.C. Molloy and N. Singh, *Dalton Trans.*, **2011**,40, 623.

PP-50

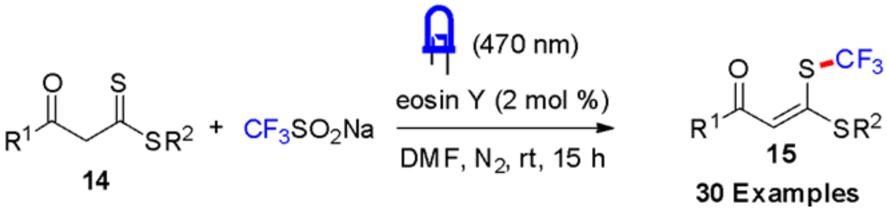
HAT and Complementing MS-CPET Strategy of Eosin-Y in Visible-Light-Photocatalysis

Sonam Soni*

Department of Chemistry, Sunbeam Women's College Varuna, Varanasi

Email- sonamsoni.bhu@gmail.com.

A photoinduced method has been developed for the metal- and oxidant-free trifluoromethylation of β-ketodithioesters, specifically targeting thioxo sulfur, at room temperature. The process demonstrates notable Z/E-stereoselectivity using the cost-effective Langlois' reagent (sodium triflinate, CF_3SO_2Na) in the presence of Eosin Y, functioning as a hydrogen atom transfer (HAT) catalyst. The reaction progresses through a disulfide intermediate, disulfanediylbis(3-(alkylthio)-1-phenylprop-2-en-1-one) (a dimer of β-ketodithioester), followed by a reverse hydrogen atom transfer (RHAT) cycle facilitated by Eosin Y. This straightforward and efficient procedure offers a direct pathway to trifluoromethylated α-oxoketene dithioacetals, yielding good to excellent results and accommodating various synthetically valuable functional groups with different electronic and steric properties.



Reference:

- Soni, S., Pali, P., Ansari, M. A., & Singh, M. S. (2020). Visible-light photocatalysis of Eosin Y: HAT and complementing MS-CPET strategy to trifluoromethylation of β-ketodithioesters with Langlois' reagent. *The Journal of Organic Chemistry*, *85*(15), 10098-10109.

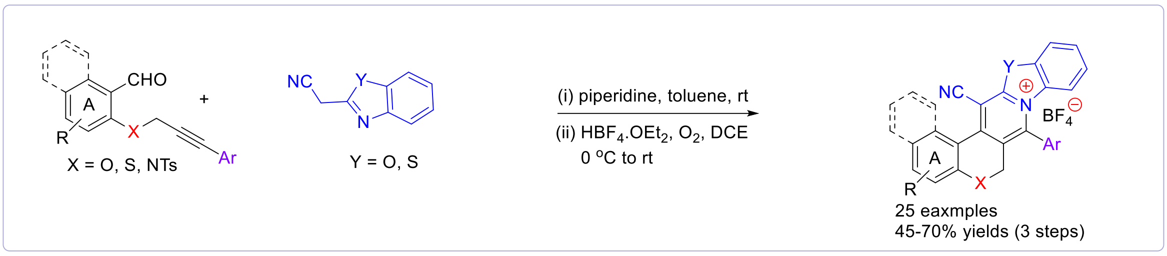
PP-51

Synthesis of azonia aromatic heterocycles bearing 6-6-6-5-6 pentacyclic core via intramolecular [4+2]-cycloaddition and oxidative aromatization reaction sequence in one-pot

*Karmdeo Prajapati, Manoj Kumar Saini, Ashok K. Basak**

Department of Chemistry, Institute of Science, Banaras Hindu University, Varanasi-221005

Cationic aza-heterocycle-fused compounds have gained wide applications in material science, biological applications, and synthetic organic chemistry.[1] In this report, synthesis of benzothiazolochromenopyridinium tetrafluoroborates, a novel molecular scaffold, bearing 6-6-6-5-6 pentacyclic core is described that proceeds via (i) piperidine catalyzed Knoevenagel condensation between 2-propargyloxyarylaldehydes bearing internal alkynes and 2-benzothiazoleacetonitrile (ii) intramolecular formal [4+2]-cycloaddition and (iii) crucial molecular oxygen mediated oxidative aromatization reaction sequence in one-pot.[2] These quaternary pyridinium salts are obtained at ambient temperature under transition-metal-free conditions in good to high yields.



Keywords: novel azonia heterocycle synthesis, 6-6-6-5-6 pentacyclic core, one-pot metal-free synthesis, molecular oxygen as green oxidant

References:

1. (a) Jortzik, E.; Zocher, K.; Isernhagen, A.; Mailu, B. M.; Rahlfs, S.; Viola, G.; Wittlin, S.; Hunt, N. H.; Ihmels, H.; Becker, K. *Antimicrob. Agents Chemother*. **2016**, *60*, 115−125. (b) Bhadra, K.; Kumar, G. S. *Med. Res. Rev.* **2011**, *31*, 821−862. (c) Pinheiro, G. E. G.; Ihmels, H.; Dohmen, C. *J. Org. Chem.* **2019**, *84*, 3011−3016. (d) Toriumi, N.; Asano, N.; Miyamoto, K.; Muranaka, A.; Uchiyama, M. *J. Am. Chem. Soc.* **2018**, *140*, 3858−3862. (e) Ohno, Y.; Ando, S.; Furusho, D.; Hifumi, R.; Nagata, Y.; Tomita, I.; Inagi, S. *Org. Lett*. **2023**, *25*, 3951−3955. (f) Yip, W.-M.; Yu, Q.; Tantipanjaporn, A.; Chan, W.-C.; Deng, J.-R.; Ko, B. C.-B.; Wong, M.-K. *Org. Biomol. Chem.* **2021**, *19*, 8507−8515. (g) Tantipanjaporn, A.; Kung, K. K.-Y.; Wong, M.-K. *Org. Lett.* **2022**, *24*, 5835−5839. (h) Bosch, P.; Marcelo, G.; Matamoros-Recio, A.; Sucunza, D.; Mendicuti, F.; Domingo, A.; Vaquero, J. J. *Dyes Pigm*. **2021**, *19*, 109443.
2. Saini, M. K.; Prajapati, K.; Basak, A. K.; *J. Org. Chem*. **2023** *(under minor revision).*

PP-52

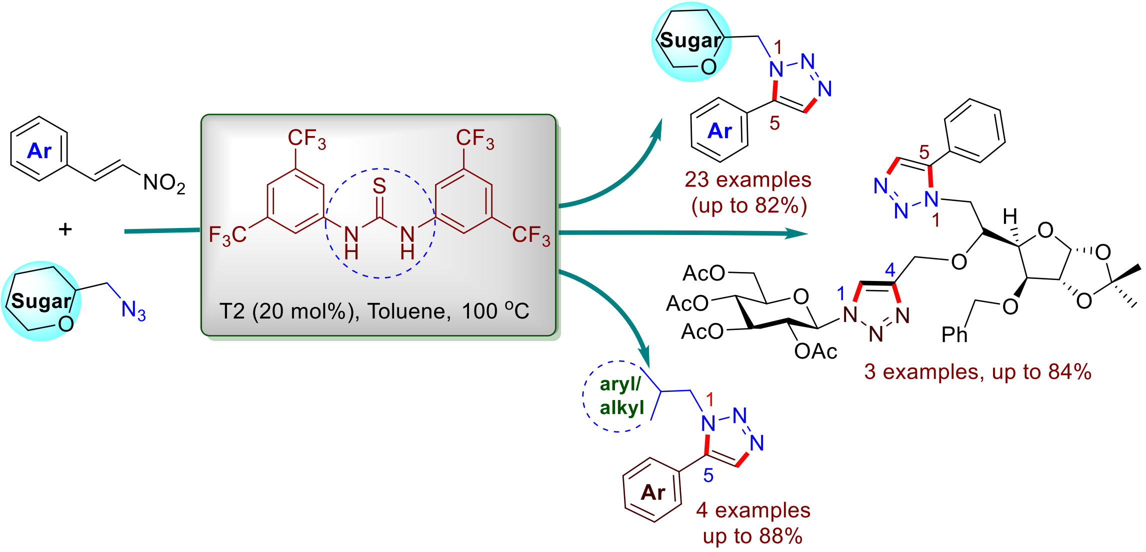
Organocatalyzed Regioselective Synthesis of 1,5-Disubstituted 1,2,3-Triazolyl Glycoconjugates

*Manoj K. Jaiswal, Mayank Singh, and Vinod K. Tiwari**

Department of Chemistry, Institute of Science, Banaras Hindu University, Varanasi-221005, INDIA

**e-mail: manoj.1991jaiswal@gmail.com, manoj_chem@bhu.ac.in*

Just after the invention of 'Click Chemistry' in 2002, the regioselective 1,2,3-triazole scaffolds have been well recognized as the functional heterocyclic core at the centre of modern organic chemistry, medicinal chemistry, and material sciences.[1] A novel organocatalyzed [3+2] cycloaddition reaction of nitroolefins with glycosyl azides has been developed for successful construction of 1,5-disubstituted triazolyl glycoconjugates.[2] This metal and acid-free, regioselective synthetic protocol proceeds in the presence of only Schreiner thiourea organocatalysts, which enable the required activation of nitroolefins through double hydrogen bonding. The straightforward, operationally simple, and regioselectivity of this methodology, complementing to the classical RuAAC catalyzed synthesis of 1,5-disubstituted 1,2,3-triazoles. In the presence of catalytic amount of Schreiner thiourea, organic azides react with a broad array of nitroolefins producing a series of 1,5-disubstituted 1,2,3- triazoles in good yields.



References:

1. (a) V. K. Tiwari, *Chem. Rec.*, **2021**, *21*, 3029. (b) Agrahari, A. K.; Bose, P.; Jaiswal, M. K.; Rajkhowa, S.; Singh, A. S.; Hotha, S.; Mishra, N.; Tiwari, V. K. *Chem. Rev.* **2021**, *12*, 7638-7956; (c) Tiwari, V. K. *et al. Chem. Rev.* **2016**, *116*, 3086-3240.
2. Jaiswal, M. K.; Gupta, A.; Yadav, M. S.; Pandey, V. K.; Tiwari, V. K. *Chem. Eur. J*, **2023**, *29*, e202301749.

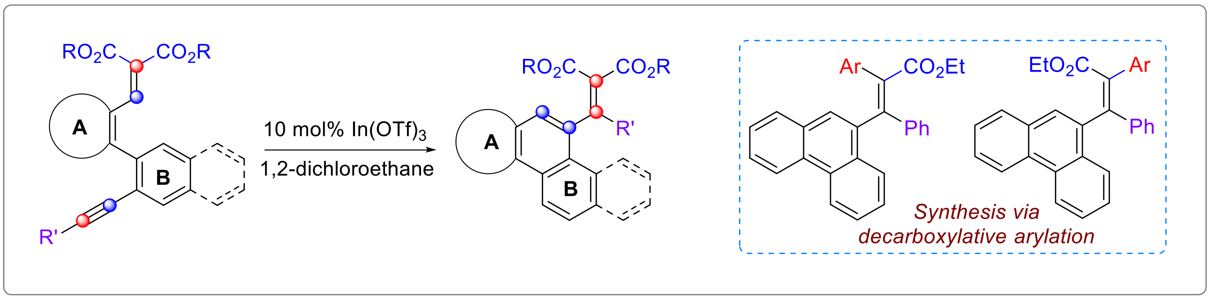
PP-53

Expeditious Synthesis of Functionalized Polycyclic (Hetero)aromatic Compounds via In(OTf)$_3$-Catalyzed Cycloisomerization of Enyne Diesters Derived from Biaryls and Related Substrates

Manoj Kumar Saini, *Ashok K. Basak**

Department of Chemistry, Institute of Science, Banaras Hindu University, Varanasi-221005

Polycyclic aromatic compounds have broad utility in core organic chemistry, materials science, and pharmaceuticals.[1] Consequently, development of efficient strategies for the synthesis of polycyclic aromatic compounds attracted interest of synthetic organic chemists worldwide. Herein, In(OTf)$_3$-Catalyzed cycloisomerization reaction is demonstrated as a versatile and highly efficient tool for the synthesis of functionalized polycyclic (hetero)aromatic compounds bearing a synthetically useful diethyl β-(hetero)arylidene malonate moiety in a step- and atom-economic manner.[2] This enyne metathesis type cycloisomerization reaction enables the synthesis of phenanthrene, benzophenanthrene, benzotetraphene, and other polycyclic (hetero)aromatic compounds. Moreover, a new avenue for the construction of triaryl groups containing all carbon tetrasubstituted olefins via Pd-catalyzed decarboxylative arylation is also demonstrated.



Keywords: Catalytic cycloisomerization of enyne diesters, Enyne metathesis, Polycyclic (hetero)aromatic compounds, Tetrasubstituted olefin synthesis.

References:

1. (a) Y. Zhang, S. H. Pun, Q. Miao, *Chem. Rev.* **2022**, *122*, 14554. (b) A. Borissov, Y. K. Maurya, L. Moshniaha, W.-S. Wong, M. Żyła-Karwowska, M. Stępień, *Chem. Rev.* **2022**, *122*, 565. (c) D. Bandyopadhyay, J. C. Granados, J. D. Short, B. K. Banik *Oncol. Lett.* **2012**, 3, 45. (d) F. F. Becker, B. K. Banik, *Front. Chem.* **2014**, *2*, 55. (e) D. Bandyopadhyay, J. L. Sanchez, A. M. Guerrero, F.-M. Chang, J. C. Granados, J. D. Short, B. K. Banik, *Eur. J. Med. Chem*. **2015**, *89*, 851. (f) E. M. Malik, C. E. Müller, *Med. Res. Rev*. **2016**, *36*, 705. (g) D. Kong, T. Cai, H. Fan, H. Hu, X. Wang, Y. Cui, D. Wang, Y. Wang, H. Hu, M. Wu, Q. Xue, Z. Yan, X. Li, L. Zhao, W. Xing, *Angew. Chem. Int. Ed.* **2022**, *61*, e202114681. (h) N. Zhang, L. Yang, W. Li, J. Zhu, K. Chi, D. Chang, Y. Qiao, T. Wang, Y. Zhao, X. Lu, Y. Liu, *J. Am. Chem. Soc.* **2022**, *144*, 21521.
2. Saini, M. K.; Prajapati, K.; Sharma, R.; Basak, A. K. *Adv. Synth. Catal.* **2023**, *365*, 2211–2217.

PP-54

N-(4-fluorobenzyl) N-(pyridin-2-ylmethyl) derived transition metal dithiocarbamate complexes: Synthesis, characterization and Antihistaminic activity

KM Riya Patel[a], *Anupam Singh*[a], *Lal Bahadur Prasad*[a*]

[a]*Department of Chemistry, Institute of Science, Banaras Hindu University, Varanasi 221005, India*

**Corresponding authors Email: lbprasad@bhu.ac.in*

N-(4-fluorobenzyl) N-(pyridin-2-ylmethyl) dithiocarbamate ligand in the form of its potassium salt (KL) and its Co(III), Ni(II), Cu(II), Zn(II), and Cd(II) complexes (1-5) respectively have been synthesized and fully characterized by elemental analysis and various spectroscopic techniques like FTIR, UV-Vis, ^{1}H & ^{13}C NMR, and mass spectroscopy. Ligand (KL), complexes 1 and 2 were also characterized by single-crystal X-ray data. XRD data reveals the octahedral geometry of complex 1 around Co(III) center and the square planar geometry of complex 2 around Ni(II) center. The crystal structures of complexes 1 and 2 are also stabilized by various intermolecular and intramolecular interactions. Thermogravimetric analysis of complexes 1-5 has also been performed and suggests the formation of metal sulfide as the final decomposition product. The antihistaminic activity of Ligand-KL, and complexes1-5 were evaluated in mice using clonidine-induced catalepsy and haloperidol-induced catalepsy models. The results showed that these synthetic compounds have antihistaminic potential to inhibit clonidine-induced catalepsy, possess antihistaminic activity, and may be targeted for different allergic conditions.

Keywords: Dithiocarbamate; metal complexes; spectroscopy, thermogravimetric analysis; antihistaminic activity.

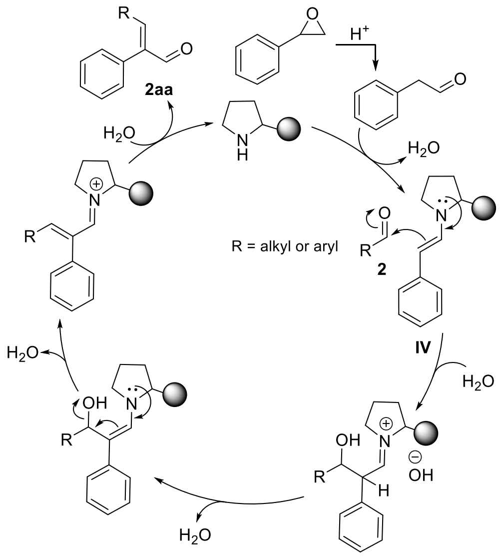
PP-55

Synthesis, characterization and anti-inflammatory activity of metal complexes derived from cyclohexyl and naphthalen-1-ylmethyl functionalized dithiocarbamate ligands

Trishna[a]*, Anupam Singh*[a]*, Lal Bahadur Prasad*[a*]
[a]*Department of Chemistry, Institute of Science, Banaras Hindu University, Varanasi 221005, India*
**Corresponding authors Email: lbprasad@bhu.ac.in (L. B. Prasad)*

Cyclohexyl and naphthalen-1-ylmethyl functionalized dithiocarbamate ligand in the form of its potassium salt (KL) has been synthesized and characterized. Further its transition metal Co(II), Ni(II), Cu(II), and Zn(II) complexes **1-4** have also been synthesized and characterized by elemental analysis and various spectroscopic techniques like FTIR, UV-Vis, ^{1}H & ^{13}C NMR, and mass spectroscopy. Ligand was also characterized by single crystal X-ray data. Magnetic moment values and d-d transition of complexes suggest tetrahedral geometry of Co(II) complex while square planar geometries of Ni(II) and Cu(II) complexes. The thermal degradations study of the complexes has been studied by thermogravimetric analysis (TGA) which indicates that metal sulfides is formed as final entity. The anti-inflammatory activity of Ligand-KL, and complexes1-4 at a concentration of 25 μg/ml, 50 μg/ml, 75 μg/ml and 100 μg/ml were evaluated using four in vitro-based assays i.e. hemolysis inhibition, proteinase inhibition, protein denaturation inhibition, and lipoxygenase inhibition using UV/VIS spectrometer at particular wavelength. The results were compared using standard drug, Ibuprofen at similar concentration. Cu(II) complex was found more significant towards the in-vitro anti-inflammatory activity out of the four above models.

Keywords: Dithiocarbamate; metal complexes; spectroscopy, thermogravimetric analysis; anti-inflammatory.



PP-56

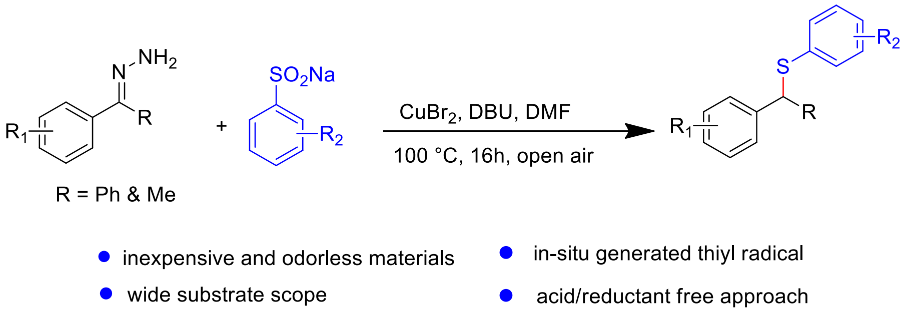
Copper-Catalyzed Thiolation of Hydrazones with Sodium Sulfinates: A Straightforward Synthesis of Benzylic Thioethers

*Aditya Rai, Anand Kumar Pandey, and Krishna Nand Singh**

Department of Chemistry, Institute of Science, Banaras Hindu University, Varanasi-221005, India.

<u>*Email*</u>*: - aadigzp@gmail.com*

A facile and sustainable protocol for the thiolation of hydrazones with sodium sulfinates has been developed in the presence of $CuBr_2$ and DBU in DMF to afford diverse benzylic thioethers (Scheme 1). Control experiments reveal a radical pathway involving a thiyl radical as a key intermediate.



Scheme 1 Synthesis of benzylic thioethers.

Reference: A. K. Pandey, S. Chand, A. K. Sharma, and K. N. Singh, *J. Org. Chem.* **2023**, *88,* 475-482.

PP-57

Triazine and Thiophene-Containing Conjugated Polymer Network Emitter-Based Solution-Processable Stable Blue Organic LEDs

Anamika, Biplab Kumar Kuila

Department of Chemistry, Institute of Science, Banaras Hindu University, Varanasi, U.P., India, 221005

Email: bkkuila.chem@bhu.ac.in

The development of solution-processable fluorescent materials with blue electroluminescence has recently attracted considerable research interest for organic light-emitting diode (OLED) applications. Whereas, conjugated polymer frameworks (CPF) have attained tremendous research interest due to their vast potential in a variety of cutting edge applications like photocatalysis[1], sensing[2], gas storage, energy storage[3], and so on. These framework materials, without sidechains or functional groups on their back bone, are generally insoluble in common organic solvents and less solution processable for electronic device applications[4,5]. Herein, we have reported two triazine based highly fluorescent and wide band gap donor-acceptor conjugated polymer framework (CPF) by coupling 3-substituted thiophene (donor) unit with triazine ring (acceptor) through a phenyl ring spacer.. OLEDs based on these CPF as emitter shows the maximum external quantum efficiency of 2.3 % with maximum brightness of 2541 cd/m^2 and a maximum current efficiency of 2.8 cd/A with blue emission.

References:

(1) Wada, Y.; Kubo, S.; Kaji, H. Adamantyl Substitution Strategy for Realizing Solution-Processable Thermally Stable Deep-Blue Thermally Activated Delayed Fluorescence Materials. Adv. Mater. 2018, 30, 1705641.

(2) Ghanem, B. S.; Swaidan, R.; Eric, L.; Pinnau, I. Ultra-Microporous Triptycene-based Polyimide Membranes for High-Performance Gas Separation. Adv. Mater., 2014, 26, 3688-3692.

(3) Ghasimi, S.; Prescher, S.; Wang, Z. J.; Landfester, K.; Yuan J. Y.; Zhang, K. A. I. Heterophase Photocatalysts from Water-Soluble Conjugated Polyelectrolytes: An Example of Self-Initiation under Visible Light. Angew. Chem. Int. Ed., 2015, 54, 14549 -14553.

(4) Bohra, H.; Li, P.; Yang, C.; Zhao, Y.; Wang, M. Greener" and modular synthesis of triazine-based conjugated porous polymers via direct arylation polymerization: structure–function relationship and photocatalytic application. Polym. Chem., 2018, 9, 1972-1982.

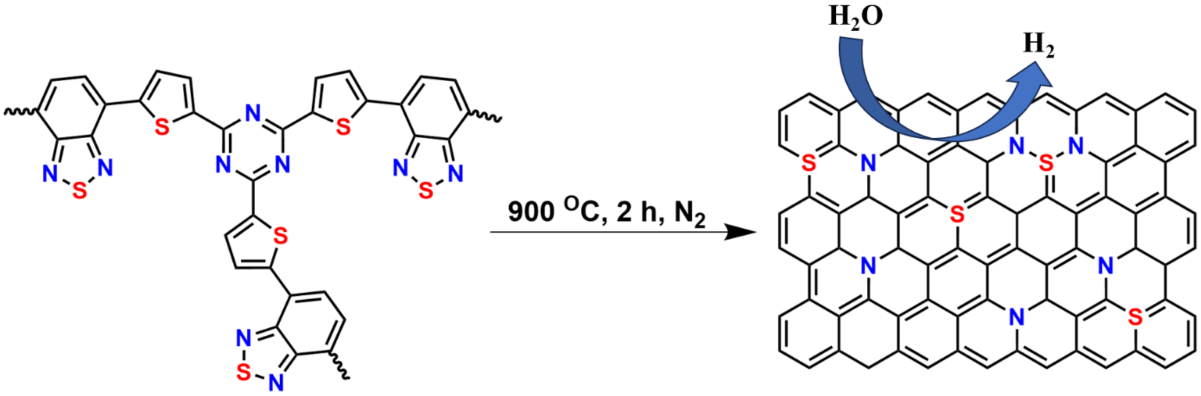
(5) Wang, L.; Zeng, C.; Xu, H.; Yin, P.; Chen, D.; Deng, J.; Li, M.; Zheng, N.; Gu, C.; Ma, Y. A highly soluble, crystalline covalent organic framework compatible with device implementation. Chem. Sci., 2019,10, 1023-1028.

PP-58

Nitrogen and sulphur Co-doped carbon material derived from conjugated porous polymer for Metal-free Hydrogen Evolution Reaction and Supercapacitor applications

Arpita Maurya, Biplab Kumar Kuila
Department of Chemistry, Institute of Science, Banaras Hindu University, Varanasi, Uttar Pradesh, 221005, India
Email: bkkuila.chem@bhu.ac.in

To cope with the developing and fast-changing energy storage needs and environment-friendly green fuels it is important to develop highly active materials for electrocatalytic and supercapacitor applications.[1,2] In the last few decades heteroatom-doped carbon materials have shown their superior activity for these applications.[3] Here, we have developed novel triazine and Benzothiazole-based conjugated polymer frameworks which are then graphitized at 900 ^{0}C temperature to yield N, S co-doped carbon. The prepared material then showed very good activity towards self-supported metal-free HER showing low overpotential and good taffel value. Along with this the N, S co-doped carbon materials also show its applicability for the energy storage application as supercapacitors. It has shown good capacitance even at high current densities with exceptional cyclic stability.



So, these types of materials are strong contenders for metal-free electrocatalysis and supercapacitor applications for future energy conversion and storage. The present study also sheds some light on designing better electrocatalysts and energy storage devices based on heteroatom-doped carbonized framework materials.

References:

1. Allen, M. R.; Frame, D. J.; Huntingford, C.; Jones, C. D.; Lowe, J. A.; Meinshausen, M.; Meinshausen, N. Warming Caused by Cumulative Carbon Emissions towards the Trillionth Tonne. *Nature* **2009**, *458* (7242), 1163–1166. https://doi.org/10.1038/nature08019.
2. Hoffert, M. I. Farewell to Fossil Fuels? *Science (80-.).* **2010**, *329* (5997), 1292–1294. https://doi.org/10.1126/science.1195449.
3. Hu, C.; Dai, L. Multifunctional Carbon-Based Metal-Free Electrocatalysts for Simultaneous Oxygen Reduction, Oxygen Evolution, and Hydrogen Evolution. *Adv. Mater.* **2017**, *29* (9), 1604942. https://doi.org/10.1002/adma.201604942.

PP-59

Mechanism deciphering interaction characteristics of the antidepressant drug trazodone with double stranded DNA: Multi-spectroscopic analysis

Ambrish Kumar[1], Moumita Saha[1], Kamalakanta Behera[2*], Shruti Trivedi[1]*
[1]Department of Chemistry, Intitute of Science, Banaras Hindu University, Varanasi-221005
[2]Department of Chemistry, University of Allahabad, Prayagraj.
*Corresponding author

Abstract

Deoxyribonucleic acid (DNA) is an important genetic substance in the organism, which plays an extremely significant role in the process of human life, such as gene expression, gene transcription, mutagenesis, and carcinogenesis. DNA is frequently the main molecular target for natural and synthetic organics. Trazodone (TZD) is a triazolopyridine derivative anti-depressant drug that inhibits the reuptake of serotonin and blocks histamine and alpha-1-adrenergic receptors. This research intends to lighten the interaction between TZD and sodium salt of salmon testis DNA by using molecular multi-spectroscopic techniques and help overcome the knowledge gap in pharmacokinetics. Interesting changes are observed in the characteristic UV-VIS spectra of DNA and Fluorescence spectra of TZD. From Circular dichroism Spectroscopy, it is evident that TZD has significantly changed the base pair stacking of DNA. Competitive study with minor groove binder displays no change, manifest TZD does not bind to DNA through the minor groove. An experiment with NaCl shows there is no ionic interaction between TZD and DNA as well. Titration of TZD in the presence and absence of DNA with KI quencher shows K_{sv} values 3.92 M^{-1} and 9.84 M^{-1} respectively, which proves intercalation binding of TZD drug. Titration of drug DNA complex against urea, a well-known DNA denaturing agent, also demonstrates the intercalatory nature of TZD.

Keywords: Anti-depressant, Drug-DNA interaction, DNA, Spectroscopy, Trazodone.

PP-60

Highly sensitive electrochemical sensor for individual and simultaneous detection of Pb (II) and Hg (II) ions based on ZnO modified g-C_3N_4 **nanocomposite**

Vikas Jangra[1]*, Narvadeswar*[2]*, Dr. Piyush Kumar Sonkar**[2]*, Dr. Lal Bahadur Parsad**[1]*,*
[1]*Department of Chemistry, Banaras Hindu University, Varansi-221 005, India*
[2]*Department of Chemistry, MMV, Banaras Hindu University,Varansi-221 005,*
**Correspondance : piyushchem.mmv@bhu.ac.in, lbprasad@bhu.ac.in*

Heavy metal contamination of the environment is a global concern primarily because these metals may accumulate in the human body and lead to major health issues. Therefore, it is crucial to have a reliable technique for determining the concentration of heavy metals. Herein, we have reported a reliable method for simultaneous detection of Pb^{2+} and Hg^{2+} ions by Differential Pulse Voltammetry (DPV) using glassy carbon electrode modified with a ZnO@**g-C_3N_4** nanocomposite. X-ray diffraction (XRD), Scanning electron microscopy (SEM), and Fourier transform infrared (FTIR) methods were used to investigate the morphology and structure. The electrochemical performance of the as-synthesized nanomaterial was characterized by cyclic voltammetry (CV), Differential Pulse Voltammetry (DPV) and impedance spectroscopy (EIS). ZnO@g-C_3N_4 nanocomposite demonstrated exceptional electrochemical performance with higher catalytic activity, lower working potential (-0.56 V) for Pb^{2+} and (0.25 V) Hg^{2+}, and low charge transfer resistance.

PP-61

Design, Synthesis And Characterization Of 1,3,5-Tris((arylselanyl)methyl) mesitylene Moieties

*Avinash Chaurasia, Shekhar Makar and Abhishek Kumar**

Department of Chemistry, Institute of Science, Banaras Hindu University, Varanasi-221005, Uttar Pradesh (India)

**** Corresponding Email:** abhi.chem@bhu.ac.in*

Organoselenium chemistry is now a well-established field of research and recent advances have been brought about by the potential applications of selenium compounds in the fields of organic synthesis, biochemistry, xerography, semiconductors and metal-ligand chemistry. The unique chemical and biological activity of organoselenium compounds also make them versatile and useful in the above mentioned applications. In this context multidentate organoselenium species and their metal complexes continues to be an active area of research in inorganic and organometallic chemistry. We have now successfully synthesized a series of flexible tridentate Se_3 type moieties bearing the formula 1,3,5-tris((arylselanyl)methyl) mesitylene. The synthesized compounds were characterized by various physicochemical techniques such as multinuclear (^{1}H, ^{13}C{^{1}H} & ^{77}Se) NMR, FTIR, UV-visible spectrophotometry and High resolution mass spectrometry. The synthesized moieties exhibit excellent binding affinity toward d^{10} metal ions such as Zn^{2+}, Cd^{2+}, Hg^{2+}.

References :-

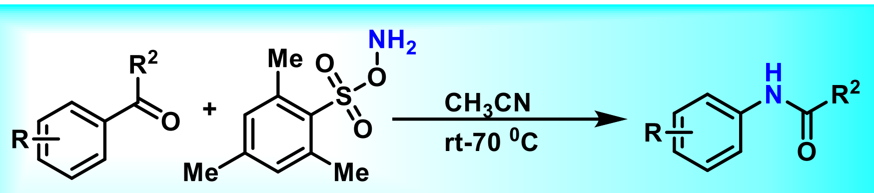
(1) Kumar, A.; Yadav, M. K.; Singh, J.; Butcher, R. J. *Dalton Transactions* **2019**, *48* (17), 5627–5636.
(2) Reich, H. J.; Hondal, R. J. *ACS Chemical Biology* **2016**, *11* (4), 821–841.
(3) Mukherjee, A. J.; Zade, S. S.; Butcher, R. J.; Sunoj, R. B. *Chemical Reviews* **2010**, *110* (7), 4357–4416.
(4) Arora, A.; Oswal, P.; Rao, G. K.; Kumar, S.; Kumar, A. *Dalton Transactions* **2021**, *50* (25), 8628–8656.

PP-62

Direct synthesis of secondary amides from ketones through Beckmann rearrangement using O-(mesitylsulfonyl)hydroxylamine

Abhishek Maurya, Dr. Jawahar L. Jat
Department of Chemistry, School of Physical and Decision Sciences
Babasaheb Bhimrao Ambedkar University (A Central University)
Lucknow, UP, India, 226025
Email-jawaharlj@bbau.ac.in, mabhishek5678@gmail.com

The formation of the amide bonds (–C(O)–NR_2) is one of the most important organic reactions as the amide bond is a typically fundamental chemical bond that widely occurs in natural and industrial products, such as polypeptide protein, pesticide, polymer materials, and medicine. Secondary amides containing molecules such as Axitinib (anticancer drugs), Spilanthol (antimicrobial, and antifungal activities), Penicillin G (Antibiotic), Tetrahydrolipstatin (antiobesity agent) shows different kind of pharmacological activities. They are also used as reactive intermediates in organic synthesis for attaining sundry of valuable nitrogen-containing products. Herein, we have developed a highly efficient direct method for the synthesis of secondary amides and lactams from ketones using O (mesitylsulfonyl)hydroxylamine (MSH). The reactions proceed rapidly at room temperature under mild condition without requiring any additive, and tolerate multiple functional groups. A simple aqueous work-up often furnished the products in excellent yield with high purity.



- One pot, metal and additive-free
- Broad substrate scope, functional group tolerance
- Water soluble byproduct, column chromatography-free process

Keywords: Ketone, Secondary amide, Lactams.

References:

Dinesh Chandra, Saumya Verma, Chandra Bhan Pandey, Ajay K. Yadav, Puneet Kumar, Bhoopendra Tiwari, **Jawahar L. Jat**. ***Tetrahedron Lett.*, 2020**, 61(18), 151822.

PP-63

Selective detection of nitroaromatic analyte through 2D Cd(II) coordination polymer

*Shiva and Nidhi Goel**

Department of chemistry, Institute of Science, Banaras Hindu University, Varanasi-221005, Uttar Pradesh, India.

Email: shiva.chemistry17@bhu.ac.in; nidhigoel.chem@bhu.ac.in

Porous coordination polymers, or PCPs, have attracted a lot of attention in the last twenty years due to their wide range of uses.[1-3] In this work, we have successfully created a new mesoporous Cd-CP through a solvothermal reaction, which is known as [Cd(7-aminonaphthalene-disulphonate)$_2$(1,2-bis(4-pyridyl)ethane)$_4$]$_n$.CH$_3$OH. Using elemental analysis, FT-IR spectroscopy, powder X-ray diffraction (PXRD), thermogravimetric analysis (TGA), and single crystal X-ray diffraction methods, the resultant Cd-CP was systematically characterized. Single crystal X-ray diffraction revealed the formation of a two-dimensional framework within the Cd-CP. In addition, the Cd-CP showed exceptional luminescence characteristics and proved to be a useful chemosensor for the specific identification of 2,6-dinitrophenol among other nitroaromatic analytes. These findings highlight the promising attributes of the synthesized Cd-CP for diverse applications in chemical sensing and materials science.

References:

(1) Mansoorianfar, M.; Nabipour, H.; Pahlevani, F.; Zhao, Y.; Hussain, Z.; Hojjati-Najafabadi, A.; Hoang, H. Y.; Pei, R.; *Environ. Res.,* **2022**, *214*, 114113.

(2) Goel, N.; Kumar, N.; *RSC Adv.,* **2018**, *8* (20), 10746–10755.

(3) Wang, X.; Liu, Y.; Lin, H.; Xu, N.; Liu, G.; Wang, X.; Chang, Z.; Li, J.; *CrystEngComm,* **2020**, *22* (40), 6626–6631.

PP-64

Sodium-Ion-Conducting Hydrogel Material: Synthesis, Characterization and Conductivity Studies

Shashikant Yadav, S. Krishnamoorthi[*]
Department of Chemistry, Institute of Science, Banaras Hindu University, Varanasi, India
Email: shashikant10@bhu.ac.in, skmoorthi@bhu.ac.in

Herein we have reported single sodium ion conducting pseudo solid polymer electrolyte material, was synthesized successfully using sodium;3,4,5,6-tetrahydroxyoxane-2-carboxylate (ALG) and sodium salt of poly (acrylic Acid): SPA in the water as solvent via solution cast technique. This pseudo-solid polymer material allows Na^+ cation transport inside the matrix. The FTIR technique confirmed the appreciable interaction between the sodium alginate and sodium polyacrylate polymer. This amorphous polymer material has good flexibility, tensile strength, and good elasticity which provides a better electrode-electrolyte interface. The material shows electrical conductivity in the range of 10^{-5} S/cm at room temperature and 10^{-4} S/cm at higher temperatures (>40°C). The material shows electrochemical stability of 2.26V owing to a very good amount of current density with ≈ 97% ionic transport number for the sodium ion. The material shows drift ionic velocity in the range of 10^{-4} m/s and ionic mobility in the order of 10^{-6} m^2/Vs at room temperature. It shows the matrix ionic diffusivity constant in the order of 10^{-7} m^2/s. It possesses low activation energy for ionic movement inside the matrix of 0.465 eV. The matrix shows the correlated type of hopping. An appreciable amount of capacitance is associated with the matrix with minute electrode contribution.

PP-65

Unveiling the catalytic potential of silicomolybdic acid in crafting diverse biologically relevant organic compounds.

Neeraj K. Sah,[a] *Dr. rer. nat. Somenath Garai** [a]
[a] *Department of Chemistry, Institute of Science, Banaras Hindu University, Varanasi 221 005, Uttar Pradesh, India;*

Heteropolyacid are well known Lewis acid catalysts owing to their distinctive physicochemical characteristics. Silicomolybdic acid (SMA) is one of the most explored heteropolyacid, which also has several technological features that are particularly helpful, such as easy recovery and handling that is safer for the environment, in addition to their very strong acid strength. Additionally, SMA has much more Bronsted acidic sites as compared to the acidity of conventional mineral acid catalysts, the solubility of it in most organic solvent as well as in water makes it best acid catalyst to frequently utilize it for both homogeneous and heterogeneous catalytic processes. On the other hand, in nature, nitrogen containing heterocyclic compound are increasingly prevalent as structural building blocks of significant bioactive substances like antibiotics, vitamins, hormones, and others. Chromene derivatives, Imidazopyrimidine derivatives and xanthene derivatives are some examples of biological significant heterocyclic compound. Although, various techniques and several Lewis acid catalyst has been employed for the synthesis of these derivatives but the use of most promising acid catalyst SMA for the preparation of these derivatives is yet to be done. The unique properties of SMA have prompted us to investigate its catalytic activity towards the synthesis of abovementioned organic compounds.

PP-66

Synthesis and Characterization of Graphene based Nanocomposite Materials and its Electrochemical Application for Detecting Phenolic Compounds

*Shivani Shukla, Ida Tiwari**

Banaras Hindu University, Department of chemistry, Varanasi, India-221005

Email: *shivanishukla509@gmail.com*

Herein, we had prepared and characterized tin doped cobalt oxide and graphene-based nanocomposite material (Sn-Co_3O_4@GO). The prepared nanocomposite was further characterized by fourier transform infrared spectroscopy, X-Ray diffraction, and transmission electron microscopy which confirms the successful synthesis of Sn-Co_3O_4@GO. Moreover, to shows its electrochemical sensing application we had drop cast the prepared Sn-Co_3O_4@GO nanocomposite on the glassy carbon electrode for the electrochemical sensing of phenolic compounds (PC). The common and ongoing source of environmental contamination among various toxic pollutants are those compounds which are based on phenols. Further, PC are the byproducts that are released from oil and carbon industries and then it enters into water and soil through waste matter discharges. This leads to environmental contaminants and is indirectly related to human health hence, PC monitoring is crucial to reduce its deadly impact on environment and human beings. Therefore, we have prepared electrochemical sensor using Sn-Co_3O_4@GO nanocomposite for the analysis of phenolic compounds using cyclic voltammetry and differential pulse voltammetry techniques.

PP-67

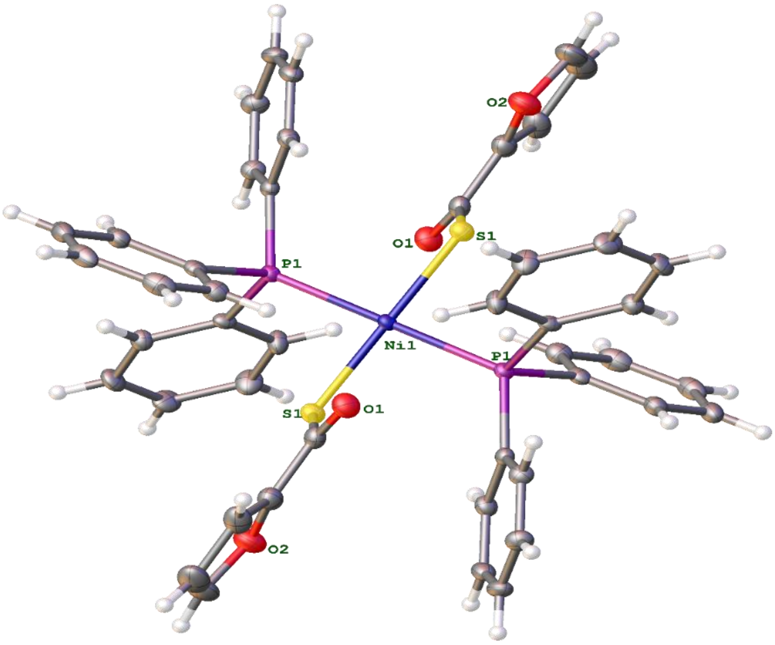
Nickel(II) carbothioate complex incorporated graphene oxide-polyvinylidene fluoride ternary composite film: Preparation, structural features, dielectric, and electrical characteristics

*Akash Shrivastav, Nishtha Chaturvedi, Raj Kumar Sahani, and Subrato Bhattacharya**

Graphene oxide-based materials are well known for their electrical properties. Novel ternary composite films (PVDF-GO-FK-31) were prepared by introducing a metal complex, for the first time, in a graphene oxide-PVDF polymer matrix (where PVDF = polyvinylidene fluoride; GO = graphene oxide; FK-31 = [Ni(PPh$_3$)$_2$(SCOf)$_2$], SCOf = furan-2-thiocarboxylate). In these composites, the graphene oxide shows strong interfacial bonding with the PVDF matrix due to the incorporation of the FK-31 molecules. The experimental results show that the incorporation of FK-31 into the PVDF-GO matrix greatly improves the dielectric constant and suppresses dielectric loss values. The composites thus may be used as dielectric materials for electronic capacitors.

Keywords: Graphene oxide; Polyvinylidene fluoride; Dielectric properties of composite.

Crystal structure of [Ni(PPh$_3$)$_2$(SCOf)$_2$]



PP-68

Untangling the Molecular Interaction: Spectroscopic Insights into DNA-Cobalt Complex

*Anant Kumar Singh, Komal Kumari, Dr. Surajit Rakshit**
Department of Chemistry, Institute of Science, Banaras Hindu University, Varanasi, Uttar Pradesh-221005, India.
anantks099@gmail.com, srakshit.chem@bhu.ac.in

DNA is the most significant macromolecule present in living things. It is not only necessary for physiology but also for carrying genetic information and controls the creation of proteins and enzymes through the translation of genetic information and transportation duplication. At the intersection of molecular biology, medicine, and chemistry, there is now active research being done to better understand how drug molecules interact with DNA. Based on the importance of metal-centered complex (drug) that can interact with DNA, this work is focused on the Cobalt based complexes. Cobalt is accepted as an essential metal element widely distributed in the biological systems such as cells and body, and thus the interaction of DNA with cobalt complex has attracted much attention. The metal complex (drug) acts as an effective DNA binder based on studies in the presence of DNA. DNA interaction studies were carried out via UV-Vis absorption spectroscopy, emission spectroscopy, circular dichroism spectroscopy and thermal denaturation. The binding constant of the complex with DNA has also been calculated. The study of competitive binding with ethidium bromide (EB) indicates the binding mode of the complex with DNA. Structural changes are observed by circular dichroism spectroscopy. The thermal denaturation process was performed to evaluate the melting temperature of DNA.

Key words: DNA, Cobalt complex, Spectroscopy, Binding constant, Interaction.

PP-69

Development of a multifunctional fluorescent probe based on carbon quantum dot/gum arabic stabilized silver nanocomposite for rapid detection of hydrogen peroxide and Hg^{+2} ion in aqueous solution

*Shukla Majhi, Debanjan Guin**
Department of Chemistry, Institute of Science, Banaras Hindu University, Varanasi-221005
Uttar Pradesh
E-mail: shukla123majhi@gmail.com

Here we constructed a sensitive multifunctional ‘off-on’ fluorescent probe via in-situ synthesis of carbon quantum dots composite silver nanoparticles (CQDs@GA-Ag NPs) for selective and sensitive detection of hydrogen peroxide (H_2O_2) and mercury ion (Hg^{+2}). The composite was prepared in a simple and green manner using naturally occurring gum Arabic (GA) polymer. Electron microscopy measurement clearly shows that CQDs are attached to the surface of Ag NPs. The fluorescence intensity of CQDs was dramatically quenched in the synthesized nanocomposite via the inner filter effect (IFE) mechanism. After the addition of H_2O_2 to the nanohybrid system, Ag NPs got oxidized leading to the formation of Ag^+ ions, and concomitantly, CQDs regained their photoluminescence (PL) property, facilitating the detection of H_2O_2 with extremely low detection limit of 1.02 uM. Furthermore, the developed nanocomposite was applied for heavy metal ion detection, particularly Hg^{+2}, obtaining a remarkably low detection limit of 1.92 uM. Real water samples were also successfully analyzed for both H_2O_2 and Hg^{+2}, with a recovery range of 90% and 95% respectively. The developed probe was extremely selective over a wide range of interfering ions and substances.

Keywords - Carbon quantum dots, GA-Ag NPs, ‘off-on’ mechanism, IFE, H_2O_2, Hg^{+2}

References:

(1) Mu, X., et al., A sensitive “off-on” carbon dots-Ag nanoparticles fluorescent probe for cysteamine detection via the inner filter effect. Talanta, 2021. **221**: p. 121463.

(2) Zhang, X., et al., A carbon dots functionalized paper coupled with AgNPs composites platform: Application as a sensor for hydrogen peroxide detection based on surface plasmon-enhanced energy transfer. New Journal of Chemistry, 2021. **45**(13): p. 6025-6032

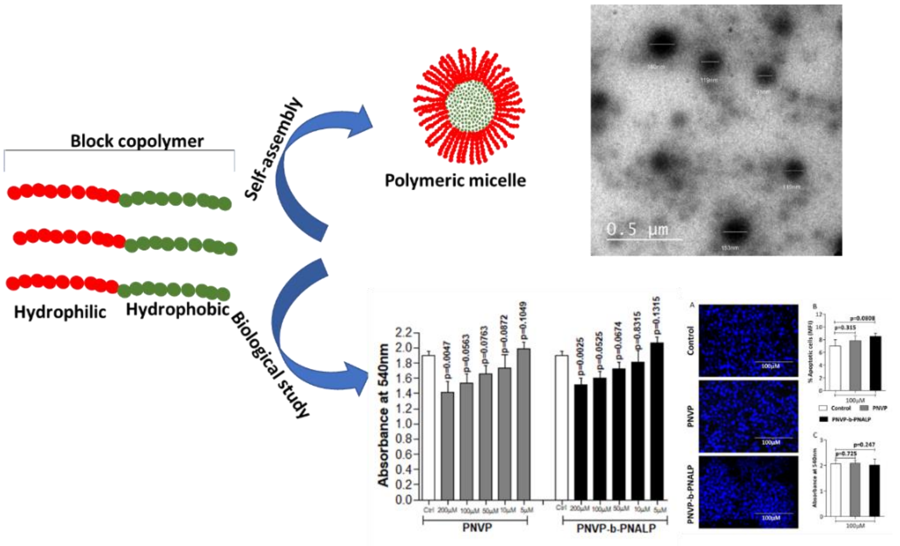
(3) Zhou, Q., et al., Measurement of mercury with highly selective fluorescent chemoprobe by carbon dots and silver nanoparticles. Chemosphere, 2021. **274**: p. 129959

PP-70

Synthesis & characterization of amino acid-based acrylamide derived amphiphilic block copolymer using a new xanthate and its influence on cell cytotoxicity & cell viability

*Megha Keshari, Shere Afgan , Krishtan Pal , Koushik Nandy, Paramjeet Yadav, Sheetal Jaiswal , Rajan Singh , Rakesh K. Singh [2], Rajesh Kumar [*1]*
[1]Department of Chemistry, Institute of Science, Banaras Hindu University, Varanasi 221005, UP, India
[2]Department of Biochemistry, Institute of Science, Banaras Hindu University, Varanasi 221005, UP, India

Amino acid-based polymers were developed for their unique properties, resembling biocompatible polymers that offer sensitive capabilities for various medicinal and biological tasks, including drug release control and biochemical sensing. To achieve this, poly(N-vinylpyrrolidone) (PNVP) and its block copolymer, poly(N-vinylpyrrolidone)-b-poly(N-acryloyl-L-phenylalanine) (PNVP-b-PNALP), were synthesized utilizing the xanthate ethyl 2-((isopropoxycarbonothioyl)thio)-2-methylpropanoate (IPX), known for effective control in RAFT polymerization. The molar mass-conversion plot displayed a linear relationship, affirming pseudo-first-order kinetics, with molar mass distribution (Đm) between 1.50 and 1.24. Both polymers underwent comprehensive characterization through methods such as 1H NMR, FTIR, DSC, TGA-DTA, GPC, and XRD analysis. TEM and DLS analysis of the aqueous solution of the block copolymer (PNVP-b-PNALP) revealed self-assembly behavior, forming structures sized between 119 and 160 nm, including a few smaller particles of 91 nm. Toxicity assessment was conducted on macrophages (RAW 264.7) and cancer cells (MCF7) at varying polymer concentrations (200–0.75 μM). The polymers showed non-toxic attributes, with no significant changes in cell proliferation even at higher concentrations (up to 100 μM). However, the polymers induced apoptosis-like changes in cancer cells up to 100 μM, although these effects were not statistically significant.



PP-71

Comparative Study of Natural and Synthetic Dyes on DSSCs: an experimental and computational approach

Anamika Chaudhari, Aman Kumar, Suman Kushwaha
Department of Chemistry, Institute of Science, Banaras Hindu University, Varanasi,
Uttar Pradesh, 221 005, India.
Corresponding authors; E-mail addresses: sumankush@bhu.ac.in

This research work explores the use of both natural pigments and synthetic dye as sensitizer for dye sensitized solar cells (DSSCs). We investigate their optical and electronic properties, as well as their ability to bind to semiconductor surfaces. Anthocyanin dye extracted from pomegranate (*Punica granatum*) fruit, bitanin pigment from beet root (*Beta vulgaris*) and the commercially available organic dye rose bengal were tested. Density functional theory (DFT) and time-dependent density functional theory (TD-DFT) studies have been also performed to gain insight at molecular levels of the tested dyes. DSSCs were fabricated and overall efficiencies (η) of 0.34 %, 0.3 % and 0.25 % were obtained for the anthocyanin, betanin and rose bengal sensitized dyes, respectively. The results specify that anthocyanin can act as promising photo-sensitizer for DSSCs compared to betanin and rose bengal sensitizer.

Keywords; Dye-sensitized solar cells, Anthocyanin, Betalains, Xanthane sensitizer, DFT and TD-DFT etc.

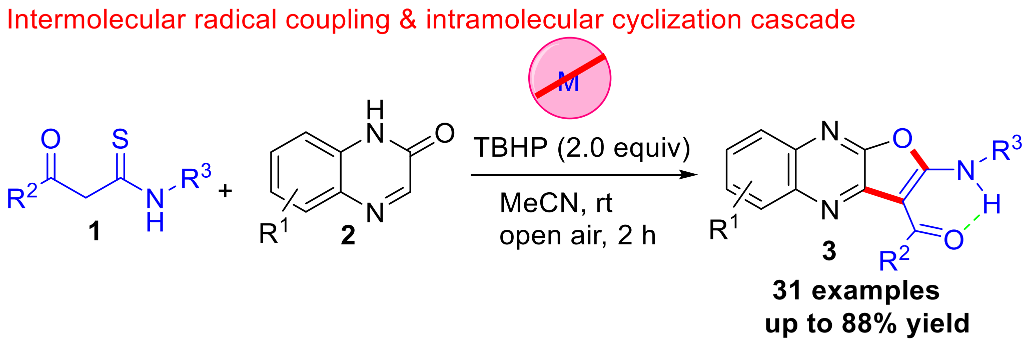
PP-72

TBHP-Mediated Intermolecular Radical Coupling and Intramolecular Cyclization Cascade: Access to Furo[2,3-b]quinoxalines and their Photophysical Study

Subhasish Ray, Vipin Kumar, Saurabh Singh, Krishanu Bandyopadhyay, Satyen Saha and Maya Shankar Singh**

A cascade one-pot strategy to construct furo-fused quinoxalines upto 88% yields has been devised from readily accessible β-ketothioamides and quinoxalin-2-ones in open flask at room temperature under TBHP mediated conditions. The method is step-/pot-/carbon economic, metal-/catalyst-free, devoid of toxic reagents with 31 examples. Mechanistic studies revealed that the overall reactivity relies on the seamless integration of intermolecular radical coupling and intramolecular cyclization *via* desulfhydration of C=S bond cleavage. Generation of H_2S as the only by-product makes this process highly attractive. Furthermore, the photophysical behaviour of the furo-fused quinoxalines has also been studied.

Keywords: Radical Coupling, TBHP-mediated, Intramolecular Cyclization



PP-73

Biosynthesis of TiO_2 nanostructures using *camellia sinensis* extract (polyphenols) and Investigation of their execution as Photoanodes in Photovoltaic device

Sudhanshu Kumar, Aman Kumar, Suman Kushwaha
Department of Chemistry, Institute of Science, Banaras Hindu University, Varanasi,
Uttar Pradesh, 221 005, India.
E.mail addresses: sumankush@bhu.ac.in

Phenolic compounds in particular, can play a significant role in reducing metal ions to form nanoparticles (NPs). As a result, NPs produced using different *Camellia sinensis* varieties may exhibit distinct properties. Therefore, in this work, a variety of *Camellia sinensis* types, including green, white, black, oolong, pu-erh have been used to synthesize TiO_2 NPs. The prepared TiO_2 NPs were comprehensively characterized for particle size, morphology, purity, composition, crystalline nature, structural, electrochemical and photovoltaic capabilities. The as synthesized titanium oxide (TiO_2) NPs were spherical in shape and particle size of ranged from 10-20 nm with little agglomerations. For DSSC application, thin films of synthesized TiO_2 NPs were prepared. Overall efficiency = 3.0 %, J_{SC} = 9.72 mA/cm^2, V_{OC} = 660 mV and FF= 0.46 was achieved with the DSSC made up with green tea mediated TiO_2 NPs based photo anode. Due to high phenolic content and good reductive properties, TiO_2 NPs prepared using green tea extract were highly crystalline in nature, have high surface area, high roughness factor, good stability which results in maximum dye loading and increases in overall conversion efficiency.

Keywords: Green synthesis, TiO_2 NPs, *camellia sinensis* extract, polyphenols, DSSC, photoanode.

PP-74

A new simple colorimetric ICT based fluorescent molecular probe for specific detection of Cu^{2+} and ClO^- ions

*Mohammed Kaleem, Ravisen Rai, Rimpi Bhandari, Arvind Misra**
Department of Chemistry, Institute of Science, Banaras Hindu University, Varanasi, UP, INDIA.
E-mail addresses: arvindmisra2003@yahoo.com, amisra@bhu.ac.in

A new simple molecular probe **3** based on 2, 3-diaminomalionitrile and tetrasubsituted imidazole moiety, have been synthesized and characterized. The probe **3** showed good photophysical behavior due to intramolecular charge transfer (ICT) process, upon interaction with different types of metal ions probe **3** showed high selectivity with Cu^{2+} ion in ACN/H_2O (9.5:0.5, v/v) medium. Probe **3** reacted with Cu^{2+} ion through de-diaminomaleonitrile reaction which disrupted the ICT mechanism by breaking the donor and acceptor linkage resulting in a remarkable change of the emission intensity. Job's plot analysis showed that the 1:1 stoichiometry between probe **3** and Cu^{2+} ion. The limit of detection was found to be 17 nM. Upon interaction with different anions probe **3** showed high selectivity with ClO^- ion with similar mechanism of Cu^{2+} ion. Job's plot analysis showed that 1:1 stoichiometry between probe 3 and ClO^- in ACN/H_2O (9.5:0.5, v/v) medium. The limit of detection was found to be 18.5 nM. The mechanism of interaction Cu^{2+} and ClO^- ions has been confirmed by NMR titration studies and HRMS analysis.

References

(1) T. Shu, X. Deng, C. Dong, Y. Ruan and Y. Yu, Diaminomalionitrile-based Fluophores as Highly Selective Sensing Platform for Cu^{2+}, Analytical Sciences 2019,35.
(2) Y. Ning, J. Cui, Y. Lu, X. Wang, C. Xiao, S. Wu, J. Li, Y. Zhang, De novo design and synthesis of a novel colorimetric fluorescent probe based on naphthalenone scaffold for selective detection of hypochlorite and its application in living cells, Sensors and Actuators B 269 (2018) 322–330

PP-75

Haloperoxidase-mimicking activity of 2D CuO nanosheets for the colorimetric detection of H_2O_2 and Glucose

Renuka Singh, *Debanjan Guin*

Department of Chemistry, Institute of Science, Banaras Hindu University, Varanasi-221005

Uttar Pradesh

E-mail: ***renukasingh@bhu.ac.in***

Nanomaterials-based enzymes, also known as nanozymes, are nanoparticles exhibiting enzyme-like catalytic activities and have been widely studied over many years. Among them, 2D copper oxide nanosheets (CuO NSs) have received growing interest across diverse research areas to catalyse new reactions, and their applications in academia, industry and commerce. We have synthesized CuO NSs by exploiting an effective approach of sugar blowing method. The nanosheets were characterized by several techniques like X-ray powder diffraction (XRD), transmission electron microscopy (TEM), X-ray photoelectron Spectroscopy (XPS) and Fourier Transform Infrared Spectroscopy (FTIR). Impressively, CuO NSs possess haloperoxidase (HPO) like catalytic activity which catalyses the oxidation of halide ions by H_2O_2 giving rise to reactive chlorine species (RCS). A sensitive and selective colorimetric sensor was then demonstrated via the oxidation of chromogenic substrate 3,3,5,5-tetramethylbenzidine (TMB) by the novel nanoenzyme CuO through the generation of RCS for H_2O_2 and glucose detection with a limit of detection of 2 uM and 10 uM respectively. Additionally, the methodology is validated for the analysis of glucose in real samples.

Keywords: CuO Nanosheets, Haloperoxidase activity, nanoenzyme, Glucose, H_2O_2, reactive chlorine species

References:

1. Cormode, D.P., Gao, L. and Koo, H., 2018. Emerging biomedical applications of enzyme-like catalytic nanomaterials. *Trends in biotechnology*, *36*(1), pp.15-29.
2. Wang, L., Hou, J., Liu, S., Carrier, A.J., Guo, T., Liang, Q., Oakley, D. and Zhang, X., 2019. CuO nanoparticles as haloperoxidase-mimics: Chloride-accelerated heterogeneous Cu-Fenton chemistry for H2O2 and glucose sensing. *Sensors and Actuators B: Chemical*, *287*, pp.180-184.
3. Guo, T., Xu, T., Xia, W., Carrier, A.J., Wang, L. and Zhang, X., 2021. Graphene oxide and CuO double quantum dot composites (GOQD-q-CuO) with enhanced haloperoxidase-like activity and its application in colorimetric detection of H2O2 and glucose. *Materials Chemistry and Physics*, *260*, p.124126.
4. Wang, L., Miao, Y., Lu, M., Shan, Z., Lu, S., Hou, J., Yang, Q., Liang, X., Zhou, T., Curry, D. and Oakes, K., 2017. Chloride-accelerated Cu-Fenton chemistry for biofilm removal. *Chemical Communications*, *53*(43), pp.5862-5865.

PP-76

Antiproliferative activities based on Ni(II) and Co(II) complexes of 1-picolinoyl-4-phenyl-3-thiosemicarbazide: Synthesis, crystal structure, and photoluminescence study

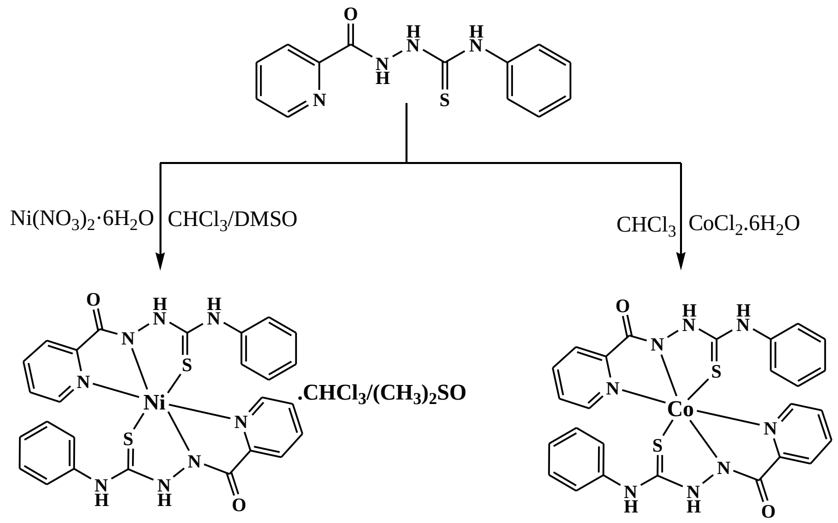
*Suryansh Chandra and Manoj Kumar Bharty**

Department of Chemistry, Institute of Science, Banaras Hindu University

Email: suryansh95chandra@gmail.com

Tel: (+91) 8960313174

Platinum and ruthenium complexes have long been used as chemotherapeutic agents despite having certain disadvantages such as neuropathy and nephrotoxicity [1]. This encouraged researchers to replace platinum-based drugs with suitable alternatives and hence numerous transition metal complexes have been synthesized and tested for their anticancer activities [2]. Keeping the above facts in view, we have synthesized $[Ni(Hppts)_2].CHCl_3$ (**1a**), $[Ni(Hppts)_2].(CH_3)_2SO$ (**1b**) and $[Co(Hppts)_2]$ (**2**) complexes of 1-picolinoyl-4-phenyl-3-thiosemicarbazide (H_2ppts). The synthesized complexes have been characterized by UV-vis., Infrared, NMR spectrometry and also by single-crystal X-ray diffraction data. Result derived from photoluminescent properties interprets that complex **1a** showed better fluorescence behavior than H_2ppts and complex **2**. The tumoricidal properties of H_2ppts**,** complexes **1a** and **2** were examined against DL cells and standard MTT test was used to assess the cytotoxicity of H_2ppts, complexes **1a** and **2.** The viability of DL cells was more effectively inhibited by complex **1a** than by the H_2ppts and complex **2**. Complex **1a** reduced cell proliferation and viability in a concentration-dependent manner. Complex **1a** displays IC_{50} value around 40 µg/mL. The result shows that complex **1a** has high anti-neoplastic activity on DL cells at low doses. Moreover, DAPI staining was used to assess the effect of complex **1a** treatment on apoptosis related alterations of nuclear morphology. The study showed that, in treated samples (20, 40, and 80 µg/mL), complex **1a** treatment increased the number of DAPI positive cells than that of control group.



$[Ni(Hptsc)_2].CHCl_3$ (**1a**), $[Ni(Hptsc)_2].(CH_3)_2SO$ (**1b**)

$[Co(Hptsc)_2]$ (**2**)

Scheme 1: Synthesis of the complexes **1a**, **1b** and **2**

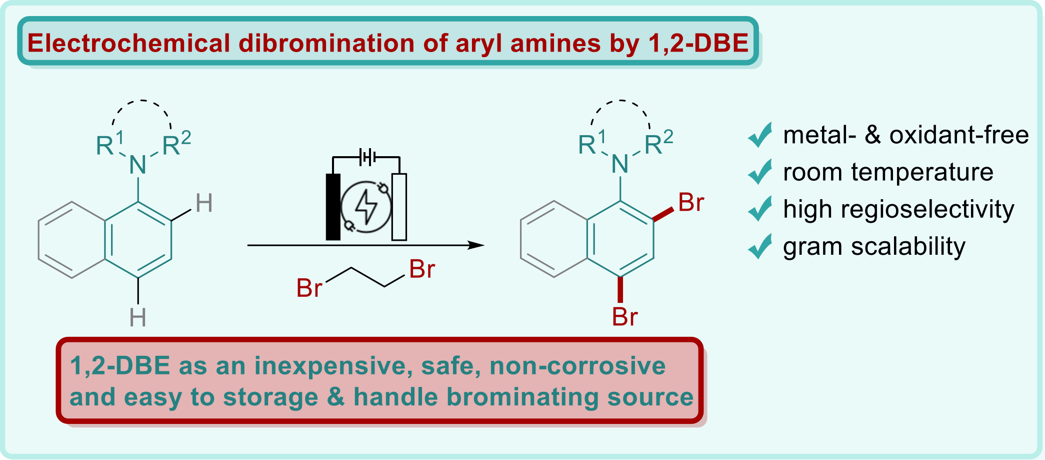
PP-77

Aromatic $C(sp^2)$–H functionalization by consecutive paired electrolysis: Dibromination of aryl amines with dibromoethane at room temperature

Malkeet Singh, Gaurav Shukla, Anup Kumar Yadav and Maya Shankar Singh[*]

Department of Chemistry, Institute of Science, Banaras Hindu University, Varanasi 221005, India

A facile and efficient electrochemical method for the dibromination of aryl amines by double functionalization of aromatic $C(sp^2)$□H (both *para* and *ortho*) under metal- and external oxidant-free conditions at room temperature is demonstrated using 1,2-dibromoethane to dibrominate a wide range of N-substituted aryl amines in a simple setup with C(+)/Pt(-) electrodes under mild reaction conditions. This transformation proceeds smoothly with a broad substrate scope affording the valuable and versatile N-substituted 2,4-dibromoanilines in moderate to excellent yields with high regioselectivity. In this convergent paired electrolysis, anodic oxidation and cathodic reduction occur simultaneously to generate two intermediates, which are then coupled to furnish the product. It represents a distinctive approach to challenging redox-neutral reactions. The versatility of the electrochemical *ortho*-, *para*-dibromination was reflected by unique regioselectivities for challenging aryl amines and gram-scale electrosynthesis without the use of a stoichiometric oxidant or an activating agent.



PP-78

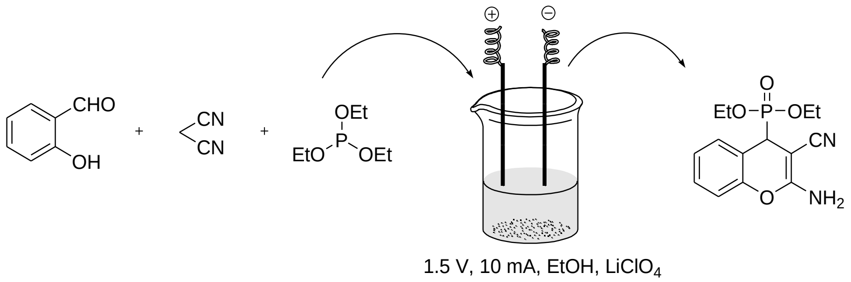
Electrochemically induced an efficient, simple, non-catalytic synthesis of β-phosphonomalonates via multicomponent reaction

Phool Chandra[a], *Vinay K. Singh*[b,c]*, *Renu Singh*[a]*
[a]*Maharishi University of Information Technology, Lucknow*
[b]*Green Synthesis lab, D.N. P.G. College, Gulaothi, Bulandshahr (An Affiliated College of C.C.S University Meerut)*
[c]*Electrochemical laboratory of green synthesis, Department of Chemistry, University of Allahabad, Allahabad 211002, India*
E-mail address: pcschem@gmail.com

Electrochemically induced an efficient and economical method has been developed for synthesis of β-phosphono malononitriles via condensation of various aldehyde, malononitrile and phosphite ester at room temperature. The present protocol highlights cost efficient, one pot, easy workup, environmentally benign process. Over the last decades, multicomponent reactions[1] become the most promising alternative approach for the synthesis of phosphorous-carbon bond. The strategy has significant advantages over classical stepwise approaches, as it proceeds with the formation of several bonds and the construction of molecule from simple precursors in a single synthetic step without isolation of intermediates, results in eco-friendly reaction with excellent yield. Electro- organic synthesis[2] is another powerful, versatile, and environmentally friendly protocol for synthesis of biologically and medicinally active compound. In recent years, electro synthetic, multicomponent reactions (EMCRs) have been used extensively to prepare biologically active compounds. As the particular method eliminates the hazardous chemicals, adverse reaction condition, minimise expensive catalyst and follow the green chemistry principle.[3] In an electrochemical reaction, electric current acts as an inexpensive and potentially renewable reagent to proceed the reaction. Extensive research on electro-organic synthesis, become revolutionized alternative technique for organic synthesis.

Keywords: Three component reaction, β-Phosphonomalonate, Malononitrile, Nucleophilic addition reaction Electrochemically induced.

Scheme 1. Synthesis of β-phosphonomalonate



PP-79

Hydrophilic Silver Nanoparticle Infused Polyester Fabric with L-Lysine Grafted Graphene Oxide for Catalytic Degradation and SERS-based Detection of Eight Industrial Contaminants

Keshav Sharma, *Debanjan Guin*
Department of Chemistry, Institute of Science, Banaras Hindu University, Varanasi-221005
Uttar Pradesh, India
E-mail: meetkeshavattri@gmail.com

We report on the surface modification of low-cost flexible polyester fabric (PET) cloth through the assembly of hydrophilic silver nanoparticles (Ag NPs) on L-Lysine (LYS) functionalized graphene oxide (GO) (Ag@LYS-GO/PET), tailored for integrated applications in catalysis and surface-enhanced Raman scattering (SERS) for reduction and sensing of eight industrial water pollutants, The successfully fabricated Ag@LYS-GO/PET substrate was validated through a comprehensive array of characterization techniques, including SEM, EDX, XRD, XPS, and Raman analyses, confirming homogeneous deposition of Ag NPs across the surface of the LYS-GO/PET, which is a direct consequence of electrostatic interactions between Ag ions and the amino groups inherent in the LYS functionalized GO. Further, the Ag@LYS-GO/PET substrate has been employed as a catalytic platform for the sodium borohydride-based reduction of various nitrophenols, namely 4-Nitrophenol (4-NP), 2-Nitrophenol (2-NP), 2,4,6-Trinitrophenol (2,4,6-TNP), as well as Methyl orange (MO) and Methyl red (MR) dyes, with high stability and reproducibility. The pseudo first-order rate constant values for 4-NP, 2-NP, 2,4,6-TNP, MO, and MR were determined to be 5.4×10^{-3} s^{-1}, 4.2×10^{-3} s^{-1}, 1.4×10^{-3} s^{-1}, 1.9×10^{-3} s^{-1}, and 3.0×10^{-3} s^{-1}, respectively. Additionally, the Ag@LYS-GO/PET substrate served as a remarkably sensitive and flexible platform for SERS, enabling the detection of organic dyes like Rhodamine B (RhB), Rhodamine 6G (R6G), and Methylene blue (MB) with enhancement factors (EF) of 3.0×10^4, 2.4×10^3, and 7.5×10^3, respectively. The SERS stability and reproducibility of the Ag@LYS-GO/PET substrate were also studied concerning R6G dye and the results were promising. Moreover, our fabrication approach offers a straightforward pathway to cost-effective functional substrates based on polyester fabric cloth, catering to a range of multichannel applications.

Keywords: Wastewater treatment, Catalysis, SERS, Raman, Silver nanoparticles, Flexible support

References

1. Sharma, K., et al., Silver nanoparticles decorated on graphene oxide modified polyester fabric: Catalytic reduction of 4-nitrophenol, organic dyes and SERS application. Journal of Physics and Chemistry of Solids, 2022. 165: p. 110640.
2. Liu, A., et al., Ag-coated nylon fabrics as flexible substrates for surface-enhanced Raman scattering swabbing applications. Journal of Materials Research, 2020. 35(10): p. 1271-1278.
3. Sharma, K., et al., Covalent functionalization of graphene oxide with l-lysine for highly sensitive and selective simultaneous electrochemical detection of rifampicin and acetaminophen. Journal of Applied Electrochemistry, 2023.

PP-80

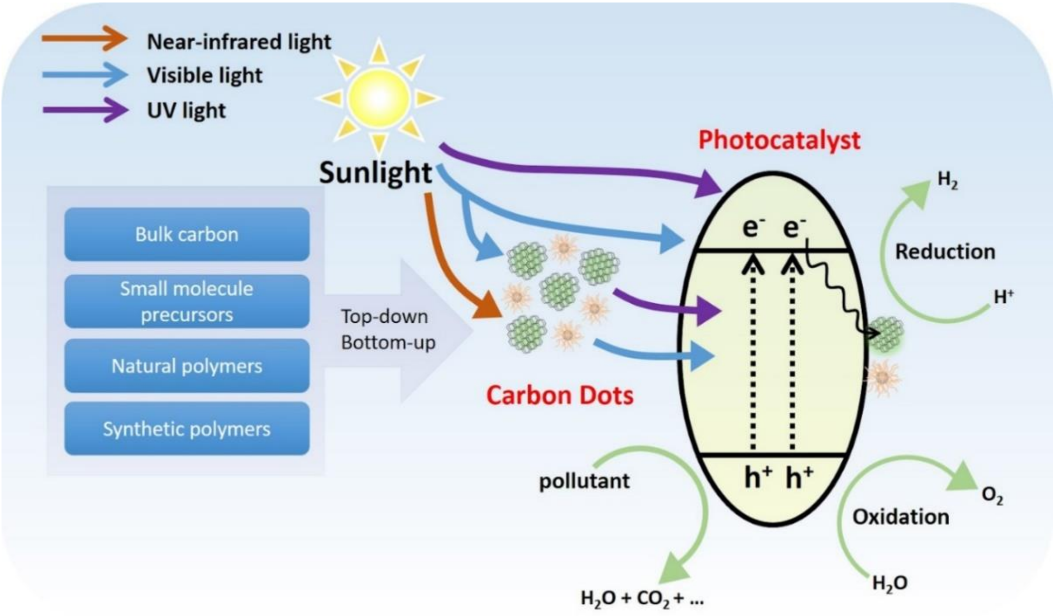
Photo-Catalytic Application of Carbon Nanoparticles

Mansi Srivastava, *Sonam Soni**

Department of Chemistry, Sunbeam Women's College Varuna,Varanasi

Email- mansisrivastav800@gmail.com, sonamsoni.bhu@gmail.com.

In Present era, carbon-based nanoparticles (CNPs) have emerged as a highly promising class of materials employed as visible-light photocatalysts. The adoption of CNPs in photocatalysis is primarily motivated by their swift electron mobility, expansive surface area, robust physicochemical stability, and the flexibility to employ various synthetic strategies from diverse precursors. Moreover, the photocatalytic efficacy of CNPs is substantially influenced by surface modifications, doping, the presence of defects, confinement, and morphology. The varied potential applications of CNPs, encompasses photocatalysis for organic compound transformations, specific instances of organic pollutant photodegradation, photocatalytic hydrogen generation, oxygen evolution, water splitting, photoreduction of CO_2, NO_x removal, and the production of photocatalytic solar fuels and related substances.



PP-81

A PET based pH-responsive bridged organic scaffold exhibiting sensitivity for Lysosome and Hg^{2+} ion through fluorescence *Off–On–Off* response

Rimpi Bhandari[a], *Ravisen Rai*[a], *Mohammed Kaleem*[a], *Nikita Shraogi*[b§], *Satyakam Patnaik*[b§]
and Arvind Misra[a]*
[a]*Department of Chemistry, Institute of Science, BHU, Varanasi 221005 UP, INDIA*
[b]*CSIR-Indian Institute of Toxicology Research (CSIR-IITR), Lucknow-226001, UP, INDIA*
**Corresponding author: amisra@bhu.ac.in; arvindmisra2003@yahoo.com*

A 1,5–bis(1,4-piperazinyl–naphthalimide–*N*–ethylmorpholine) pyridine based flexible fluorescence probe **7** is designed, synthesized, and its photophysical behavior has been examined in different media. The photophysical behavior of probe **7** in phosphate (PBS) buffer (10% DMSO) showed pH sensitivity and selectivity for Hg^{2+} ion in solution and live cell with a change in naked-eye sensitive visible color. In acidic medium ($pH \leq 6$) probe **7** showed enhanced (~21 fold) "turn–On" emission, while at $pH \geq 7.4$ probe **7** remained in the "turn–Off" state. The observed fluorescence "turn–On" response is attributed to inhibition in photoinduced electron transfer (PET) process. Jobs plot analysis revealed a 1:2 stoichiometry for an interaction between probe **7** and Hg^{2+} ion with good limit of detect (LOD) 5.78×10^{-8} M (57nM). The reversibility in complexation and the mode of interaction were confirmed by EDTA and through NMR and HRMS spectroscopic data. MTT assay and cell imaging studies showed biocompatibility of the probe **7** to detect lysosomes and Hg^{2+} ion in A549 cells.

References:

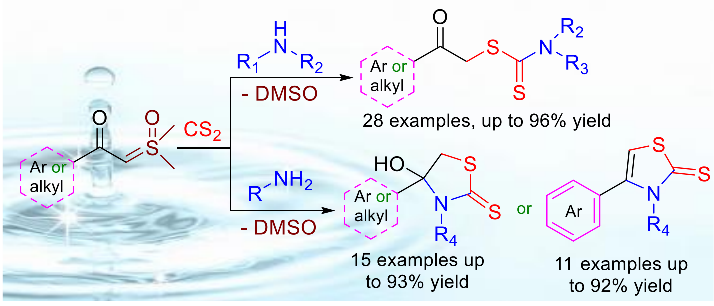
[1] C. D. Duve, R.Wattiaux, Functions of lysosomes, Annu. Rev. Physiol., 28 (1966) 435-492.
[2] T.W. Clarkson, L. Magos, G. J. Myers, The Toxicology of mercury-current exposures and clinical manifestations, N Engl. J. Med. Review article, 349 (2003) 1731-1737.

PP-82

Multicomponent Reaction of CS_2, Amines, and Sulfoxonium Ylides in Water: Straightforward Access to *β*-Keto Dithiocarbamates, Thiazolidine-2-thiones, and Thiazole-2-thiones

*Naveen Kumar and Satyendra Kumar Pandey**
Department of Chemistry, Institute of Science, Banaras Hindu University,
Varanasi, 221005, India
**Corresponding Author: Telephone number: +91-700-934-6528*
E-mail address: skpandey.chem@bhu.ac.in

Through a multicomponent reaction involving CS_2, amines, and sulfoxonium ylides, a simple, versatile, and catalyst-free synthesis approach for *β*-keto dithiocarbamates, thiazolidine-2-thiones, and thiazole-2-thiones has been disclosed. In the presence of CS_2 and secondary amines, *β*-keto sulfoxonium ylides produced *β*-keto dithiocarbamates, while dehydration of primary amines produced thiazolidine-2-thiones or thiazole-2-thiones in an acidic setting. The reaction has a broad substrate range and high functional group tolerance with minimal operational complexity. The entirety of the talk will be devoted to discussing the specifics of the synthetic approach.[1] The specifics of the findings will be shared at the poster presentation session.



References:

1. **Kumar, N.**; Sharma, A.; Kumar, U.; Pandey, S. K. *J. Org. Chem.* **2023**, *88*, 6120−6125.

Synthesis of Functionalized *S*-Benzyl Dithiocarbamates from α-Aryl diazoesters via Multicomponent Reactions with Carbon Disulfide and Secondary Amines

*[1]*Kumar N., [1]Rapelly, V., [1]Kandasamy, J.*

[1] Department of chemistry, Indian Institute of Technology (BHU), Varanasi, Uttar Pradesh-India; Email: nitinkumar.rs.chy21@itbhu.ac.in

Triflic acid promoted multicomponent synthesis of functionalized *S*-benzyl dithiocarbamates from α-aryl diazoesters, carbon disulfide and amines is reported *via* multicomponent reaction. The reactions proceeded at room temperature and gave the desired dithiocarbamates in good yields. Wide-substrate scope and easy operations are the important features of this methodology.

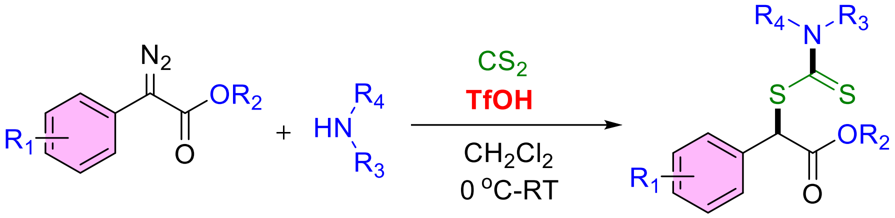


Figure 1. Synthesis of S-benzyl dithiocarbamates from α-aryl α-diazoesters.[1]

References

[1] Kumar. N, Venkatesh. R, & Kandasamy. J, *Organic & Biomolecular Chemistry.*, **2022,** *20,* 6766-6770.

PP-84

Photoredox Catalysed Benzylic C(sp^3)-H Functionalisation: A Strategy to Construct Important Heterocyclic Frameworks and Total synthesis of (+)-Centrolobine and (-)-Codonopsinine

*Km Swati Sharma and Ganesh Pandey**
Department of Chemistry, Institute of Science, Banaras Hindu University, Varanasi-221005 (U. P.), India. E-mail: ganesh.pandey1@bhu.ac.in

A mechanistically intriguing photoredox catalytic cycle is designed for the benzylic C(sp3)-H functionalization to form carbon-heteroatom (C-X) bonds directly. The utility of this redox photocycle is demonstrated as a general heterocyclisation strategy to construct lactones, lactams, cyclic ethers and cyclic amines. High yields of cyclo-etherification and -amination reaction has led to the total synthesis of (+)-Centrolobine and (-)-Codonopsinine, respectively.

PP-85

High-performance transparent conductive graphitic carbon ultrathin film

Amresh Kumar Singh[1] *and Monalisa Pal*[1]*
amaresh_1@bhu.ac.in, monalisa@bhu.ac.in
[1]*Department of Chemistry, Institute of Science, Banaras Hindu University*
Varanasi-221005, India

Graphitic carbon film, a member of the graphene family, has not attracted much attention despite of their potential advantages in synthetic method as well as in optical and electromechanical properties. This academic disinterest is due to the lack of low-cost methods for synthesizing ultra-thin films with properties comparable to graphene. In this study, we proposed the direct synthesis of ultrathin graphitic carbon film on various target substrates. We prepared an amorphous carbon ultrathin film in a microwave oven and used it as a transferable precursor film to transform it into a graphitic carbon ultrathin film. The thickness of ultra-thin graphitic carbon film was controlled in the range of 0.7 to 12 nm. Graphitic carbon ultrathin film has opto-electro-mechanical properties comparable to graphene, work function comparable to graphene (4.57 eV), high transparency with relatively low sheet resistance (83% at 1.1 kΩ sq^{-1}), stable electrical resistance upon folding, anti-oxidation, excellent flexibility, and chemical protection. This very thin graphitic carbon layer is expected to have various practical applications as a substitute for graphene. For example, we demonstrated a highly flexible pixelated display fabricated using ultrathin graphitic carbon films as electrodes in an alternating current electroluminescence (ACEL) devices.

Reference: J. Mater. Chem. C, 2020, 8, 9243--9251

PP-86

Design, synthesis & structural characterization of Bidentate Organoselone moieties

*Sanjana Srivastav, Debnarayan Nandi and Abhishek Kumar**
Department of Chemistry, Institute of Science, Banaras Hindu University, Varanasi-221005, Uttar Pradesh (India)
****Corresponding email:-** abhi.chem@bhu.ac.in*

The organoselone moieties have attracted a great deal of attention in pharmaceutical and material chemistry. In particular, Imidazole selones are used for the inhibition of lacto peroxidase-catalyzed oxidation, as analogue of antithyroid drug methimazole. In view of their importance, the development of an efficient and facile synthetic route for obtaining organoselone moieties is highly desirable.Therefore our current focus is on development of facile synthetic route for obtaining bis-Imidazole selones can bind with a number of selenophilic metal ions such as Ag^+, Hg^{2+} etc. We have now successfully synthesized a few examples of bis-Imidazole selone moieties using mesitylene backbone. The synthesized compounds have been well characterized by various physiochemical technique such as multinuclear (^1H, $^{13}C\{^1H\}$ & ^{77}Se) NMR, FT- IR, HRMS and Single Crystal X-ray diffraction studies.

Reference:

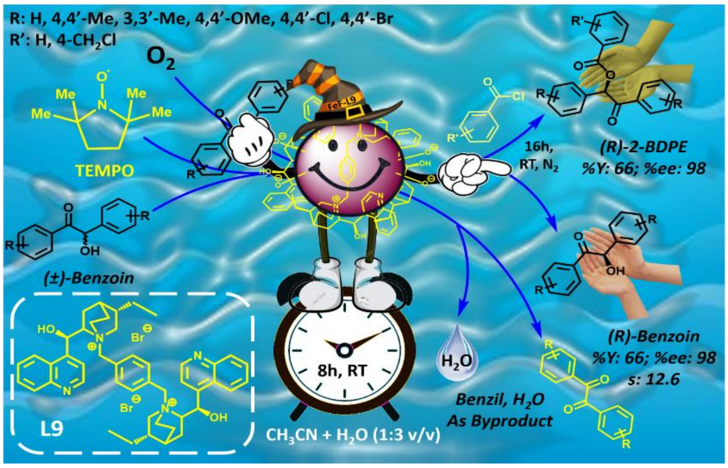
1. Prabusankar, G.; Sathyanarayana, A.; Srinivas, K.; Suresh, P.; Nath, I. *ChemistrySelect* **2018**, *3* (4), 1294–1299.
2. Roy, G.; Jayaram, P.; Mugesh, G. *Chemistry-An Asian Journal* **2013**, *8* (8), 1910-1921..

PP-87

Enantiospecific 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]*
[a] *Department of Chemistry, CAS, Banaras Hindu University, VNS-221005, Uttar Pradesh, India*
[b] *Department of Chemistry, KGTM, North Bengal University, Darjeeling-734104, Assam, India*
[c] *Department of Chemistry, Yogi Vemana University, Kadapa-516005, Andhra Pradesh, India*

The static or dynamic resolution of racemic mixtures offer facile and affordable mode 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 not synthetic extension. We report novel chiral hydrocinchonine gemini surfactant modified magnetite heterogeneous nanohybrid that could affored 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

1. P. Muthupandi, S.K. Alamsetti, G. Sekar, **2009**, *Chem. Comm.* (22), 3288-3290.
2. M. Shaikh, M. Sahu, P.K. Gavel, K.V.S. Ranganath, **2015**, *Catal. Comm.* 64, 18-21.
3. P.K. Gupta, N. Kumar, A. Mujumder, M. Pandey, P.V. Reddy, K.V.S. Ranganath, **2023**, *Asian J. Org. Chem.*, e202300325.

PP-88

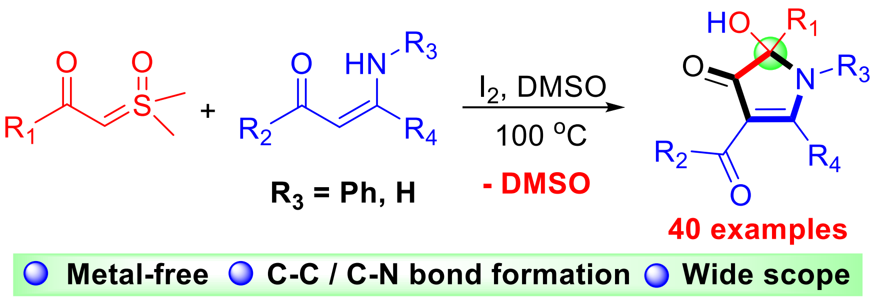
I_2-DMSO-Mediated Cascade Cyclization of *β*-Ketosulfoxonium Ylides and *β*-Enaminones: Synthesis of Quaternary Carbon Centered 2-Hydroxy-pyrrol-3(2*H*)-ones

*Rahul Kumar Saini, Paran J. Borpatra, and Satyendra Kumar Pandey**

Department of Chemistry, Banaras Hindu University, Varanasi Uttar Pradesh 221005, India

Email: skpandey.chem@bhu.ac.in

A novel I_2-DMSO-mediated cascade cyclization approach for the construction of 2-hydroxy-pyrrol-3(2*H*)-one scaffold from readily accessible *β*-ketosulfoxonium ylides and *β*-enaminone derivatives has been developed. This cascade transformation generates one C-C and one C-N bond in one pot under mild and metal-free conditions with broad functional group tolerance. In addition, this method added an active hydroxyl group to a quaternary carbon center.[1] The specifics of the findings will be shared at the poster presentation session.



Reference:

1. Saini, R. K.; Borpatra. P. J.; Pandey, S. K. *Eur. J. Org. Chem*.**2023**, *23*, e202300693.

PP-89

Tuning of Frontier Orbital Energy Levels of Fluorene Based Conjugated Porous Organic Polymer Through Introducing Electron Deficient Group for Improving Organic Photocatalysis

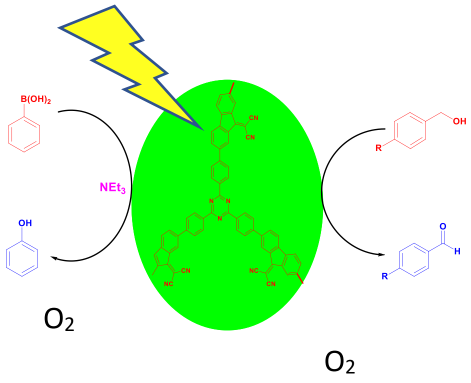
Raj Laxmi, *Biplab K Kuila*

Department of Chemistry, Institute of Science, Banaras Hindu University, Varanasi, U.P., India, 221005

Email: bkkuila.chem@bhu.ac.in

Conjugated porous organic polymers (CPOPs) are multifunctional materials that combine high surface areas with extended conjugation and porosity, making them ideal for applications like degradation, catalysis, and gas adsorption separation.[1-2] Recently, photo-catalytic organic synthesis has drawn tremendous research attention due to its favorable environmental benefits, simple setup, and mild reaction conditions.[3]

Here, we have demonstrated a novel strategy to boost organic photocatalytic activity, by engineering donor ability based on triazine based CPOP through design of fluorene-based building blocks with electron deficient group precisely positioned in the structures. Both theoretical calculations and experimental studies revealed that the CPOPs that contains fluorene moiety with CN group at 9th position exhibited the best performance [TOF (mmol $g^{-1}h^{-1}$) = 13.33 and 10.9 in 3Watt blue and white light respectively] compared to others and also much higher than the state of art photocatalysts. The high performance can be attributed to the lower band gap, suitable positioning of the HOMO/LUMO energy levels, enhanced charge transfer efficiency, and low recombination rate of electrons and holes in CPOP3. The current work contributes a fundamental insight into the structure-property relationship for photocatalysis applications of CPOP and gives guidelines for the design of efficient photocatalysts for organic reaction by small structural modification of single monomeric unit of the polymer.



References

(1) Kaur, P.; Hupp, J. T.; Nguyen, S. T. Porous Organic Polymers in Catalysis: Opportunities and Challenges. *ACS Catalysis* **2011**, *1* (7), 819–835.

(2) Dawson, R.; Cooper, A. I.; Adams, D. J. Nanoporous Organic Polymer Networks. *Progress in Polymer Science (Oxford)* **2012**, *37* (4), 530–563.

(3) Bohra, H.; Li, P.; Yang, C.; Zhao, Y.; Wang, M. “greener” and Modular Synthesis of Triazine-Based Conjugated Porous Polymers: Via Direct Arylation Polymerization: Structure-Function Relationship and Photocatalytic Application. *Polymer Chemistry* **2018**, *9* (15), 1972–1982.

PP-90

Copper-catalyzed chemoselective oxidative *o*-aroylation of 2-acetylphenols, alkyl salicylates and 1,3-dicarbonyl compounds using styrene derivatives

Upendra Kumar, Naveen Kumar and Satyendra Kumar Pandey*

Department of Chemistry, Institute of Science, Banaras Hindu University, Varanasi-221005, India

E-mail: up32sahu@gmail.com

Transition metal-based catalysis has emerged as a promising approach to a variety of chemical transformations.[1] Esterification is also not remained unimpaired to above technique to developed C-C and C-X (O, N, S) bond formation. Esterification is one of the most fundamental and important basic reactions in organic synthesis, because ester group are very important and abundant scaffolds found in natural products, medicinally relevant molecules, and functional materials.[2] An attractive approach is the direct catalytic transformation of alcohols to esters, without the use of the corresponding acid or acid-derivative.[3] Esterification done by using transition metal like Pd, Rh, Ru and Cu which is supported by some directing group.[4] Mostly transition metal esterification are known via acid or acid derivative.[5] Cu (II) metal catalysed esterification reported for direct oxidised alkylbenzene, benzaldehyde, benzyl alcohol and dibenzyl ethers which can also serve as o-aroylation or benzoylation source using only Cu (II) salts. Our approach for the preparation of phenol ester of 2-hydroxyacetophenone and alkyl 2-hydroxybenzoate using terminal alkene serve as o-aroylation in the presence Cu (II) metal and TBHP as oxidising agent. This protocol provides an efficient synthesis of phenol esters in good to excellent yields with high chemoselectivity. This method represents an alternative protocol for classical esterification reactions. The details of reactions strategy and mechanism will be presented.

References:

1. Ackermann, L.; *Chem. Rev.*, **2011**, *111*, 1315.
2. Park, J.; Han, S. H.; Sharma, S.; Shin, Y.; Mishra, N.K.; Kwak, J. H.; Lee, C.; Lee, J.; Kim, I. S. *J. Org. Chem.* **2014**, *79*, 4735.
3. Rout, S.; Guin, S.; Banerjee, A.; Khatun, N.; Gogoi, A.; Patel, B. K. *Org. Lett.* **2013**, *16*, 4106.
4. Wang, W.; Luo, F.; Zhang, S.; Cheng, J. *J. Org. Chem.*, **2010**, *75*, 2415.
5. Liu, Z.; Ma, Q.; Liu, Y.; Wang, Q. *Org. Lett.*, **2014**, *16*, 236.

Amorphous metal oxide on carbon support as bifunctional catalyst for oxygen electrocatalysis

*Varsha Singh, Vikram Rathour, Smita Singh, and Vellaichamy Ganesan**
Department of Chemistry, Institute of Science
Banaras Hindu University, Varanasi-221005, UP, India
E-mail: velganesh@yahoo.com and velgan@bhu.ac.in

It has been estimated that by the year 2050, the global energy demand will increase by double. The disturbed chain of supply and demand of fuels, mainly fossil fuels have urged researchers worldwide to find alternative sources of energy. In this regard, fuel cells and rechargeable metal-air batteries have garnered the attention of researchers owing to their high power density, zero carbon emission, and high energy efficiency. Oxygen reduction reaction (ORR) and oxygen evolution reaction (OER) are the two important reactions in rechargeable metal-air batteries. However, it should be noted that the ORR is limited by the use of expensive catalysts (like platinum on carbon, Pt/C) and the OER suffers from sluggish kinetics. Thus, designing a single catalyst that can efficiently catalyze both ORR and OER is important. Amorphous transition metal oxides are being synthesized as efficient bifunctional catalysts mainly due to variable oxidation states, loose active sites, and high stability. However, they suffer from poor conductivity and catalyst passivation during long-term use. To overcome these problems, carbon supports like graphene, mesoporous carbon nitride, and carbon nanotubes are used. In this work, amorphous metal oxide on carbon support has been synthesized and demonstrated as the efficient catalyst for both OER and ORR. The catalyst and the control samples were physiochemically characterized by powder X-ray diffraction, X-ray photoelectron spectroscopy, etc. The activity of the catalyst towards the oxygen electrocatalysis was studied using cyclic voltammetry and hydrodynamic-linear sweep voltammetry techniques. The catalyst exhibits a high positive onset potential for the ORR and a very low overpotential for the OER with high stability during long-term use.

References

1. Singh, S., Yadav, M., Singh, D.K., Yadav, D.K., Sonkar, P.K. and Ganesan, V., 2022, *New Journal of Chemistry*, *46*(28), pp.13422-13430.
2. Rathour, V., Singh, S., Singh, V., Singh, D.K., Yadav, M., Tiwari, A., and Ganesan, V., 2023, *Material Advances, under review*
3. Singh, V., Singh S., Rathour, V., and Ganesan, V., *Manuscript under preparation*.

Acknowledgments

SERB and IoE grant of BHU for financial assistance and CSIR for the JRF and SRF.

PP-92

1,4- naphthoquinone-Isoniazid hybrid molecules as potential broad spectrum antituberculosis agents

Satyam Srivastava and Harish C. Upadhyay[*]

Laboratory of Chemistry, Department of Applied Sciences, Rajkiya Engineering College (Affiliated with Dr. A.P.J. Abdul Kalam Technical University, Lucknow), Churk, Sonbhadra-231206, India

As one of the leading causes of illness and mortality worldwide, tuberculosis (TB) is a highly transmissible and frequently severe airborne disease that is brought on by the (Mtb). Nearly 10.6 million persons were predicted to have contracted tuberculosis in 2021, up 4.5% from 2020, according to the World Health Organization's Global TB report-2022. Beginning with streptomycin, and the novel drugs isoniazid (INH), pyrazinamide, ethionamide, rifampicin, and ethambutol as first-line drugs are getting failed due to development of resistance. It has been noticed that medications that target several targets may be more effective, less likely to cause resistance, and have fewer side effects rather than those traditionally acting on single target. Consequently, the pattern of drug molecules has changed from "one molecule-one target" to "one molecule-multi-target" which can be achieved by clubbing two or more scaffolds in to 'hybrid' molecules. Herein, we synthesized various hybrid molecules taking isoniazid and 1,4- naphthoquinone, a class of organic compounds that have been shown to possess antimicrobial activity. A total of seventeen derivatives were synthesized, characterized by NMR and mass spectroscopic analysis. The samples are under biological evaluation. The suitable *in silico* parameters support isoniazid-1,4- naphthoquinone derivatives as potential broad spectrum antituberculosis agents.

Keywords: Anti-tuberculosis; Isoniazid; 1,4- naphthoquinone; In silico; Drug resistance

……………………………………………………………………………………

*Corresponding author. Mobile: (+91) 9415164409;
E-mail: harishcu@gmail.com, harishcu@recsonbhadra.ac.in

Synthesis and Analysis of Properties of some Bimetallic Nanoparticles

Vidusha Singh, N. P. Singh, and Abhishek Singh**

Department of Chemistry, Udai Pratap College Varanasi, Uttar Pradesh

Along with the coordination capabilities of noble metals, recent advances in nanotechnology and material science provided new research junctures in academic research as well as in industry, which formulizes advanced applications including medical ones. Noble metal nanoparticles play a significant role in the field of biomedicine such as in the preparation of antimicrobial and antiviral agents, drug carriers, diagnostics and imaging probes.

In this work, we have performed the synthesis of bimetallic nanoparticles, as from the name, they are composed of two different metal elements. Bimetallization enhances the original single metal catalytic properties and results in improved characteristics. The addition of the second metal permits control of activity, stability and selectivity of the catalyst in certain reactions with their high surface area and presence of multiple surfaces for catalysis, resulting in high competence.

References:

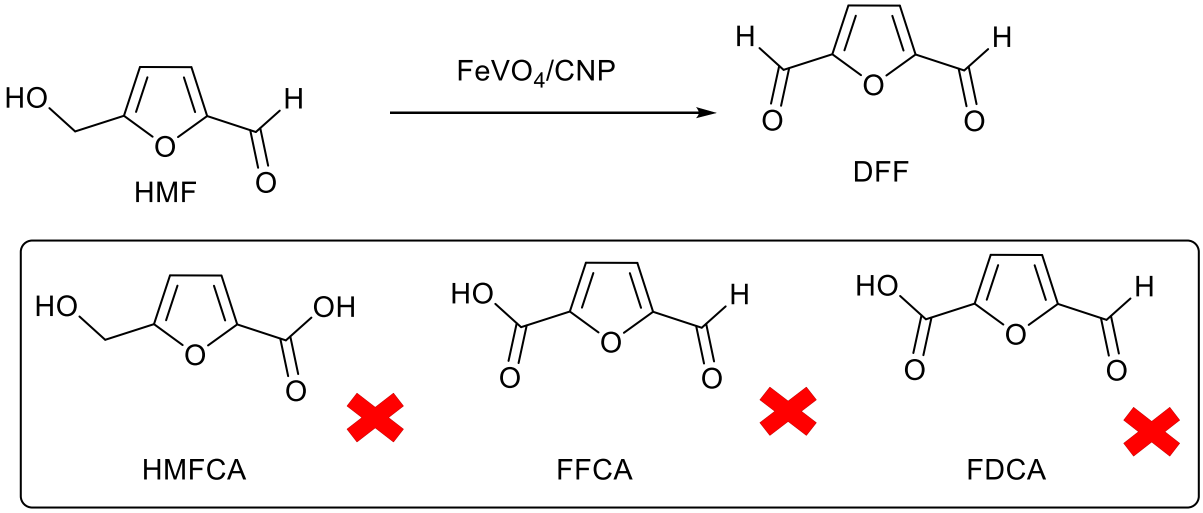
1. Sànchez-López E. et al. metal based nanoparticles as antimicrobial agents:an overview. Nanomaterials 10, 292 (2020).
2. Padilla-Cruz, A.L., Garza-Cervantes, J.A., Vasto-Anzaldo, X.G. *et al.* Synthesis and design of Ag–Fe bimetallic nanoparticles as antimicrobial synergistic combination therapies against clinically relevant pathogens. Sci Rep 11, 5351 (2021). https://doi.org/10.1038/s41598-021-84768-8
3. Ramsurn H and Gupta R. B. Chapter 15 - Hydrogenation of Nanoparticle Catalysts in *New and Future Developments in Catalysis.* Elsevier, Amsterdam, 2013 pp 347-374. https://doi.org/10.1016/B978-0-444-53874-1.00016-0

PP-94,

Design and Synthesis of Carbon-Entrapped Bimetallic Oxide as a New Hybrid Material for the Oxidation of 5-Hydroxymethylfurfural (5-HMF) to 2,5-Diformylfuran (DFF)

*Rama Jaiswal and Kalluri VS Ranganath**
Department of Chemistry, Banaras Hindu University, Varanasi
E-mail: ramaruby39@gmail.com and ranganath.chem@bhu.ac.in

Development of new materials for catalytic applications is one of the rapidly growing research areas. The selective oxidation of 5-hydroxymethyl furfural (HMF) to 2,5-diformylfuran (DFF) is one of the rapidly growing research area due to having its own importance in the fuel technology. The usual byproducts obtained in this process are FDCA, FFCA and HMFCA. However, in this process we did not get all these products . Here we report a new heterogeneous catalyst for the oxidation of HMF to DFF in aqueous medium using a carbon soot (from candle light) deposited on bimetallic oxide i.e. Fe_3O_4@C and CNP/$FeVO_4$. (Scheme 1).



Scheme 1: Selective Aerobic Oxidation of 5-HMF to DFF in an aqueous medium.

References:

1. P. Pal, S. Saravanamurugan, *ChemSusChem* **2019**, *12*, 145
2. R. Jaiswal, KVS Ranganath, *J. Inorg. Polym. Chem* **2021**, *31*, 4504-4511
3. R. Jaiswal, M. Pandey, A. Kiran Kumar, KVS Ranganath, ChemistrySelect **2023**, *8(30)*, e20232075
4. M. Pandey, R. Jaiswal, P. K. Gupta, KVS Ranganath, Inorg. Chem. Commun 2022, *146*, 110226

Electrochemical Biosensor for the Analytical Detection of Dopamine Based on PDDA/Multiwalled Carbon Nanotubes Modified Glassy Carbon Electrode

A.K. Upadhyay[1], D.M. Upadhyay[2], D.K.dubey and Dr. Amit Jaiswal*

[1]*Department of Chemistry, Sunbeam College for Women, Bhagwanpur, Varanasi-221005*
[2]*Department of Physics, Sunbeam College for Women, Bhagwanpur, Varanasi-2210053*
[3]*Department of Math, Sunbeam College for Women, Bhagwanpur, Varanasi-221005*
[4]*Department of Physics, Sunbeam College for Women, Bhagwanpur, Varanasi-2210053*
Email- up.arun@gmail.com

Neurotransmitters are biochemical molecules that transmit a signal from a neuron across the synapse to a target cell, thus being essential to the function of the central and peripheral nervous system. Dopamine is one of the most important catecholamine neurotransmitters since it is involved in many functions of the human central nervous system, including motor control, reward, or reinforcement. Fabrication of analytically reliable electrochemical biosensors for dopamine is highly essential to understand various biological processes. Here, we proposed a novel and reliable electrochemical sensing platform for the monitoring of cell-secreted dopamine based on Poly(diallyldimethylammonium chloride) (***PDDA***) decorated with multi-wall carbon nanotubes (MWCNTs) nanocomposite, which is incorporated in ormosils hybrid nanocomposite and the interconnectivity between PDDA and carbon nanotubes endow the nanocomposite with the enhancing conductivity and electrochemical activity. The PDDA-MWCNTs hybrid modified electrode exhibited excellent electrocatalytic ability for the selective detection of dopamine with a wide linear range (4 nM to 1 μM) and a low detection limit (3 nM). The developed dopamine biosensor sensor has a fast response time less than 5 sec.

* Corresponding author

Key words- Dopamine, MWCNT, Ormosils, PDDA

PP-96

DNA/protein binding and anticancer activity of ruthenium (II) arene complexes based on quinoline dipyrrin

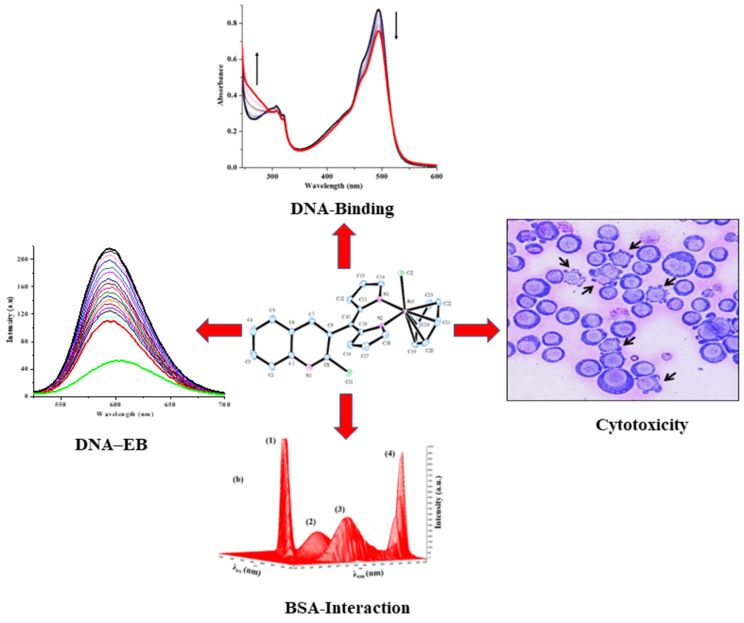
*Nikhil Kumar Singh, and Daya Shankar Pandey**

Department of Chemistry, Institute of Science,

Banaras Hindu University, Varanasi – 221 005 (U.P.), India

Arene ruthenium complexes [(η^6–arene)Ru(**L**)Cl] (η^6–arene = benzene, **R1**; *p*-cymene, **R2**) containing the chelating ligand **(2–chloro–3–(di(1H–pyrrol–2–yl)methyl)quinoline)** (L) **have been synthesized and carefully characterized by various studies (^{1}H and ^{13}C NMR, IR, ESI–MS, UV–vis). Structure of** R1 **has been verified by X–ray single crystal analyses. Binding of the complexes with calf thymus DNA (CT–DNA) have been investigated by** absorption titration, ethidium bromide (EB) displacement **and viscosity measurements. Experimental binding constants (5.1x10^4 M^{-1},** R1; **5.7x10^4 M^{-1},** R2) **suggested appreciable bonding of complexes with CT–DNA. Fluorescence, synchronous and 3D fluorescence spectroscopic studies showed that complexes strongly bind with bovine serum albumin. Intercalative interaction of the complexes with DNA has been further supported by DFT studies. Our studies have shown potential anticancer activity of both complexes** R1 **and** R2 **against T cell lymphoma.**

Keywords: Ruthenium complexes, BSA/DNA interaction, and cytotoxicity.



References:
1. Pandey et al., Dalton. Trans. **2018**, 47, 17500–17514.
2. Pandey et al., Inorg. Chem. **2013**, 52, 3687–3698.

Magnesium Oxide Nanosheets/Polyaniline Nanocomposite integrated Glassy Carbon Electrode as an Electrochemical sensing platform for the Detection of Dopamine and 4-Nitrophenol

Ashish Kumar, *Chandra Shekhar Pati Tripathi**
Department of Physics, Institute of Science, Banaras Hindu University, Varanasi Uttar Pradesh, India -221005
E-mail: verma.as.1994@gmail.com

The present work focuses on devising an electrochemical sensor, based on magnesium oxide (MgO) and polyaniline (PANI) nanocomposite modified glassy carbon electrode (GCE), with remarkable sensitivity for the rapid detection of Dopamine (DA) and 4-Nitrophenol (4-NP). 2-D MgO nanosheets were synthesized by a simple one-step sugar-blowing method and PANI was produced through oxidative polymerization of aniline. The nanocomposite (PANI/MgO-NSs) was formed by simply blending MgO nanosheets with PANI. The as-synthesized materials were characterized by Transmission electron microscopy (TEM), X-ray diffraction (XRD), and Fourier transform infrared spectroscopy (FT-IR) for their morphological and microstructural properties. The as-synthesized materials were further electrochemically characterized using Cyclic Voltammetry (CV) and Electrochemical Impedance Spectroscopy (EIS) techniques. Owing to the lowest charge transfer resistance and highest electrochemically active surface area, PANI-MgO/GCE substantially enhances the electrocatalytic oxidation of DA and the reduction of 4-NP. The analytical performance of PANI-MgO/GCE towards detecting DA and 4-NP was investigated using the more sensitive technique, Differential Pulse Voltammetry (DPV). PANI-MgO/GCE exhibited linear response within a concentration range of 5-80 μM for DA, achieving a limit of detection (LOD) of 0.75 μM and linear responses in the concentration ranges of 5−25 μM and 30−70 μM for 4-NP, with a low LOD of 2.6 μM. The developed sensor showed excellent reproducibility, high sensitivity, and selectivity and was also effectively utilized in real sample monitoring.

References

[1] X. Liu and J. Liu, *View* **2021**, *2*, 20200102;
[2] M. Lakshmanakumar, N. Nesakumar, A. J. Kulandaisamy and J. B. B. Rayappan, *Measurement* **2021**, *183*, 109873.
[3] a) A. M. Abdel-Aziz, H. H. Hassan and I. H. Badr, *ACS omega* **2022**, *7*, 34127-34135

PP 98

Dielectric and Electrical Characteristics of $Bi_{2/3}Cu_{2.9}Ni_{0.1}Ti_4O_{12}$ ceramic

Biswajit Jena, Vishnu Shankar Rai and K.D. Mandal*
Department of Chemistry, Indian Institute of Technology (Banaras Hindu University), Varanasi-221005
Email: biswajitjena.rs.chy22@itbhu.ac.in

ABSTRACT

We have investigated a low temperature chemical route of the synthesis and measured the dielecrtric and electrical characteristics of the $Bi_{2/3}Cu_{2.9}Ni_{0.1}Ti_4O_{12}$ ceramic. The synthesized material was sintered at 1123 K for 8 h in this study. The phase formation of the material was examined by the XRD pattern. The dielectric constant was observed as 1940 for $Bi_{2/3}Cu_{2.9}Ni_{0.1}Ti_4O_{12}$ ceramic at 470 K and 100 Hz. The tangent loss value for $Bi_{2/3}Cu_{2.9}Ni_{0.1}Ti_4O_{12}$ ceramic was obtained as 0.08 at 310 K and 10 kHz. The electrical conductivity of $Bi_{2/3}Cu_{2.9}Ni_{0.1}Ti_4O_{12}$ ceramic fluctuate with temperature in the range of 300-500 K, satisfying the Arrhenius equation and producing a nearly single slope. The calculated specific capacitance of $Bi_{2/3}Cu_{2.9}Ni_{0.1}Ti_4O_{12}$ based electrode is 38 F/g.

Keywords: Chemical route, XRD, Dielectric Properties, Cyclic Voltammetry.

PP 99

Graphene-Infused Conducting Polymers for Advanced Applications

*Rocky Kashyap and Ekta Sonker**
Department of Chemistry, Deen Dayal Upadhyay Gorakhpur University, 273009
**ektasonkar3@gmail.com*

Abstract

Graphene was first produced and identified by group of Andre Geim and Konstantin Novoselov and in 2010 they got Nobel prize in physics for this finding. Graphene is a single layer of carbon atoms arranged in a hexagonal lattice, has emerged as a revolutionary material with extraordinary electronic, mechanical and thermal properties. Graphene's exceptional electrical conductivity and transparency make it an ideal candidate for the next generation of electronic devices and complements the properties of conducting polymers. Some common conducting polymers include polyaniline, polypyrrole, and polythiophene. These polymers exhibit semiconducting or conducting behavior due to their conjugated structures. When graphene is introduced into these polymer matrices, it can enhance the overall electrical conductivity of the composite. The improved electrical performance of these materials makes them promising candidates for advanced applications in energy storage, sensing, and electronic devices. The compatibility of these composites with scalable fabrication processes is emphasized, making easier for cost-effective and large-scale production. In conclusion, the incorporation of graphene into conducting polymers has led to the development of composite materials with enhanced properties, making them valuable for various applications.

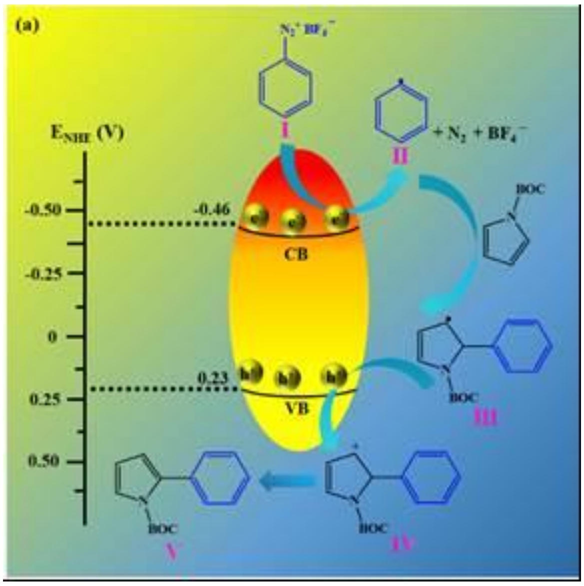
PP 100

A Photocatalytic C-H Activation for the Arylation of Heteroarenes by Using Ultrathin Bismuthene Nanosheets

Ajit Kumar Singh, Arindam Indra[a],*

[a]Department of Chemistry, Indian Institute of Technology (BHU), Varanasi, UP-221005, India. Email: arindam.chy@iitbhu.ac.in

Abstract: Bismuthene, 2D nanosheets of bismuth with a graphene-like structure, has recently been explored for the electrochemical and photocatalytic energy conversion processes. The optimized band structure tuned electronic properties, and the contribution from the f-orbitals make it a unique material in the field of catalysis. Although a growing interest on bismuthene-catalyzed energy conversion processes has been observed, its use for organic transformation is rarely studied. Herein, we have demonstrated the synthesis of ultrathin bismuthene nanosheets and its use for the photocatalytic C-H arylation of heteroarenes. In the presence of light, bismuthene catalyzes the generation of aryl radicals from diazonium salt which is trapped in the presence of suitable heteroarenes (thiophene, furan, and pyrrole), leading to C*sp*^{2}-C*sp*^{2}(-) coupling to form aryl-functionalized heteroarenes. A series of aryldiazonium salts having electron donating and withdrawing groups produce moderate to high yield reacting with heteroarenes. Interestingly, the catalyst can be recycled for five times with a minimum loss of activity. Further, the photoredox reactions has been extended for the borylation of diazo salt.



Scheme. Reaction mechanism of the photocatalytic C-H activation by the Bismuthene photocatalyst.

List of Sponsors

Tokyo Chemical Industry (India) Pvt. Ltd.
Moving Your Chemistry Forward

ACS

Reaxys®
Improved synthetic planning with Reaxys

ELSEVIER

SERB INDIA

BANARAS HINDU UNIVERSITY

INSTITUTIONS OF EMINENCE (IoE) SCHEME

Advance Quality Traders	Uma Scientific Traders	Gyan Scientific Traders

Compiled by Dr. Kanak Roy
Thanks to Satyam, Avinash, Ritesh, Priya, and Sanjana for their help.