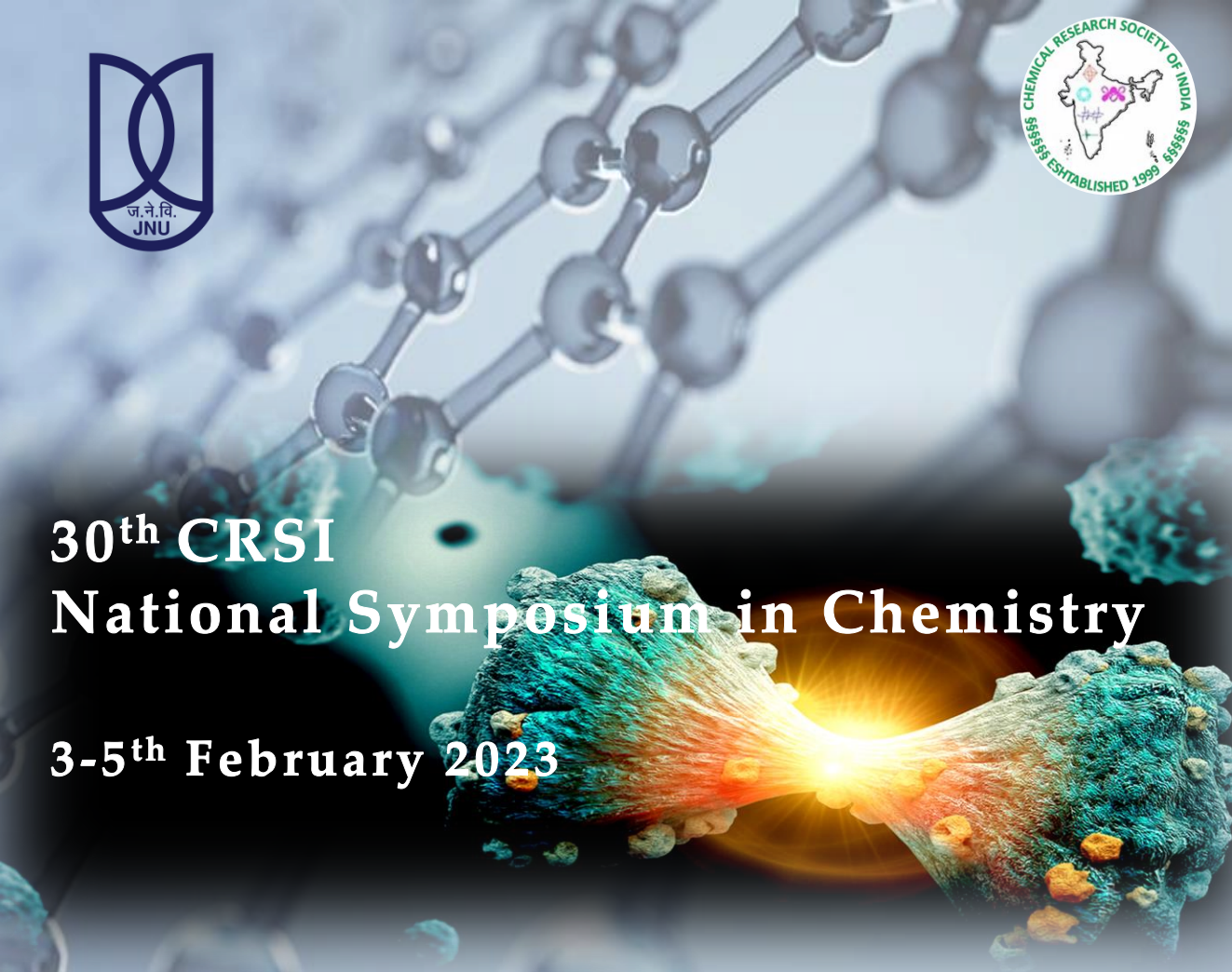

30th CRSI National Symposium in Chemistry

3-5th February 2023

Organized by
SCMM & SPS
Jawaharlal Nehru University
New Delhi, India

ROYAL SOCIETY OF CHEMISTRY

2023

Abstract Book

प्रोफेसर शांतिश्री डी. पंडित
कुलगुरु
Professor Santishree D. Pandit
Vice-Chancellor

जवाहरलाल नेहरू विश्वविद्यालय
JAWAHARLAL NEHRU UNIVERSITY
नई दिल्ली-११००६७
NEW DELHI-110067

It is a matter of great pride and honour that Jawaharlal Nehru University (JNU) will be hosting the National Symposium in Chemistry (NSC) of Chemical Research Society of India (CRSI) and a joint symposium with Royal Society of Chemistry (RSC) for the first time. The symposium will be jointly organized by Special Centre for Molecular and the School of Physical Sciences. CRSI has recognised the need to promote quality research in chemistry and foster talent in the form of recognition at various levels. Since the inception of CRSI, the National Symposia in Chemistry have a history of providing a platform for meaningful scientific exchange that has made a profound difference to the community of chemists in the country. The 30th conference in the series will be held during 2-5 February 2023 with JNU as the host institute. This year, the 16th edition of the CRSI Royal Society of Chemistry (CRSI-RSC-16) symposium on 2nd February 2023 will be dedicated to "***Health and Well-being***" which has been the central focus during the time of COVID-19 Pandemic. Needless to say, research in the interdisciplinary area of health has a strong bearing on the well-being of our society and plays a crucial role towards realizing the mission of Atmanirbhar Bharat (self-reliant India).

During the past five decades, JNU has emerged as a world-renowned institution in the country emphasizing quality research and teaching in the fields of pure and applied sciences, social sciences, international studies and humanities. Currently, there are 14 schools, 07 special centres and several centres within the schools in the university. JNU was accredited with A++ grade by the NAAC for the period 2017-2022. JNU has consistently ranked number 2 among all universities by NIRF, Government of India. JNU received the Visitor's award of "Best University" in the year 2017 from the President of India. From being a student at the University to being its first female Vice Chancellor, I can proudly say that JNU stands for Inclusion, Integrity and Innovation.

I congratulate the organising team for their hard work and meticulous planning in conducting the 30th CRSI NSC and wish them a grand success. As the head of the Institution, I would like to heartily welcome all the delegates and participants of the symposium to JNU as the nation celebrates Azadi ka Amrit Mahotsav and hope that you have a wonderful time and enriching experience during the symposium.

Santishree Pandit
13/1/23

Prof. Santishree Dhulipudi Pandit

Message from the President, CRSI

I am glad that the Special Centre for Molecular Medicine and the School of Physical Sciences, Jawaharlal Nehru University, New Delhi are jointly hosting the 30th National Symposium in Chemistry of Chemical Research Society of India (CRSI-NSC-30) and the 16th joint symposium with the Royal Society of Chemistry (CRSI-RSC-16) during 2-5 February 2023. The theme of the CRSI-RSC-16 will be "Health and Wellbeing".

The CRSI was established in 1999 as a part of the celebration of 50th year of India's independence. Since then, it has played a pivotal role in promoting chemical science by bringing together chemists on a platform through the organization of symposia. Currently, there are more than 3500 life members of the CRSI which have deep international cooperation with the RSC, American Chemical Society (ACS), Asian Chemical Editorial Society (ACES), commonwealth Chemistry (CC), etc. The CRSI acknowledges the contributions of chemists in the form of various awards and medals.

This year's highlights of the program will be lectures by CRSI medal recipients, endowment lectures, and CRSI-RSC lectures. There will be poster presentations spanning all areas of Chemistry. I am quite sure that the delegates and participants would benefit immensely from this symposium.

On behalf of the CRSI, I would like to extend a very warm welcome to all the eminent delegates from academia and industry as well as young researchers to this symposium.

I wish you great success for the symposium.

Sincerely,

VKSingh

Prof. Vinod K. Singh
President, CRSI

सत्यमेव जयते
स्वच्छ भारत
एक कदम स्वच्छता की ओर
आज़ादी का अमृत महोत्सव

डॉ. एस. चंद्रशेखर
Dr. S. Chandrasekhar

सचिव
भारत सरकार
विज्ञान एवं प्रौद्योगिकी मंत्रालय
विज्ञान एवं प्रौद्योगिकी विभाग
Secretary
Government Of India
Ministry of Science and Technology
Department of Science and Technology

18th January, 2023

MESSAGE

I am pleased to know that the 30th National Symposium of the Chemical Research Society of India (CRSI-NSC-30) and the 16th CRSI Royal Society of Chemistry (CRSI-RSC-16) Symposium Series in Chemistry is being organised by the Special Centre for Molecular Medicine and the School of Physical Sciences, Jawaharlal Nehru University during February 2-5, 2023.

It is heartening to note that one of the main objectives of CRSI is to organize events including conferences, seminars, workshops, symposia etc., which provide an excellent platform for exchange of ideas in all branches of chemistry. This facilitates effective networking amongst researchers working in chemistry and allied disciplines. Further, CRSI also aims to encourage and foster talent in chemistry through various awards for the outstanding contributions of researchers at appropriate levels.

The National Symposium in Chemistry aims to provide a forum for scientists, teachers and students to discuss the recent developments in chemical sciences. In addition, one of the main objective of the symposium is also to create opportunities for exchange of ideas and to build long lasting collaborative endeavours in the frontier areas of chemistry. The focus area of this year's Symposium i.e. "Health and Well-being" is contemporary and of paramount importance in the current times. As we celebrate Azadi ka Amrit Mahotsav (75th anniversary of Indian Independence), I sincerely hope that the deliberations during the symposium will generate innovative ideas contributing to the dream of self-reliant India (*Atma-nirbhar Bharat*).

I extend my best wishes to the organizing team at JNU and welcome all participants.

I wish the event a grand success.

(S. Chandrasekhar)

Technology Bhavan, New Mehrauli Road, New Delhi - 110016
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Message from Convenor and Co-Convenors

Dear Delegates,

Greetings from the Organizing Committee, 30th CRSI-NSC & 16th CRSI-RSC Symposium Series in Chemistry!

On behalf of the Special Centre for Molecular Medicine (SCMM), School of Physical Sciences (SPS), and the organizers at Jawaharlal Nehru University (JNU), New Delhi, we welcome you all to the 30th CRSI-NSC & 16th CRSI-RSC Symposium Series in Chemistry scheduled from 2nd to 5th February 2023 at Jawaharlal Nehru University, New Delhi. The symposium is jointly organized by the Special Centre for Molecular Medicine and the School of Physical Sciences, Jawaharlal Nehru University, New Delhi. The 16th joint symposium with the Royal Society of Chemistry CRSI-RSC-16 is scheduled on 2nd Feb. 2023 and the theme of the CRSI-RSC-16 will be "***Health and Wellbeing***". The 30th National Symposium in Chemistry of Chemical Research Society of India (CRSI-NSC-30) will begin on 3rd February 2023. The symposium includes Medal lectures, CRSI-RSC lectures, and Endowment Lectures from distinguished Scientists. Apart from these lectures, more than 250 posters will be presented by young researchers during the symposium. There will be an RSC-CRSI panel discussion on "***Chemistry for India's Health Equity***" and Prof. Javed Iqbal has kindly agreed to chair the panel.

The symposium will start at 9.30 AM on 2nd February and will continue till 2.00 PM on 5th of February, 2023 aiming to showcase the research activities of faculty members/scientists and research scholars from various top-notch institutions all over India. The purpose of this symposium is to serve as a platform for collaborations between academic institutions and industry. This prestigious conference also provides a platform, where researchers from academia & industry, teachers, and students across the country come together and deliberate the recent advances in the area of chemical sciences.

Once again, we wish you all an engaging and productive conference participation. Our best wishes for the conference and hope it will be in great success.

Prof. Vibha Tandon
(Convenor)

Prof. Akhilesh K. Verma (Co-Convenor)

Prof. Ram Sagar Misra
(Co-Convenor)

PATRON

Prof. Santishree D. Pandit
Vice Chancellor, JNU

PRESIDENT CRSI

Prof. Vinod K. Singh

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(Convenor)

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7. Dr. Dinabandhu Das (SPS, JNU)
8. Any Finance representative of SCMM, SPS, & JNU

SPEAKERS

Prof Goverdhan Mehta
University of Hyderabad
(Junjappa-Ila Endowment Lecture)

Prof. Richard Winpenny
University of Manchester, UK
(Animesh Chakravorty Endowment Lecture)

Prof. Ram Seshadri
University of California, Santa Barbara
(CNR Rao Award Lecture)

Dr. Rajesh S. Gokhale
Secretary, DBT
(CRSI-RSC Lecture)

Dr. Radha Rangarajan
Director, CSIR- CDRI
(CRSI-RSC Lecture)

Prof. Stuart John Conway
University of Oxford, UK
(CRSI-RSC Lecture)

Dr. Vidya Ramadas
Director, Enveda Biosciences
(CRSI-RSC Lecture)

Prof. M. Carmen Galan
University of Bristol, UK
(CRSI-RSC Lecture)

Dr. Ana Rodriguez-Mateos
King's College, London
(CRSI-RSC Lecture)

Dr. Souvik Maiti
CSIR- IGIB
(CRSI-RSC Lecture)

CRSI Medal Lectures

Prof. Vishwakarma Singh
IIT Bombay
Gold Medal Lecture

Prof. S. Ramasesha
IISc Bangalore
Gold Medal Lecture

Prof. K. N. Singh
BHU, Varanasi
Silver Medal Lecture

Prof. Sanjay Mathur
Univ. of Cologne, Germany
(CRSI Medal Lecture)

CRSI Bronze Medal Lectures

Dr. Amit Kumar
IIT- Patna

Prof. Baskar Sundaraju
IIT- Kanpur

Prof. D. Mukherjee
Bose Institute, Kolkata

Dr. Sakya S. Sen
CSIR- NCL

Dr. Debasis Banerjee
IIT- Roorkee

Prof. J Sankar
IISER- Bhopal

Dr. Joydev K. Laha
NIPER, Mohali

Dr. S. A. Babu
IISER Mohali

Dr. KRS Chandrakumar
BARC, Mumbai

Prof. M. Sankar
IIT- Roorkee

Dr. P. C. Ravikumar
NISER- Bhubaneswar

Prof. Sujit K. Ghosh
IISER Pune

Dr. Prathama S. Mainkar
CSIR- IICT

Prof. R Kothandaraman
IIT- Madras

Prof. Rodney A. Fernandes
IIT- Bombay

Dr. Tharamani C. Nagaiah
IIT- Ropar

30th CRSI-NSC & 16th CRSI-RSC Symposium Series in Chemistry

Venue: Auditorium 1, Convention Centre, JNU

16th CRSI-RSC Symposium

February 02, 2023 (Thursday)
One Day Symposium on "Health and Well Being"

08:30-09:30	**REGISTRATION**
09:30-10:15	**Welcome Address by RSC Representatives and Convener of CRSI**
Session I 10:15-11:15	**Chairpersons:** Prof. Sandeep Verma, IIT Kanpur & Prof. Rakesh K. Tyagi, SCMM, JNU
10:15-10:45	**Special Lectures** ***Dr. Rajesh S. Gokhale***, Secretary DBT, New Delhi **Title:** Fostering Biotech Innovation and Bioeconomy
10:45-11:15	***Professor Carmen Galan,*** University of Bristol, UK **Title:** Photoresponsive Ligands to Modulate G-quadruplex DNA
11:15-11:45	**High Tea**
Session II 11:45-13:15	**Chairperson:** Prof. H. Ila, JNCASR, Bangalore & Prof. D. S. Reddy, CSIR-IICT, Hyderabad
11.45-12:15	***Dr. Radha Rangarajan,*** CSIR-CDRI, Lucknow **Title:** Developing Drugs for India: Opportunities and Challenges
12:15-12:45	***Prof. Stuart J. Conway,*** University of Oxford **Title:** Chemical Approaches to Targeting and Imaging Tumour Hypoxia
12:45 -13:15	***Dr. Souvik Maiti***, CSIR- IGIB, New Delhi **Title:** Correcting Genes with Precision: An Indigenous Approach
13:15-14:15	**Lunch**
Session III 14:15-15:45	**Chairpersons:** Prof. Chinmay K. Mukhopadhyay, SCMM, JNU & Prof. Gobardhan Das, SCMM, JNU
14:15-14:45	***Dr Ana Rodrigez-Mateos,*** King's College, London **Title:** Nutrition's Dark Matter: Beyond Traditional Nutrients
14:45-15:15	***Dr. Vidya Ramadas,*** Medicinal Chemistry, Enveda Biosciences, Hyderabad **Title:** Discovery of New Drugs and Associated Challenges from a Chemist Perspective
15:15-15:45	***Dr. Sam Jones,*** *University of Manchester* **Title:** Virucidal Antivirals - Preparing for the next pandemic
15:45-16:15	**Tea/Coffee Break**
16:15-17:45	RSC-CRSI Panel Discussion on **"Chemistry for India's Health Equity"** **Moderator:** Prof. Javed Iqbal, Incor Renovis Labs Pvt Ltd., Hyderabad **Panelists:** Prof. Sandeep Verma, IIT Kanpur; Dr. P. K. Jadav, Enveda Biosciences, Hyderabad: Dr. Sanjay Mishra, DBT, New Delhi; Dr. BVNBS Sarma, Sai Life Sciences, Hyderabad
19:30 onwards	**Dinner for CRSI-RSC Delegates**

30th CRSI-National Symposium in Chemistry

Venue: Audi 1, Convention Centre, JNU

February 03, 2023 (Friday)

08:30-09:30	**REGISTRATION**
9:30-10:45	**INAUGURATION** & Presidential Address by **Prof. Vinod K. Singh**, President CRSI & IIT Kanpur
10:45-11:15	**Tea/Coffee Break**
Session 1 **11:15-13:15**	**Junjappa-Ila Endowment Lecture 2023** **Chairperson:** Prof. S. Chandrasekaran, IISc., Bangalore
11:15-11:55	***Prof. Goverdhan Mehta***, *HCU, Hyderabad* **Title:** Chemistry – A Pivotal Science for Sustainability of People and the Planet
	CRSI Silver Medal Lecture **Chairperson:** Prof. T. Punniyamurthy, IIT Guwahati
11:55-12:35	***Prof. Krishna Nand Singh***, Banaras Hindu University, Varanasi **Title:** Some Advancements in Organic Synthesis Using New Synthons and Decarboxylative Coupling Reactions
	CRSI Bronze Medal Lectures **Chairperson:** Dr. Vijay Pal Singh Rawat, SCMM, JNU
12:35-12:55	***Dr. Rodney Fernandes,*** *IIT Bombay* **Title:** Total Synthesis of γ-Lactone and THF Natural Products
12:55-13:15	***Dr. Debasis Banerjee,*** *IIT Roorkee* **Title:** Hydrogen Borrowing and Interrupted Hydrogen Borrowing Catalysis; Applications and Mechanistic Studies
13:15-14:00	**Lunch Break and Photo Session**
14:00-16:00	**POSTER PRESENTATIONS-I (Poster Nos. P001-P130)** **Chairpersons:** Prof. Bijoy Kuanr, SPS, JNU; Prof. Parthasarathi Das, IIT-ISM, Dhanbad; Prof. G. Sekar, IIT Madras; Prof. Ravi P. Singh, IIT, New Delhi; Dr. D. K. Mohapatra, CSIR-IICT, Hyderabad; Dr. Jaydeep Saha, CBMR, Lucknow; Dr. Dinabandhu Das; Dr. Debamalya Roy, DRDO - DMSRDE, Kanpur; Dr. Pijus K. Sasmal, SPS, JNU, and Dr. Manoj Munde, SPS, JNU.
14:00-15:30	**COUNCIL MEETING** Only for Council Members, **Venue**: Meeting Room Convention Center, JNU
15.30-16.00	**Tea/Coffee Break**
Session 2 **16:00-18:10**	**CRSI Medal Lecture** **Chairperson:** Prof. Sourav Pal, Ashoka University, Haryana
16:00-16:30	***Prof. Sanjay Mathur***, University of Cologne, Germany **Title:** Chemically Processed Functional Ceramics for Energy and Health Applications

	CRSI Bronze Medal Lectures **Chairperson:** Prof. Uday Maitra, IISc. Bangalore & Prof. Kamal K. Kapoor, Jammu University
16:30-16:50	***Dr. Sakya Singha Sen,*** CSIR-NCL Pune **Title:** The Chemistry of Silicon in Low Oxidation State
16:50-17:10	***Dr. Sujit Kumar Ghosh,*** IISER Pune **Title:** Functional Microporous Materials for Industrially Relevant Hydrocarbons Separation
17:10-17:30	***Dr. Tharamani C. Nagaiah,*** IIT Ropar **Title:** Hydrogen production from waste H_2S pollutant
17:30-17:50	***Prof. Basker Sundararaju,*** IIT Kanpur **Title:** Does Oxidation State Matter in Cobalt-Catalyzed Sustainable Transformations?
17:50-18:10	**SPECIAL SESSION** *RSC Presentation and Discussion on the Draft of **"Gender Diversity in India"***
19:30 Onwards	**Dinner**

30th CRSI-National Symposium in Chemistry

February 04, 2023 (Saturday)

Session 3 **09:30-11:00**	**CNR Rao Award Lecture** **Chairperson:** Prof. K. N. Ganesh, IISER, Tirupati
9:30-10:00	***Prof. Ram Sheshadri,*** University of California, Santa Barbara **Title:** Chemistry and Design in Magnetic and Battery Materials
	CRSI Bronze Medal Lecture **Chairperson:** Prof. J. K. Bera, IIT Kanpur & Prof. G. Mugesh, IISc. Bangalore
10:00-10:20	***Prof. R. Kothandaraman,*** IIT Madras, Chennai **Title:** In-situ Restoration of Energy Delivery in an Organic Flow Battery
10:20-10:40	***Dr. J. Sankar,*** IISER, Bhopal **Title**: Efficient routes to harvest energy from solar radiation using conjugated molecules as antenna complexes
10:40-11:00	***Dr. KRS Chandra Kumar,*** BARC, Mumbai **Title:** Theoretical Insights into the Activation of Covalent Bonds under Nanoconfinement
11:00-11:30	**Tea/Coffee Break**
Session 4 **11:30-12:50**	**CRSI Bronze Medal Lectures** **Chairperson:** Prof. H. N. Ghosh, BARC, Mumbai & Prof. Ranjana Aggarwal, CSIR- NIScPR, New Delhi
11:30-11:50	***Prof. M. Sankar,*** IIT Roorkee **Title:** π-Extended Porphyrins and Their Analogues: Synthesis, Spectral, and Redox Properties and Their Application in Sensing, Nonlinear Optics and Catalysis

11:50-12:10	***Dr. Debaraj Mukherjee***, Bose Institute, Kolkata **Title:** Recent Development on Construction of Various Aromatic Chiral Cores from Glycals
12:10-12:30	***Dr. P. C. Ravi Kumar,*** NISER Bhubaneswar **Title:** Palladium-Catalyzed C-C bond Cleavage of Carbocyclic Strained Systems: A Useful Strategy in Organic Synthesis
12:30-12:50	***Dr. S. A. Babu,*** IISER Mohali **Title:** Palladium-(II)-Catalyzed C-H Functionalization of Diastereotopic C-H Bonds
12:50-14:00	**Lunch Break**
14:00-16:00	**POSTER PRESENTATIONS-II (Poster Nos. P131-P262)** **Chairpersons:** Dr. Raja Angamuthu, IIT, Kanpur; Dr. Arnab Bhattacharjee, SCIS, JNU; Dr. Neel S. Bhavesh, ICGEB, New Delhi; Dr. Anil Kumar, BITS Pilani; Dr. Srabani Taraphder, IIT Kharagpur; Dr. Ankita Rai, SPS, JNU; Dr. Supriya Sabbani, SPS, JNU; Dr. Vijay Goel, SPS, JNU and Dr. Amit Kumar, IIT Patna
15:30-16:00	**Tea/Coffee Break**
Session 5 **16:00-18:50**	**Gold Medal Lecture** **Chairperson:** Prof. Vinod K. Singh, IIT, Kanpur, and Prof. N. Sathyamurthy, IISER Mohali
16:00-16:40	***Prof. Vishwakarma Singh,*** IIT Bombay **Title:** Molecular Complexity from Aromatics: Concept, Strategy, and Reality
16:40-17:20	***Prof. S. Ramasesha,*** IISc. Bangalore **Title:** Importance of Electron Repulsions
17:20-18:50	**Presentation of Medals and General Body Meeting**
19:30 onwards	**Dinner**

February 05, 2023 (Sunday)

Session 6 **09:30-10:45**	**CRSI Bronze Medal Lecture** **Chairperson:** Prof. A. K. Ganguli, IIT Delhi & Prof. Rajiv Bhat, SBT, JNU
09:30-9:50	***Dr. Prathama Mainker,*** CSIR-IICT, Hyderabad **Title:** Easy access to diverse natural products through aryne insertion
09:50-10:10	***Dr. Amit Kumar***, IIT Patna **Title:** Glycosylation and Glycodiversification: An Important aspect of Carbohydrate Chemistry
10:10-10:30	***Dr. Joydev Laha,*** NIPER Mohali **Title:** Opportunities and Challenges in the Synthetic Process Development for Pharmaceuticals

10:30-11:00	**Tea/Coffee Break**
Session 7 **11:00-12:00**	**Presentation by DRDO Delegate and BARC** **Chairperson:** Prof. Ram Vishwakarma; CSIR Distinguished Scientist, CDRI Lucknow & Prof. D. S. Rawat, University of Delhi
11:00-11:20	***Dr. Debmalya Roy***, DMSRDE, DRDO, Kanpur **Title:** Stretchable and Printable Nanocomposite Materials for Remote Monitoring of Physiological Parameters
11:20-11:40	***Dr. Jyotirmayee Mohanty,*** BARC, Mumbai **Title***:* Cucurbituril-based Supramolecular Assemblies: Prospective Applications
11:40-12:00	***Dr. Puja Panwar Hazari***, INMAS (DRDO), Delhi **Title**: Cyclotron-Produced Innovative Radionuclides for Theranostic Applications
Session 8 **12:00-13:30**	**Animesh Chakravorty Endowment Lecture 2023** **Chairperson:** Prof. S. Chandrasekhar, Secretary DST, New Delhi
12:00-12:40	***Prof. Richard Winpenny***, University of Manchester, UK **Title:** Synthesis and Study of Polymetallic Cage Complexes Involving Molecular Magnetism
12:40-12:50	**CRSI-ACS Best Poster Awards**
12:50-13:00	***Dr. Rupam Dinda,*** NIT, Rourkela **Presentation by Organizers of 31st CRSI-NSC from Rourkela**
13:00-13:10	**Concluding Remarks** ***Prof. Vinod K. Singh,*** President CRSI
13:10-13:30	**Vote of Thanks** ***Prof. Neelima Gupta,*** Secretary, CRSI **Co- Convenor** 30th CRSI-NSC, JNU
13:30-14:30	**Lunch and Departure**

Special Award Lectures

Junjappa-Ila Endowment Lecture 2023

Chemistry – A pivotal Science for Sustainability of people and the planet

Prof Goverdhan Mehta
University Distinguished Professor &
Dr. Kallam Anji Reddy Chair
University of Hyderabad

Prof. Goverdhan Mehta, *FRS*
University Distinguished Professor &
Dr. Kallam Anji Reddy Chair
University of Hyderabad

Prof Goverdhan Mehta received his Ph.D. from Pune University and did his post-doctoral research at Michigan State University under Prof. Don Farnum and at the Ohio State University under Prof. Paul G. Gassman. He joined IIT Kanpur in 1969 and remained there until 1977. From 1977 to 1998, he was a Professor of Chemistry at the University of Hyderabad; from 1998 to 2010, he was a Professor at the Indian Institute of Science Bangalore. He was Vice-Chancellor, University of Hyderabad, from 1994–98 and Director Indian Institute of Science, Bangalore, from 1998–2005. From 2010 onwards, he is University Distinguished Professor and Dr. Kallam Anji Reddy Chair at the Department of Chemistry, University of Hyderabad, India. Prof. Mehta has authored more than 450 research papers. He is a recipient of over 40 Honorary Doctorates from India/abroad and has delivered over 300 invited/plenary lectures at Universities/Institutions across the world.

Research Interests:

- Design and reactivity of novel molecular objects and entities, total synthesis of complex bioactive natural products.
- Creation of NCE's for drug discovery, origin, and control of stereogenesis
- Crystal engineering of conformationally locked polyols and photodynamic therapy of cancer.
- More recently he is involved in profiling and promoting chemical sciences as 'sustainability science'.

Awards/Recognitions:

- Fellow of the Royal Society (2005)
- Prof Mehta is a Fellow of all three National Science Academies in India and a Fellow of the World Academy of Sciences (TWAS).
- Padma Shri (2001); Shanti Swarup Bhatnagar Prize (1978)
- President, Chemical Research Society of India (2002-2005)
- President, Association of Indian Universities (2003)
- President of ICSU (2005-2008)
- Chairperson, National Accreditation and Assessment (NAAC) (2006-2012)
- Chairman, Board of Governors, Indian Institute of Technology Jodhpur (2014-2018).

Animesh Chakravorty Endowment Lecture 2023

From Rings to Nanostructures

Prof. Richard Winpenny
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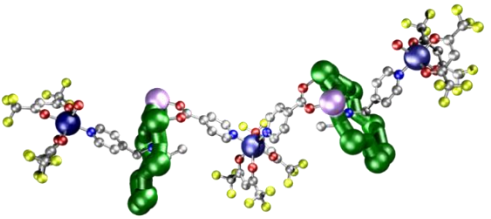

Around fifteen years ago it was proposed that molecular magnets could be used as qubits for quantum information processing.[1,2] The major advantage that molecules possess over other proposed hardware is the potential to control inter-spin interactions. We are pursuing chemistry to link together heterometallic rings to make large supramolecular structures that bring together multiple such potential qubits. These include [13] rotaxanes grown around a $\{Pd_6\}$ octahedron,[3] and attachment of $[10^{14}]$ rings to a bead producing a form $[10^{14}]$ rotaxane.[4] In some cases, we can include switchable units that allow us to propose strategies to implement entangling gates such as the CNOT or the $\sqrt{\text{iSWAP}}$ gate.[5] In other cases we have attempted to build supramolecules that could model decoherence in quantum teleportation.

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Richard Winpenny obtained both his degrees from Imperial College London; his Ph.D. studies were with Prof. David Goodgame on metal-organic frameworks. After a postdoctoral position with Prof. John Fackler Jr., at Texas A&M University he joined the staff at the University of Edinburgh in 1990. In 2000 he moved to Manchester as a Professor of Inorganic Chemistry in 2000. He has published around 420 papers witan a h-index of 78.

Research Interests:

- Coordination and supramolecular chemistry
- Molecular magnetism
- Nanofabrication

Awards and Honours:

- Royal Society of Chemistry Dalton Division Horizon Prize 2021 (lead of prize-winning Molecular Magnetism team)
- Royal Society of Chemistry Ludwig Mond Prize 2016
- Royal Society of Chemistry Emerging Technologies Winner for Materials 2016 (for spin-out Sci-Tron Ltd)
- Royal Society of Chemistry Tilden Prize 2011
- Royal Society Wolfson Merit Award 2009-2014
- Member Academia European
- Fellow of the Learned Society of Wales elected 2016
- Fellow of the Royal Society of Chemistry elected 2011

CNR Rao Award Lecture

Chemistry and Design in Magnetic and Battery Materials

Prof. Ram Seshadri

Distinguished Professor, Materials Department, and Department of Chemistry and Biochemistry, University of California

Email: seshadri@mrl.ucsb.edu

Advancing the goal of materials-by-design requires the ability to screen materials for function. This is the almost trivial first step *en route* to a paradigm of dialing up the optimal material structure and composition to serve a particular function. Several issues that make even this task of screening somewhat complex. The first is that many properties of interest are not tractably calculated in a reliable way, because the underlying science is as-yet not established. The second is that materials optimization is frequently based on much more than a single performance criterion. In this talk, I will describe a computational proxy that has allowed us to establish guidelines to find better magnetocaloric materials.[1] I will separately discuss the chemistry of early 4d transition metals and how some of them, within specific crystal structural families, could be employed in fast-charging batteries,[2] including through the use of metal-metal bonding to control the voltage and enhance structural rigidity during lithium insertion/de-insertion.[3]

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1. Bocarsly, J. D.; Levin, E. E.; Garcia, C. A. C.; Schwennicke, K.; Wilson, S. D.; Seshadri, R.; *Chem. Mater.*, **2017**, *29*, 1613–1622.
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Prof. Ram Seshadri

Distinguished Professor,
Materials Department, and Department of
Chemistry and Biochemistry, University of California
Email: seshadri@mrl.ucsb.edu

Ram Seshadri received his PhD in Solid State Chemistry in 1995 from the Indian Institute of Science (IISc), Bangalore, working under the guidance of Professor C. N. R. Rao FRS. After some years as a postdoctoral fellow in France (Bernard Raveau) and Germany (Wolfgang Tremel), he returned to IISc as an Assistant Professor in 1999. He moved to the Materials Department (College of Engineering) at UC Santa Barbara in 2002. Since 2020, he is a Distinguished Professor in the Materials Department and the Department of Chemistry and Biochemistry. He is also the Fred and Linda R. Wudl Professor of Materials Science and Director of the Materials Research Laboratory: A National Science Foundation Materials Research Science and Engineering Center (NSF-MRSEC). His work, embodied in over 400 journal publications, broadly addresses the topic of structure–composition–property relations in crystalline inorganic and hybrid materials, with a focus on magnetic materials and materials for energy conversion and storage.

Awards and Honours:

- He is Fellow of the Royal Society of Chemistry, the American Physical Society, and the American Association for the Advancement of Science.
- He currently serves as an Associate Editor of the journal *Annual Reviews of Materials Research*, and Executive Editor of the journal *Chemistry of Materials*

CRSI Medal Lectures

Gold Medal Lecture

Importance of Electron Repulsions

Prof. S. Ramasesha
Solid State and Structural Chemistry Unit, IISc, Bengaluru,
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While qualitatively the role of electron repulsions is well known, their quantitative study is a grand challenge problem and numerical techniques have led the way forward. There have been many advances in their quantitative study in real systems. We have been involved in the development of ED and DMRG techniques for application to systems of interest in chemistry and physics. On the ED front, we have developed a diagrammatic valence bond (VB) method [1-3], extended to exploit the symmetry of non-Abelian point groups [4], and introduced a correction vector (CV) approach for dynamical NLO coefficients [5,6]. We also solved the problem of spin statistics violation in electron-hole recombination in light-emitting organic polymers [7,8]. In the field of magnetism, we have applied the VB method for molecular spin systems and single molecule magnets [9-12]. By developing techniques to incorporate symmetry, we targeted important excited states in conjugated polymers [13]. The CV approach has been implemented to study frequency-dependent properties of large systems. We have also developed new real-time dynamics algorithms to study spin-charge separation in conjugated polymers. We have applied the DMRG method to quantum phases in spin chains, spin ladders and skewed spin ladders.

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Prof. S. Ramasesha

Emeritus Professor and INSA Honorary Scientist
Solid State and Structural Chemistry Unit (SSCU)
IISc, Bangaluru 560012; *Email: ramasesh@iisc.ac.in*

Prof Ramasesha obtained his B.Sc (Hons., Chemistry) from Bangalore University in 1968 and M.Sc (Chemistry) from IIT, Kanpur in 1970. He continued in IIT, Kanpur for his PhD degree under Professor C.N.R. Rao's guidance and obtained his PhD in 1977. He was a postdoctoral fellow in IISc (April 1977 to September 1979), in University of Oxford (September 1979 to November 1981), in Louisiana State University (November 1981 to October 1982) and in Princeton University (October 1982 to June 1984). He joined IISc as an assistant professor in SSCU in 1984 and superannuated in 2015. From 2015 to 2020 he was an Honorary Professor at IISc and an INSA senior Scientist from 2017 till 2021. Prof. Ramasesha, during his PhD, applied classical Monte Carlo method to Anisotropic Next Nearest Neighbor Ising (ANNNI) model to explain the phenomenon of polytypism in solids and studied spin state transition in solids using path integrals. In the study of extended correlated systems, he used the valence bond (VB) basis for exact diagonalization (ED) studies. He extended the Rumer-Pauling rules, developed bit representation of VB states and introduced the correction vector (CV) technique for dynamic nonlinear optic (NLO) coefficients within the ED scheme. He modelled the electron-hole recombination process to explain apparent violation of spin statistics, developed VB basis to study Kondo chains and studied models for organic molecular magnetism, photomagnetism, magnetic anisotropy in single molecule magnets (SMM) and used Kinetic Monte Carlo method to study slow relaxation in SMMs. He solved the long-standing problem of incorporating total spin symmetry for non-Abelian point groups within the VB approach.

Awards and Honours:

Prof. Ramasesha received the INSA Young Scientists' medal, B.M. Biral Science Prize for Chemistry, Shanti Swaroop Bhatnagar Prize for Chemistry, IISc alumni award for excellence in research, CRSI Silver Medal, the J.C. Bose National Fellowship and Sir M. Visvesvaraya medal for life time achievement from Karnataka. He is an elected fellow of the Indian Academy of Sciences (IASc), Indian National Science Academy (INSA), the World Academy of Sciences (TWAS) and honorary fellow of Karnataka Science and Technology Academy.

Molecular Complexity from Aromatics: Concept, Strategy and Reality

Prof. Vishwakarma Singh
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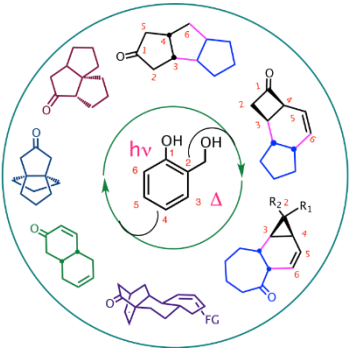

The philosophy of synthesis design from *o*-hydroxymethyl phenols, evolution of methodology and its application towards the creation of diverse molecular architectures will be presented. Oxidative dearomatization of *o*-hydroxymethyl phenols to the transient cyclohexa-2,4-dienones followed by their interception with olefins/dienes and sigmatropic shifts in the ground and excited states are the key features of our approach. Application of this concept towards the synthesis of polyquinanes, sterpuranes, platencin, atisanes, atropurpurane and other related natural products will be delineated.

References:

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5. R. Sahu; V. Singh; *Synthesis.* **2019**, *51*, 1633-1642.

Prof. Vishwakarma Singh

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Vishwakarma Singh obtained his Ph.D. degree from the University of Gorakhpur. After postdoctoral studies in India (Professor G. Mehta), Japan (Professor E. Osawa), and the USA (Professors J. B. Hendrickson and A. R. Martin), he worked at the Malti Chem Research Centre, Nandesari, Baroda, and the Maharaja Sayajirao University of Baroda (1984–1989). Subsequently, he moved to the Indian Institute of Technology Bombay and continued there as a professor of chemistry. He was a visiting professor at the department of chemistry, IISER Bhopal. Professor Singh is a recipient of several endowment awards and is a fellow of the National Academy of Sciences, India (NASI), and the Indian National Science Academy (INSA), New Delhi. He was a J.C. Bose fellow (Department of Science and Technology, New Delhi) and a chair professor (IIT Bombay).

Research Interests:

- Organic Synthesis and Photochemistry

Awards and Honours:

- Fellow of Indian National Science Academy [INSA] New Delhi, 2003.
- Award for "Excellence in Teaching", IIT Bombay, 2014, 2016.
- Institute Chair Professor, IIT Bombay, 2011-2014.
- J. C. Bose National fellowship 2010, DST, New Delhi.
- Silver & Bronze Medals, CRSI, 2010 & 2000 respectively.
- Prof. A. Srkrishna Memorial Endowment Award, IISc, Bangalore, 2018.
- Prof. K. K. Balasubramanian Endowment Award, IIT Madras, 2017.
- Prof. K. Venkatraman endowment Lecture award 2006-07, Institute of Chemical Technology, Mumbai University.
- Dr. T. R. Govindachari 60th birthday commemoration award (2001-2002) for outstanding teaching and research, by university of Madras, Chennai.
- Professor R. C. Shah Endowment award (2000) by the Department of Chemistry, Mumbai University.

CRSI Silver Medal Lecture

Some Advancements in Organic Synthesis Using New Synthons and Decarboxylative Coupling Reactions

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Department of Chemistry, Institute of Science, BHU, Varanasi-221005, India
Email: knsingh@bhu.ac.in

The present pursuit of our research group centres around the development of novel synthetic methodologies to accomplish the C-C & C-X bond formation under environmentally benign conditions. We have serendipitously discovered the use of sulfonyl hydrazide as a nucleophilic thiol equivalent and Ar-SO_2 source; and demonstrated its use in organic synthesis.[1] Some other notable contributions from our group include the decarboxylative cross-coupling/oxidative cross-coupling of *α,β*-unsaturated carboxylic acids/aryl acetic acid, and C-H activation (sp^3 & sp^2) under conventional and photoredox conditions.[2] Electrophilic as well as the nucleophilic centre is generated by the activation of benzylic C(sp^3)-H of alkyl arylacetates to construct the C-C/ C-heteroatom bond either via oxidative decarbethoxylation or by cross dehydrogenative coupling.[3] Some other methodologies have also been established using olefins, methylarenes, and *N*-methylated amines.[4]

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Prof. Krishna Nand Singh (born 1962) obtained his M. Sc. (Organic Chemistry) and Ph. D. (Chemistry) from Banaras Hindu University, Varanasi, India. After a short post-doctoral tenure, he joined the Department of Applied Chemistry, Institute of Technology (Now IIT), Banaras Hindu University as Lecturer/Assistant Professor in 1993, where he was elevated to the post of Associate Professor in 2002. He moved to the Department of Chemistry, Banaras Hindu University as a Professor of Organic Chemistry in the year 2007 and is continuing there. Prof. Singh has successfully completed 16 major research projects from different central government funding agencies. His research work has resulted in the publication of over 145 research papers in journals of international repute, with 18 students awarded with the Ph. D. Degree. His H-index is 33 (24 since 2017)) with over 3750 citations (~2100 citations since 2017) for his work from Banaras Hindu University.

Research Interests:

- Coupling Reactions, C-H Activation, Decarboxylative Coupling
- Photo redox Catalysis, Electro-organic Synthesis

Awards and Honours:

- Fellow of the Indian National Science Academy, New Delhi (2020)
- Fellow of the National Academy of Sciences, India (2016)
- Chemical Research Society of India (CRSI) Bronze Medal (2018)
- Vice-Chancellor's Award for Excellence in Research (2014).
- Invited Professor, Institute of Chemistry, University of Rennes, France (2004).
- AICTE Career Award (1995).

CRSI Bronze Medal Lecture

Glycosylation and Glycodiversification: An Important aspect of Carbohydrate Chemistry

Dr. Amit Kumar
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Carbohydrates, the vital endogenous biomolecules, found mostly in conjugation with lipids (to form glycolipids) and proteins (to form glycoproteins), are composed of various monosaccharide units linked together through *O*-glycosidic linkages. They serve for the storage of energy (starch and glycogen) and form much of the structural framework of cells and tissues (cellulose and chitin). Carbohydrate processing enzymes are responsible for making and breaking the chief glycosidic linkage and have been implicated in controlling diseases like influenza infection, cancer, AIDS, Gaucher's disease and diabetes.[1] Therefore, the formation of glycosidic bonds is one of the important aspects of carbohydrate chemistry. Anomeric trichloroacetimidates are the most effective and commonly used glycosyl donor in chemical synthesis for glycosylation reactions.[2] In recent years, many new benchtop stable and readily available glycosyl donors have been introduced in the literature.[3-4] However, still there is a large demand from organic chemists to find new glycosyl donors which favor the smooth *O*-glycoside bond formation in high anomeric selectivity. This talk will summarize the conceptually novel approach used in stereoselective glycoside bond formation and glycodiversifications.[5] The mechanistic details followed by the different catalysts and further application of these methods in the synthesis of complex saccharides will be also discussed.

References:

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5. a) Aghi,A, Baghel, A.S., Kumar, A. *Eur. J. Org. Chem*, **2022**, ASAP article, b) Shaw, M., Kumar, A., *Chemistry-An Asian Journal*, **2019**, *14*, 4651.

Dr. Amit Kumar

Associate Professor, Department of Chemistry
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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

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

Honours and awards:

- Life-member- CRSI, India
- Life-member-ISCB, India
- Life-member, ACIIT, India

Does Oxidation State Matter in Cobalt-Catalyzed Sustainable Transformations

Prof. B. Sundaraju

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Ideal chemical transformations have enormous impact on resources, energy, and environment.[1] Recent advancement in chemical synthesis have been witnessed on the use of non-toxic reagents, environmentally benign transition metals, and reagent free synthesis (energy transfer catalysis) towards the sustainable development.[2] In this regard, transition metal catalysis revolutionize the organic synthesis by minimizing the use of strong base, toxic reagents, multi-step synthesis etc. To further advance the sustainable synthesis, use of 3d-metals has been widely explored over the last decade for two sustainable catalytic processes, i.e., C-H bond functionalizations[3] and borrowing hydrogen chemistry.[4] In this lecture, I will discuss the advantages and unique reactivity of high-valent cobalt over the in-situ generated low-valent cobalt for C-H bond functionalizations and its mechanistic pathways.[5] Also, I will discuss briefly about our recent report on the discovery of new mechanism in redox active metals.[5]

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Prof. Basker Sundaraju

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Basker Sundararaju obtained his doctoral degree in 2011 from universite de Rennes1, France. He then moved to Muelheim to carry out his post-doctor research (2011-13) under the supervision of Prof. Alois Fuerstner at the Max-Planck Institute of Coal Research, Germany, supported by AvH fellowship. During his Ph.D. and post-doctoral research, he primarily focused on developing new catalytic methods using Noble metals such [Ru], [Pd] and [Ir]. In 2013, he began his independent career as an assistant professor at the department of chemistry, IIT Kanpur and subsequently raised to Associate professor in 2018. He was part of early career editorial advisory board of ACS Catalysis (2018-20) and currently serve as an associate editor of the journal heterocyclic chemistry (2019-). He has published 47 papers in his independent career (overall 65 papers) cited well over 3700 with an H-index of 33. He has collaborated with several researchers at the national and international collaboration.

Research Interests:

- 3d-Metal Catalysis
- C-H Bond Functionalization's
- Hydrogen Neutral Strategy for Sustainable Processes
- Waste-Recycling
- Asymmetric Catalysis

Awards and Honours:

- Invited to join as Fellow of Royal Society of Chemistry (FRSC) **2022**
- Guest Editor, Frontiers in Catalysis on "Perspectives in Organometallic Catalysis" **2022.**
- Founding member and Co-coordinator, Indo-UK Sustainability Chemistry Consortium **2021**
- Winner of Merck Young Scientist Award **2019**
- Selected as Top 3 finalist for Scopus Young Scientist award **2019**
- Invited to be part of selection committee member for REAXYS PhD Prize, **2019**
- Invited to serve as an Associate Editor of Journal of Heterocyclic Chemistry **2019**
- Invited as Early Career Advisory Board Member by "ACS Catalysis" **2018 & 2019**
- Awarded "P. K. Kelkar Young Faculty Research Award **2017**" by IITK, Kanpur, India.

Recent Development on Construction of Various Aromatic Chiral Cores from Glycals

Prof. Debaraj Mukherjee

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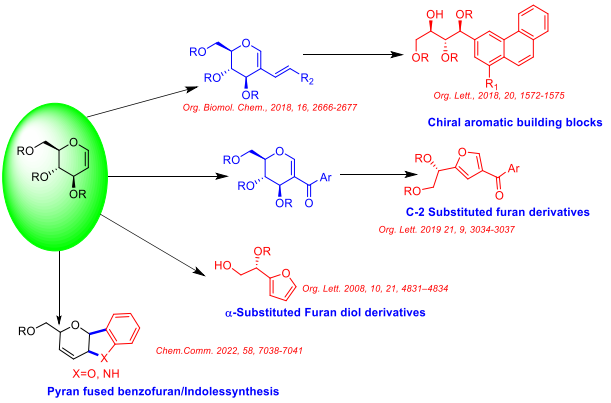

Glycals are unsaturated sugars that act as versatile chiral pool synthons in the synthesis of bioactive natural products and medicinally important compounds.[1] Glycals can be utilized to construct various carbohydrate-derived chiral intermediates which contain arrays of defined stereocenters. It is well-recognized that the synthetic utility of glycals can be further utilized through the incorporation of other reactive functional groups in addition to already existing ones, by controlling the relative configuration during the transformation. During my lecture, I will be presenting some of the recent developments from my lab exploring the new reactivity of glycals[2] and its application in the synthesis of chiral aromatic/heteroaromatic derivatives.[2]

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Prof. Debaraj Mukherjee

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Debaraj Mukherjee obtained his PhD degree in the field of synthetic carbohydrate chemistry from IICB-CSIR Kolkata under Jadavpur University, India in 2006. Thereafter, he joined as a scientist at CSIR-Indian Institute of Integrative Medicine (IIIM), Jammu in 2006 March and subsequently elevated to Principal Scientist position in 2017. He worked as Boyscast postdoctoral fellow with Prof David Crich at Wayne State University, USA (2011-2012). His scientific work has been published in ca. 100 original international publications and review articles, 2 book chapters, and 4 patents as Principal Investigator. Ten of his students have been awarded PhD and few of them have joined as faculties in IIT and Universities.

Research Interests:

- Carbohydrate Chemistry (novel methods for O-/C-/N-glycosylation, glycal chemistry, nucleoside synthesis, synthesis of oligosaccharide mimetics, new protection/deprotection strategies for monosaccharides, multicomponent tandem reactions in carbohydrates and synthesis of carbohydrate-fused bicyclic systems containing medium-ring to macrocyclic ethers, thioethers and lactones of promising therapeutic potential, non-infringing routes for the synthesis of carbohydrate-based APIs
- Medicinal Chemistry
- Natural Product Chemistry (plant, microbes)

Awards and Honours:

- D.S.T award for 'meeting with Nobel Laureates in Lindau, Germany (2002)
- Young Scientist Award in International Carbohydrate Conference at DU (2006)
- DST Boyscast fellowship (2011-2012)
- ACCTI "Dr. H.C. Srivastava Memorial Award-2019"at Lucknow
- "2020 Professor D.K. Banerjee Memorial Lecture Award" by Department of Organic Chemistry, Indian Institute of Science, Bangalore (2020)
- Invited talk at NOST-Udaipur (2019)

Hydrogen Borrowing and Interrupted Hydrogen Borrowing Catalysis: Applications and Mechanistic Studies

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Amines, amides and *N*-heterocycles are most valuable compounds ubiquitous in bioactive molecules, alkaloids, and extensively used in pharmaceuticals, agrochemicals and as ligands.[1] Therefore, catalytic selective C–N and C-C bond formation for their synthesis is an ultimate goal in chemical research. Conventional methodologies for their synthesis involve multi-step pathways and suffer from low atom economy, limited selectivity and produced stoichiometric amounts of waste.[1] Direct application of renewable alcohols as electrophilic coupling partner represents a sustainable alternative, as they can be readily available in industrial scale production from lignocellulose biomass.[1] Recently, there is a potential drive to replace the precious noble-metal catalysts using earth abundant and inexpensive non-noble metals for sustainable organic transformations.We have demonstrated a general and practical applications of various primary alcohols, including diols and amino alcohols for selective construction of numerous primary and secondary amines, amides, five or six-membered N-heterocycles, activation of weak sp^3 C-H bond of alkyl substituted N-heteroarenes to *E*-selective alkenes as well as functionalization of ketone enolates. Our recent studies on the interrupted hydrogen borrowing strategies for per-fluoroalkylation will also be discussed. A detailed mechanistic and kinetics studies were also established for such transformations.[2-6]

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1. Watson, A. J. A.; Williams, J. M. J. *Science* **2010**, *329*, 635.
2. (a) Vellakkaran, M.; Singh, K.; Banerjee, D. *ACS Catal*., **2017**, *7*, 8152–8158. (b) Singh, K.; Vellakkaran, M.; Banerjee, D. *Green Chemistry*, **2018**, *20*, 2250-2256. (c) Das, J.; Singh, K.; Vellakkaran, M.; Banerjee, D. *Org. Lett*., **2018**, *20*, 5587-5591.
3. (a) Das, J.; Vellakkaran, M.; Sk. M.; Banerjee, D. *Org. Lett*., **2019** *21*, 7514-7518. (b) Bera, S.; Bera, A.; Banerjee, D.. *Org. Lett.* **2020**, *22*, 6458–6463. (c) Bera, S.; Bera, A.; Banerjee, D. *Chem. Commun.* **2020**, *56*, 6850–6853. (d) Kabadwal, L. M.; Bera, S.; Banerjee, D. *Chem. Commun.* **2020**, *56*, 4777–4780.
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Debasis Banerjee graduated with M.Sc. degree in Organic Chemistry from Banaras Hindu University and obtained Ph.D. in organic chemistry from Indian Institute of Technology Kanpur in 2011 with Prof. M. L. N. Rao. Thereafter he moved to Leibniz Institute for Catalysis (LIKAT), Germany for a postdoctoral position with Prof. Matthias Beller (2011-14) and subsequently held another postdoctoral position (2014-2015) at the Stockholm University, Sweden with Prof. Jan-Erling Bäckvall. In 2015, he has accepted a position of Assistant Professor at the Indian Institute of Technology Roorkee (Uttarakhand, India). Currently he is an Associate Professor at the same institute from August 2020.

Research Interests:

Redox-switchable catalysis (RSC) relates to tuning the catalytic activity of a transition metal by designing a suitable ligand in combination with more abundant non-precious metals, enantioselective dual-catalysis, activation of small molecules, perfluoroalkylation technologies and heterogeneous catalysis for sustainable organic transformations.

Awards and Honours:

He is a recipient of SERB-Early Career Research Award (2016), DAE-Young Scientist Research Award (YSRA-2016) and winner of Evonik Call for Research Proposal (ECRP-2016) Award by Evonik Industries GMBH, Germany. Recently has been selected for the Thieme Chemistry Journals Award 2020. Since 2021 he is working as a Guest Editor in *Tetrahedron* and *Tetrahedron Letters* on a Special Issue based on Non-Precious Metal-Catalysis for Sustainable Organic Transformations. He has been selected for the Chemical Research Society of India (CRSI) Bronze Medal of 2023.

Near-IR Absorbing and Emitting Terrylene Diimides

Prof. Jeyaraman Sankar
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Organic near-infrared (NIR) emitters are in demand for their utility in night vision detectors, photobiomodulation and biological imaging. A handful of NIR absorbing molecular classes are known; however, reports on intense NIR emitting molecules are sparse. Longer rylene diimides such as terrylene diimides (TDIs) are important class of molecules having intense absorption and emission in the NIR range.[2] However, these larger polyaromatics hinder their synthesis, isolation and characterization due to inherent aggregation.

Herein, we present a simple method to achieve a few TDI derivatives. These new molecules have intense absorption and emission in the range of 700 nm – 900 nm. The emission quantum yields observed are some of the highest among this class of molecules (up to **93%**).[3] This work will highlight the utility of precise electronic and structural tuning necessary to achieve intense NIR absorbing and emitting molecules for modern applications.

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1. Law, K.Y.; *Chem. Rev.*, **1993**, *93*, 449-486.
2. Holtrup, F. O.; Müller, G. R. J.; Quante, H.; Feyter, S. De.; Schryver, F. C. De.; Müllen, K.; *Chem. Eur. J.*, **1997**, *3*, 219-225.
3. Mehra, K. S.; Jha, S.; Bhandary, S.; Mandal, D.; Mishra, R.; Sankar, J.; *Angew. Chem. Int. Ed.*, **2022,** *https://doi.org/10.1002/anie.202205600.*

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After completing his PhD from IIT Kanpur (2005) and JSPS Fellowship (2008) from Kyoto University, he joined IISER Bhopal as an assistant professor in 2009. Currently, he is at the same institute as a full professor. His group is interested in developing new molecules with polyaromatic backbone for modern molecular electronic applications. Metal complexes of bio-inspired macrocycles too are being investigated with the aim to utilize them as magnetic materials and redox-active catalysts.

Research Interests:

- Rylene Diimides and their optoelectronic properties
- Metal complexes of bio-inspired ligands and their coordination chemistry

Awards and Honours:

- JSPS Fellowship 2006

Opportunities and Challenges in the Synthetic Process Development for Pharmaceuticals

Dr. Joydev K. Laha

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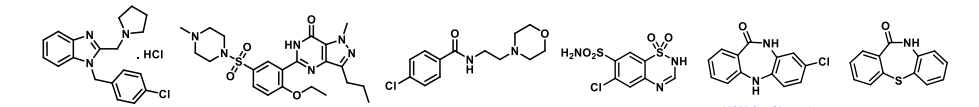
India's overwhelming dependence on China for generic active pharmaceutical ingredients (APIs) to the extent over 65 percent of the requirement is a serious concern in the production of affordable medicines used in current health care in India. While many Indian pharmaceutical companies produce generic APIs, the similar research activities in academia are rarely postulated. Evolution of innovative, cost-effective processes for generic API synthesis in academia could help promote the production of generic APIs in industry. Our group is involved in the development of new synthetic processes for APIs and Key Starting Materials (KSMs) (some selected APIs and KSM are shown below). At the beginning of the presentation, pros and cons in the synthesis of several grams of Clemizole, required for our collaborator, following procedures available in the public domain will be discussed. Subsequently, preparation of several KSM or drug intermediates featuring reduced number of steps, avoiding substrates like acid chloride, avoiding stoichiometric amount of corrosive Lewis acids, use of cheap oxidants, "reagentless" synthesis, adopting a friendly work up procedure, etc will be discussed. A major focus will be on the gradual development (first to second to third generation) of the synthesis of sildenafil, a top-selling PDE5 inhibitor drug. Some on-going efforts on various APIs under PLI scheme and underlying challenges will also be covered.



Clemizole Hydrochloride (H1 antagonist, used for allergic rhinitis) Available market price:197 USD/ 25mg

Sildenafil (PDE5 inhibitor) 53.8 USD/Kg

Moclobemide (Antidepressant) 163.5 USD/Kg

Chlorothiazide (Diuretic) 41.6 USD/Kg

KSM for Clozapine (Antipsychotic)

KSM for Quetiapine (Antipsychotic)

References:

1. Laha, J. K.; Patel, K. V.; Tummalapalli, K. S. S.; Dayal, N. *Chem. Commun*., **2016**, 52, 10245-10248.
2. Laha, J. K.; Manral, N.; Kaur H. M. *New J. Chem.*, **2019**, *43*, 7339-7343.
3. Laha, J. K.; Kaur H. M.; Hegde, S.; Gupta, A. Conditions *Org. Lett*. **2020**, *22*, 1442-1447.
4. Laha, J. K.; Gulati, U.; Gupta, A.; Indurthy, H. K., *New J. Chem.* **2021,** *25*, 2643-2648.

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Dr. Joydev Laha started his independent research career at NIPER S.A.S. Nagar on July 2011. Prior to joining the NIPER, Dr. Laha was employed on a permanent position in the Laboratory for Drug Discovery in Neurodegeneration (LDDN) at Harvard Medical School. Dr. Laha obtained a Ph.D. degree in organic chemistry from the National Chemical Laboratory at Pune under the mentorship of Prof. Ganesh Pandey. He acquired a total of about five years of postdoctoral research experiences in synthetic organic chemistry and medicinal chemistry at the North Carolina State University and Mayo Clinic in the United States. Dr. Laha has versatile research experiences including target-driven method development in organic synthesis, natural product synthesis, and medicinal chemistry research directed to structure-based drug discovery. Over the past ten years in his independent career, he has mentored two Postdoctoral Fellows, ten PhDs and seventy one Master's students. Dr Laha and his group have demonstrated translational applications (Ready-to-Transfer Technology) of laboratory concept to prepare marketed drugs including Clemizole, Metronidazole, Moclobemide, Dicholofenec, Sildenafil, and several others. He is author or co-author of over seventy-five papers published in peer-reviewed international journals and has two US Patents (and several applications filed) to his credit. He has been serving referee to the ACS, RSC, Science Direct, and Wiley journals. He has delivered invited lectures/oral presentations extensively in India and abroad. [h-index 31, i10-index-54]

Research Interests:

- Radical reactions largely using persulfates and their mechanistic study
- Synthesis of heterocycles, key starting materials and generic active pharmaceutical ingredients (APIs)

Awards and Honours:

- NIPER Innovation award 2019
- Award of appreciation by NIPER S.A.S. Nagar on the Technology Day May 11, 2018
- Rajnibhai V. Patel PharmInnova Award 2017-18 with Mr. Gurudutt Dubey

Theoretical Insights into the Activation of Covalent Bonds under Nanoconfinement

Dr. K. R. S. Chandrakumar
Theoretical Chemistry Section, Bhabha Atomic Research Centre
Email: krsc@barc.gov.in

Confinement under nano-regimes can strongly influence the electronic, catalytic and spectroscopic properties of molecular systems. The nanoconfinement can be in the form of a nanocavity, spherical sized fullerenes, organic & inorganic nanotubes, micelles, molecular organic frameworks, zeolites, etc. It can cause the molecular systems to feel very stressful which can give rise to some of the unusual and fascinating physical as well as chemical properties. These unusual properties otherwise might not be possible to achieve under normal conditions. The present talk focuses the impact of such "stressful" conditions on chemical reactions, in particular the charge-transfer and proton transfer reactions. In addition, we will also discuss one of the most important reactions, the activation of nitrogen molecules for the production of ammonia which is in general achieved by the well-known Haber–Bosch method. Herein, the challenge is the activation of nitrogen and hydrogen molecules leading to the formation of hydrazine as well as ammonia without any additional catalysts. The origin of these unusual chemical reactions under nanoconfinement has been analysed internal pressure as well as molecular crowding effects. We finally conclude that when a conducive atmosphere with a suitable cavity diameter in the nano-regime is created in a reaction medium, different chemistry or unusual phenomena can be expected.

Dr. K. R. S. Chandrakumar

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Dr. Chandrakumar received his M.Sc. in 1994 from Madurai Kamaraj University and his Ph.D. in the year 2003 from National Chemical Laboratory and Pune University, Pune under the supervision of Prof. Sourav Pal. In 2003, he joined as Dr K. S. Krishnan Research Associate at Bhabha Atomic Research Centre, Mumbai where he is now working as a senior scientific officer. He did his postdoctoral work with Prof. (Late) K. Morokuma, at Kyoto University, Japan during the year 2009-2011.

Research Interests:

- Theoretical and computational chemistry
- Development of catalysts for energy and Environment
- Materials under extreme environmental effects
- Growth mechanism and assembly of complex nanostructures

Awards and Honours:

- Young scientist award from Indian Science Congress Association (**2002**)
- Young scientist award from Indian National Science Academy (**2005**)
- Young scientist award from Department of Atomic Energy (**2007**)
- Scientific & Technical Excellence Award from Department of Atomic Energy (**2015**)

π-Extended Porphyrins and Their Analogues: Synthesis, Spectral and Redox: *Properties and Their Application in Sensing, Nonlinear Optics and Catalysis*

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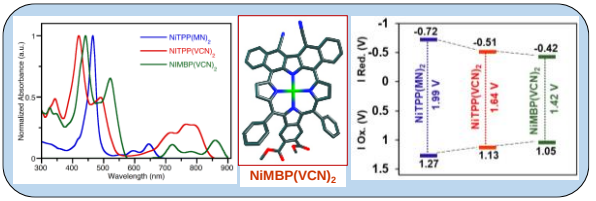

Chart 1. Molecular structure of NiMBP(VCN)$_2$ and the UV-Vis spectral features of some fused porphyrins along with their HOMO-LUMO gap.

β-Functionalization of *meso*-tetraphenylporphyrins and their analogues is of great interest since the electronic spectral and redox properties of the porphyrin π-system can be tuned by fusing the exocyclic rings to tetrapyrrole macrocycle which leads to extended π-conjugation or through peripheral functionalization.[1] Herein, we present the facile synthesis of *β*-to-*ortho*-phenyl fused porphyrins and chlorins having malononitrile or 1,3-indanedione moieties by facile oxidative fusion of *trans*-chlorins using DDQ in excellent yields under mild conditions.[1] A new series of *β*-substituted benzoporphyrins and their fused derivatives have been synthesized with good yields.[1] The synthesized fused tetrapyrroles exhibited significantly red-shifted ($\Delta\lambda_{max}$ = 16-110 nm) electronic spectral features up to 900 nm (Chart 1) due to the extended π-conjugation and twisted macrocyclic conformation (twist angle ~20-36°).[1] Further, *β*-TCBD appended porphyrins were synthesised and utilised as optical limiters.[1j] The π-extended porphyrins and corroles were utilised as excellent two-photon absorbers.[1] In this presentation, we will describe the synthesis, spectral and electrochemical redox properties of fused tetrapyrroles and their utilization in anion sensing, nonlinear optics (NLO) and catalysis in detail.

References:

1. (a) Sankar, M. *et al.*, *Green Chem.* **2019**, *21*, 1757; (b) Sankar, M. *et al.*, *J. Mater. Chem.* A **2017**, *5*, 6263; (c) Chaudhri, N.; Grover, N.; Sankar, M. *Inorg. Chem.* **2017**, *56*, 11532; (d) Chaudhri, N.; Grover, N.; Sankar, M. *Inorg. Chem.* **2018**, *57*, 6658; (e) Chaudhri, N.; Grover, N.; Sankar, M. *Inorg. Chem.* **2018**, *57*, 11349.

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Prof. M. Sankar is working as Professor at the Department of Chemistry, Indian Institute of Technology Roorkee. He obtained BSc and MSc degrees in Chemistry from the University of Madras and Madurai Kamaraj University in the year 1999 and 2001, respectively. Then he joined IIT Madras to earn his PhD in Bioinorganic Chemistry. In 2005, he joined as a postdoctoral researcher at Tel-Aviv University, Israel in the area of "Porphyrin-based Supramolecular Network Solids". In 2007, he was selected for EDIGE postdoctoral fellowship and worked at the University of Bourgogne, Dijon, France. Later he worked as a CNRS researcher at University Rennes1, France for a year. In 2009, he moved to Japan to take up JSPS fellowship sponsored by MEXT, Japan. From 2011, he is working at IIT Roorkee, Uttarakhand, India. In 2018, he worked as Bhaskara Advanced Solar Energy (BASE) Fellow at the University of North Texas, Denton, TX, USA. He has published 120 research articles in reputed international journals and 3 book chapters.

Research Interests:

- Synthesis of Novel Porphyrins and their Analogues for Solar Cell, Catalysis, Sensing, Nonlinear Optics and Phtodynamic Therapy Applications, Supramolecular Chemistry, Coordination Chemistry and Catalysis.

Awards and Honours:

- 2021 Outstanding Teacher Award, IIT Roorkee, India
- 2020 Fellow, Royal Society of Chemistry, London, UK
- 2018 BASE Fellow, University of North Texas, Denton, TX, USA
- 2018 Outstanding Researcher Award with Institute Research Fellowship, IITR
- 2009 JSPS Postdoctoral Fellowship, MEXT, Tokyo, Japan
- 2008 CNRS Research Fellowship, CNRS, Paris, France
- 2007 EDIGE Postdoctoral Fellowship, Bourgogne Research Council, Dijon, France

Palladium Catalysed C-C bond Cleavage of Carbocyclic Strained Systems: A Useful Strategy in Organic Synthesis

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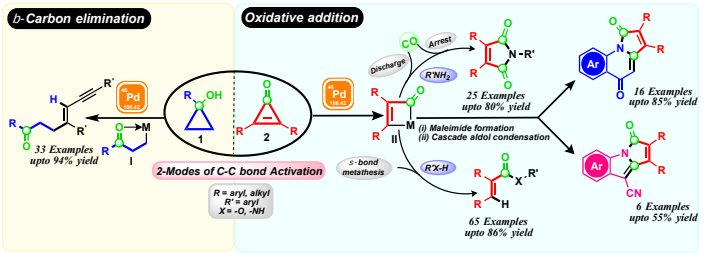
Email: pcr@niser.ac.in



Palladium catalyzed C-C bond functionalization of Cyclopropenones and Cyclopropanols

During the last century direct functionalization of inert bond such as C-C bond has been largely ignored due to its high bond strength and inertness. Since the beginning 21st century there has been renewed interest in functionalizing inert bonds through palladium catalyst for the synthesis of many useful organic molecules. As compared to C-H bond functionalization, C-C bond functionalization is far more difficult due to the high thermodynamic barrier in breaking the C-C bond. One useful strategy to overcome high thermodynamic barrier is to use strained ring systems as substrates. In our group we have employed this strategy for the synthesis of heterocycles and useful organic scaffolds. A brief overview of the works completed so far and our ongoing works will be presented.

References:

1. Pati, B. V.; Ghosh, A.; Yadav, K.; Banjare, S. K.; Pandey, S.; Lourderaj, U., Ravikumar, P. C., *Chem. Sci.*, **2022**, *13*, 2692.
2. Nanda, T.; Ravikumar, P. C., *Org. Lett.*, **2020**, *22*, 1368.
3. Nanda, T.; Biswal, P.; Pati, B. V.; Banjare, S. K.; Ravikumar, P. C., *J. Org. Chem.*, **2021**, *86*, 2682.
4. Nanda, T; Fastheem, M; Linda, A; Pati, B; Banjare, S. K; Biswal, P; and Ravikumar, P. C.; *ACS Catal.*, **2022**, *12*, 13247.
5. Nanda, T; Fastheem, M; Banjare, S. K.; Ravikumar, P. C. (*Manuscript under preparation*).

Dr. Ponneri C. Ravikumar
Associate Professor, School of Chemical Sciences,
NISER-Bhubaneswar, Odisha, India.
Email: pcr@niser.ac.in

Dr. Ponneri C. Ravikumar obtained his B.Sc. (Chemistry) and M.Sc (Organic Chemistry) from the University of Madras. He completed his Ph.D. at the Indian Institute of Science (IISc), Bangalore, India. Subsequently he moved to USA for his postdoctoral fellowship, first at Duquesne University, Pittsburgh and then at Yale University, New Haven. He joined as Assistant Professor at the Indian Institute of Technology (IIT), Mandi, Himachal Pradesh in the year 2010. He continued there until 2015, then he moved to National Institute of Science Education and Research (NISER), Bhubaneswar, Odisha, where he is currently an Associate Professor. He has received teaching excellence award as well as foundation day awards for institute service while serving at IIT Mandi. Apart from teaching and research he also served actively in administrative positions such as Associate Dean (Planning and Infrastructure) at IIT Mandi and Head, Estate Management and Works Department at NISER Bhubaneswar.

Research Interests:

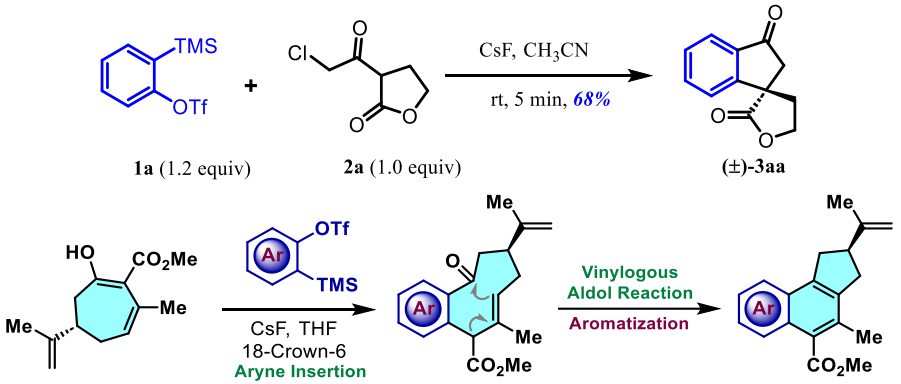
- Developing new methods for oxidative cleavage of the carbon-carbon bond of strained organic molecules such as cyclopropenone, cyclopropanol and its application to the synthesis of bioactive heterocyclic core skeletons and useful organic scaffolds
- Developing new methods for the functionalization of arenes and heteroarenes

Awards and Honours:

- Teaching Excellence Award for undergraduate teaching at IIT Mandi
- Foundation Day Award 2012 for institute service at IIT Mandi
- Foundation Day Award 2013 for institute service at IIT Mandi

Easy access to diverse natural product like scaffolds through Aryne insertion

Dr. Prathama S Mainkar
CSIR-Indian Institute of Chemical Technology
Email: prathama@iict.res.in



Arynes have been used extensively after the publication of milder reaction conditions by Kobayashi et al.[1] With Tambar and Stoltz[2] publishing a methodology for acyl alkylation of arynes, a large number of new scaffodls are being generated using the same. Our group has been working on using arynes for generating new scaffolds through modifications of some of the commonly used starting materials to generate new and interesting molecular skeletons. Some of these achievements will be presented.

References:

1. Yoshio H.; Takaaki S. Kobayashi H; *Chem. Lett.*, **1983**, *12.*, 1211-1214
2. Tambar U K.; Stoltz B M.; *J. Am. Chem. Soc.*, **2005**, *127.*, 5340-5341
3. Roy Y N.; Ghosh P. Mainkar P S; Chandrasekhar S. *Org. Lett.*, **2022**, *24.*, 5372-5375.
4. Chaitanya N K.; Rao Y N S. Mainkar P S; Chandrasekhar S *Chem. Comm.*, **2020**, *58.*, 3178-3181

Dr. Prathama S. Mainkar

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Dr Prathama Mainkar has studied in Osmania University for M. Sc., Organic Chemistry and Ph. D. was from CSIR-Indian Institute of Chemical Technology. She has:

- Published over 85 peer reviewed papers in the areas of organic synthesis and medicinal chemistry, 1 book chapter and filed 32 patents.
- Has experience in industry as well as academics.
- Developed a molecule up to Phase IIa clinical trials bought by biotech company.
- Worked on identifying new scaffolds for treatment of tuberculosis, new molecules with antiviral potential and identified new scaffolds for drug resistant bacterial infections.
- At present research is focused on developing HDAC inhibitor for the treatment of idiopathic pulmonary fibrosis for IND filing.
- Worked on kinase inhibitor for treatment of squamous small cell lung cancer.
- Has experience in synthesis of oligosaccharides and oligopeptides

Research Interests:

- Medicinal Chemistry and Drug discovery
- Synthetic Organic Chemistry and process development for API synthesis

Awards and Honours:

- Fellow, National Academy of Sciences, India
- National Tech Excellence Award for Women by TDB, GoI, 2022
- CSIR Technology Award 2021 (for Covaxin® adjuvant)
- Best Woman Scientist Award 2021 by Genesin of Education Institute
- CSIR Technology Award 2020 (for process of Favipiravir)
- CSIR-IICT Best Woman Scientist of the year 2017
- OPPI Woman Scientist Award 2016
- Fellow of Telangana Academy of Sciences, Telangana
- Research Council member, CSIR-NCL
- Advisor, Heavy Water Board, DAE

In-situ Restoration of Energy Delivery in an Organic Flow Battery

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Globally electrical energy storage cost is at least an order of magnitude higher than renewable energy generation cost. Replacing oil with elements (such as Li, V, Co etc.) imported for energy storage will keep India import-dependent. To realize India-centric solutions, technologies out of materials abundant with us are crucial. Towards this end, our group is actively utilizing robust organic redox-active materials (ORM), zinc, lead, iron, etc., for energy storage applications. Aqueous redox flow batteries (ARFB) with ORMs hold great promise in lowering the levelized costs of electricity storage and with suitable molecular engineering, ORMs could outperform their expensive inorganic counterparts. The biggest obstacles to commercializing ARFBs with ORMs are their poor stability, low solubility, synthetic cost, and capacity fade. Capacity fade can be reversible and irreversible depending on the nature of the side reactions that occur. This lecture will discuss restoring the capacity of the highly soluble quinone-based ARFB by deep electrolysis. A high capacity of > 20Ah L^{-1} coupled with affordable cost makes it a commercially worthy system for energy storage applications.

References:

1. Lixing Xia, et al.; *Sustainable Energy & Fuels*, **2022,** *6*, 2045
2. Yan Jing, et al.; *Nature Chemistry*, **2022,** *14*, 1103

Dr. Kothandaraman Ramanujam

Department of Chemistry
Indian Institute of Technology Madras
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Prof. Kothandaraman Ramanujam has completed his B.Sc. in Chemistry from Sri Vasavi College affiliated to Bharatiyar University. He obtained his M.Sc. in Applied Chemistry from Anna University in 2000. He was introduced to the field of Materials Electrochemistry by Prof. Ashok Kumar Shukla at the Solid State and Structural Chemistry Unit, Indian Institute of Science, and he obtained his Ph.D. in 2006. He is currently a professor in the Department of Chemistry, IIT Madras. Subsequently, he completed two postdoctoral stints at Michigan State University, East Lansing (2007-2009) and the National Research Council of Canada, Ottawa (2009-2011). He was a visiting faculty at the Energy, Environment & Chemical Engineering Department of Washington University, St. Louis, in 2019. He has served as guest editor in J. Electrochemical Society and J. Photochemistry and Photobiology. He has co-chaired and conducted MRSI-AGM Conclave symposium on "Batteries fuel cell and supercapacitor" in 2021. He presented Amara Raja award lecture in the national symposium on electrochemical science and technology in 2022 held at IISc. He has more than 120 paper publications, one US patent, and three Indian patents to his credit. Besides, he is the principal investigator of two nationally important centres at IIT Madras: the organic photovoltaics division of DST-IITM Solar Energy Harnessing Centre and the Potential Centre for Advanced Energy Storage and Conversion established under Institute of Eminence funding.

Research Interests:

- Batteries (Redox flow, alkali metal ion, zinc-air, photo rechargeable)
- Organic functional materials for batteries and solar cell
- Electro organic synthesis

Awards and Honours:

- Recipient of Amara Raja Award-2021 (sponsored by M/S Amara Raja Batteries Ltd.) from The Electrochemical Society of India
- Fellow of the Royal Society of Chemistry (FRSC)
- Fellow of the Academy of Sciences, Chennai, University gold medallist: B.Sc. (Chemistry)- Bharatiyar University

Total Synthesis of γ-Lactone and THF Natural Products

Prof. Rodney A. Fernandes
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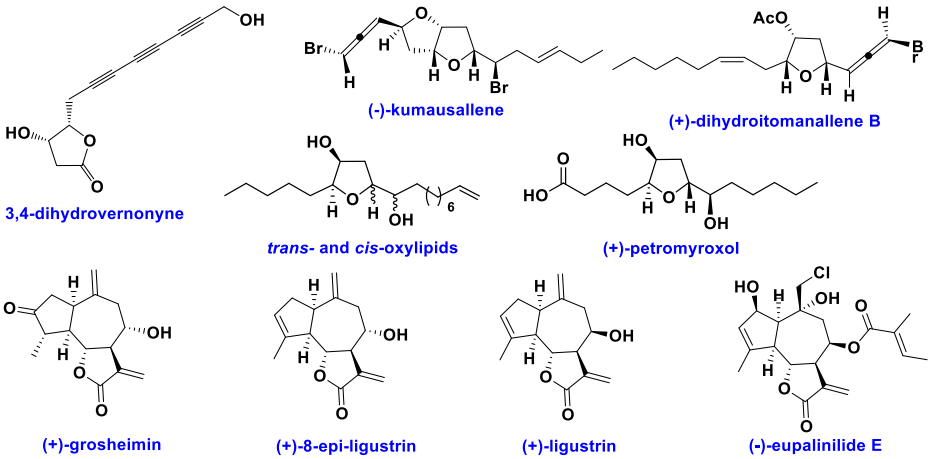

The total synthesis of selected γ-lactone and THF natural products by short synthetic sequences will be presented in this lecture. The aim was to minimise the use of protecting groups and develop step-economic synthesis.[1] Our work on the total synthesis of 3,4-dihydrovernoniyne, dihydroitomanallene B, kumausallene, oxylipids, petromyroxol and guaianolide molecules will be presented.[2]

References:

1. R. A. Fernandes, Ed.; John Wiley & Sons: Hoboken, NJ, **2018**.
2. (a) Ramakrishna, G. V.; Fernandes, R. A.; *J. Org. Chem.* **2019**, *84*, 14127. (b) Ramakrishna, G. V.; Fernandes, R. A.; *Org. Lett.* **2019**, *21*, 5827. (c) Fernandes, R. A.; Kumar, A.; Pathare, R. S.; *Chem. Commun*. **2022**, *58*, 11921. (d) Fernandes, R. A.; Ramakrishna, G. V.; *J. Org. Chem.* **2022**, doi.org/10/1021/acs.joc. 2c02094. (e) Fernandes, R. A.; Jha, A.; Gorve, D. A.; *Chem. Commun*. **2022**, under revision.

Prof. Rodney A. Fernandes

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Prof. Dr. Rodney A. Fernandes completed his Ph.D. in Organic Chemistry in Jan. 2003 at the CSIR-National Chemical Laboratory, Pune, under the guidance of Dr. Pradeep Kumar; postdoctoral research in Tohoku University, Japan, with Prof. Yoshinori Yamamoto (Jan-Dec 2004); Alexander von Humboldt fellow and then DFG postdoctoral fellow at the University of Freiburg with Prof. Reinhard Brückner (May 2004-June 2006). He started independent research at the Institute of Chemistry, UNAM, Mexico City (Sep 2006–July 2007) and then joined the Department of Chemistry, Indian Institute of Technology Bombay (IIT-Bombay), India as Assistant Professor in August 2007. He became full Professor in May 2015. Has authored 145 research publications including 5 book chapters and 8 patents. Guided 18 PhD, 8 postdoctoral and over 20 Master students. Delivered over 90 Invited and Shorts Talks in National and International Conferences and Workshops.

Research Interests:

- Asymmetric Synthesis and Total Synthesis
- Development of New Synthetic Methodologies

Awards and Honours:

- Keerti Sangoram Endowment Award 2002: Best Research Scholar by NCL Research Foundation.
- AvH Fellowship, Germany, May 2004-June 2006
- INSA Young Scientist Medal Award in 2004
- Elected Fellow of Maharashtra Academy of Sciences, 2016
- Delivered 4th Prof. S. C. Bhattacharya Memorial Lecture hosted by Prof. S. K. Paknikar Research and Education Trust, Dec. 2017, GOA
- Outstanding Reviewer Award by Chem. Commun. Journal of RSC, Sep. 2019
- Departmental Award for Excellence in Teaching, Sep. 2019, IIT Bombay.

The Chemistry of Silicon in Low Oxidation State

Dr. Sakya S. Sen
Inorganic Chemistry and Catalysis Division,
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It is matter of great pride and honour that Jawaharlal Nehru University (JNU) will be hosting the National Symposium in Chemistry (NSC) of Chemical Research Society of India (CRSI) and a joint symposium with Royal Society of Chemistry (RSC) for the first time. The symposium will be jointly organized by Special Centre for Molecular and the School of Physical Sciences. CRSI has recognised the need to promote quality research in chemistry and foster talent in the form of recognition at various levels. Since the inception of CRSI, the National Symposia in Chemistry have a history of providing a platform for meaningful scientific exchange that has made a profound difference to the community of chemists in the country. The 30th conference in the series will be held during 2-5 February 2023 with JNU as the host institute. This year, the 16th edition of the CRSI Royal Society of Chemistry (CRSI-RSC-16) symposium on 2nd February 2023 will be dedicated to "***Health and Well-being***" which has been the central focus during the time of COVID-19 Pandemic. Needless to say, research in the interdisciplinary area of health has a strong bearing on the well-being of our society and plays a crucial role towards realizing the mission of Atmanirbhar Bharat (self-reliant India).

During the past five decades, JNU has emerged as a world-renowned institution in the country emphasizing quality research and teaching in the fields of pure and applied sciences, social sciences, international studies and humanities. Currently, there are 14 schools, 07 special centres and several centres within the schools in the university. JNU was accredited with A++ grade by the NAAC for the period 2017-2022. JNU has consistently ranked number 2 among all universities by NIRF, Government of India. JNU received the Visitor's award of "Best University" in the year 2017 from the President of India. From being a student at the University to being its first female Vice Chancellor, I can proudly say that JNU stands for Inclusion, Integrity and Innovation.

I congratulate the organising team for their hard work and meticulous planning in conducting the 30th CRSI NSC and wish them a grand success. As the head of the Institution, I would like to heartily welcome all the delegates and participants of the symposium to JNU as the nation celebrates Azadi ka Amrit Mahotsav and hope that you have a wonderful time and enriching experience during the symposium.

Dr. Sakya S. Sen

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CSIR-National Chemical Laboratory,
Dr. Homi Bhabha Road, Pune-411008, India
Email: ss.sen@ncl.res.in

Dr. Sen received his Ph.D. in 2010 at the University of Göttingen, Germany. Postdoctoral work followed (2011-2013), working with Prof. Holger Braunschweig at the University of Würzburg, Germany, supported by the AvH Foundation. In 2014, he was appointed as a senior scientist at CSIR-NCL, Pune, where he is currently serving as a Principal Scientist since 2018. Dr. Sen is the recipient of CSIR-Young scientist award in 2017, INSA medal for Young Scientist in 2018, Merck Young Scientist Award, 2019, NCLRF Scientist of the year in 2020, Swarnajayanti fellowship in 2021, CRSI-Bronze Medal 2022. He has been selected as a ChemComm Emerging Investigator 2018, Early Career Advisory Board Member of ACS Catalysis (2019-2021), Young Associate of Indian Academy of Science (2017-2020) and featured in "75 under 50 Scientists Shaping Today's India" (DST) (2021).

Palladium (II)-Catalyzed C-H Functionalization of Diastereotopic C-H Bonds

Dr. S. Arulananda Babu
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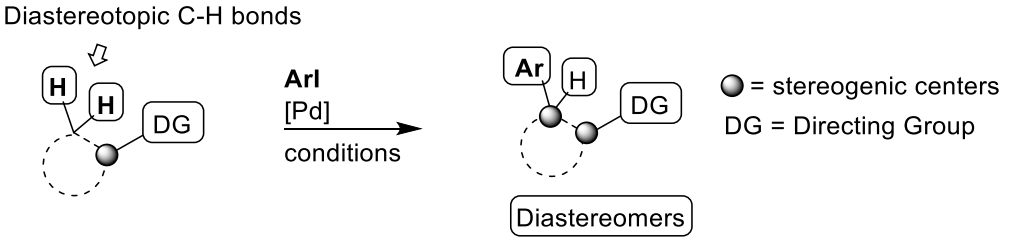
Email: *sababu@iisermohali.ac.in*

C-H functionalization of diastereotopic C-H bonds



The regio-or site-selective C–H functionalization of small organic molecules has been achieved with the help of various types of directing groups. In recent years, we have witnessed tremendous developments in the area of the Pd(II)-catalyzed, directing group site-selective C-H functionalization of carboxamides. Subsequently, the Pd(II)-catalyzed, directing group-aided functionalization method is being exploited to accomplish the stereoselective construction of stereogenic centers (adjacent or remote) in aliphatic compounds and *Z*-olefins *via* the sp^3 and sp^2 C-H bond functionalization, respectively. A glimpse of our group's contribution comprising the diastereoselective Pd(II)-catalyzed, directing group-aided functionalization of the diastereotopic C-H bonds will be presented.

References:

1. Kaur, R.; Banga, S.; Babu, S. A.; *Org. Biomol. Chem.*, **2022**, *20*, 4391.
2. Banga, S.; Kaur, R.; Babu, S. A.; *Eur. J. Org. Chem.*, **2021**, 3641.
3. Gopalakrishnan, B.; Mohan, S.; Parella, R.; Babu, S. A.; *J. Org. Chem.*, **2016**, *81*, 8988.
4. Parella, R.; Babu, S. A.; *J. Org. Chem.*, **2015**, *80*, 2339.
5. Shukla, D.; Babu, S. A.; *Adv. Synth. Catal.*, **2019**, *361*, 2075.
6. Babu, S. A.; Aggarwal, Y.; Patel, P.; Tomar, R.; *Chem. Commun.*, **2022**, *58*, 2612.
7. Tomar, R.; Suwasia, S.; Venkataramani, S.; Babu, S. A.; *Chem. Commun.*, **2022** under revision.

Dr. Srinivasarao Arulananda Babu

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Email: sababu@iisermohali.ac.in

Srinivasarao Arulananda Babu studied B.Sc. in Chemistry at Govt. Arts College, Krishnagiri, and received his B.Sc degree in Chemistry from the University of Madras (India) in 1996. He then studied M.Sc. in Organic Chemistry at AC Tech Campus, Chennai, and received his M.Sc degree (Organic Chemistry Specialization) from the University of Madras (India) in 1998. He carried out his Ph.D. work at CSIR-CSMRI, Bhavnagar (India), under the guidance of Prof. S. Muthusamy, and received his Ph.D. degree in Chemistry from Bhavnagar University (India) in 2003. He then performed a post-doctoral study with Prof. Akio Baba at Osaka University (Japan) from July 2003 to March 2005. He then worked as a designated Assistant Professor till March 2006 and then as an Assistant Professor in Baba's lab till Jan 2009. He then joined as an Assistant Professor at the Indian Institute of Science Education and Research Mohali (India) in Jan 2009. In March 2016, he was appointed as an Associate Professor at the Indian Institute of Science Education and Research Mohali (India). He served as the Head of the Department of Chemical Sciences, IISER Mohali, for a period of three years from October 2017 to October 2020. He has close to 95 publications and filed 10 patent applications (6 patents are under examination and 4 patents are granted). Nine (9) students have received PhD under his guidance and three (3) post-doctoral associates have worked in his group. Currently, he is guiding about 10 PhD students.

Research Interests:

- Stereoselective C-H activation and functionalization of small organic molecules.
- Metal-mediated stereoselective C-C bond construction reactions.
- Stereoselective synthesis of rigid unnatural amino acids and crown ether derivatives.
- Synthesis of new antimalarial and anticancer agents.

Awards and Honours:

- CSIR-SRF Dec 2000; CSIR-JRF June 1999; CSIR-LS June 1998; GATE '98: AIR = 102.
- Handai Frontier Research Center, Osaka, Post-Doctoral Fellowship

Functional Advanced Microporous Materials for Industrially Relevant Hydrocarbons Separation

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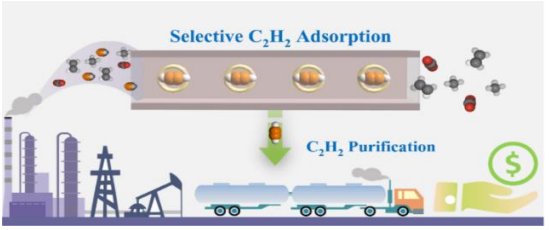
Email: sghosh@iiserpune.ac.in



Scheme 1: Diagram of MOF based C_2H_2 separation from industrial C2-C1 impurities.

Separation and purification of hydrocarbons in an energy-efficient manner is of fundamental relevance to petrochemical industries. Typically, light hydrocarbons such as acetylene and ethylene are utilized to produce several commodity chemicals, such as plastics, fibres, rubber, vinyl compounds, acrylic acid derivatives, among others. Energy-efficient selective physisorption driven C_2H_2 separation from industrial C2-C1 impurities such as C_2H_4, CO_2 and CH_4 is of great importance in the purification of downstream commodity chemicals. Under this backdrop, the industrially essential separation of benzene (Bz)/cyclohexane (Cy) and xylene isomers still prevails to be one of the most important challenges in chemical industry. Traditional purification methods viz. chemisorption, solvent extraction, azeotropic and/or fractional and/or cryogenic distillation albeit can separate these hydrocarbons, but they bear huge energy footprint, for instance, around 10–15% of the global energy is consumed in separation processes. This underscores the need to replace the existing energy-intensive purification technologies that majorly suffer from high energy footprint with energy-efficient alternatives such as recyclable/ regenerable physisorption. In this talk, I will discuss several metal-organic frameworks (MOFs) based separation and purification of hydrocarbons.

References:

1. Dutta, S.; Soumya, S.; Qazvini, O.T.; Gupta, A.K.; Sharma, S.; Mahato, D.; Babarao, R.; Ghosh S. K. *Angew. Chem. Int. Ed*. **2022**, *61*, e202114132.

Prof. Sujit K. Ghosh
Department of Chemistry, IISER Pune
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Prof Sujit K. Ghosh has obtained his Ph.D. from Indian Institute of Technology Kanpur in 2006. He then spent three years at Kyoto University (Japan) as a JSPS and CREST postdoctoral fellow before joining at IISER Pune in 2009. His research group is mainly working on development and functional studies of metal-organic frameworks (MOFs) and related advanced porous materials for chemical industry, energy and environmental applications.

Research Interests:

- Advanced functional porous materials
- Industrially relevant chemicals separation.
- Priority pollutants capture for clean drinking water.

Awards and Honours:

- CRSI Bronze Medal
- Advisory Board of ChemCommun
- Materials Research Society of India (MRSI) Medal.
- India Research Excellence - Citation Award by Clarivate Analytics.
- Alexander von Humboldt (AvH) Fellowship for Experienced Researchers, Germany.

Hydrogen production from waste H_2S pollutant

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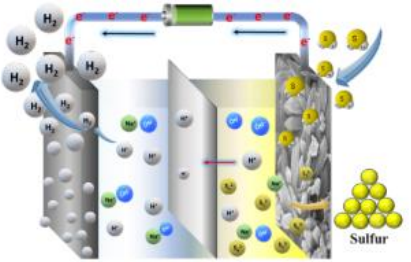

Highly efficient and cost-effective hydrogen production (H_2) promises to play a vital role in green energy production due to its high energy density, low-pollution, and renewable nature. The electrocatalytic decomposition of H_2O to H_2 and O_2 considered to be the most sustainable method for pure H2 production, unfortunately, it stumbles due to potentially uphill and energyconsuming sluggish anodic oxygen evolution reaction (OER).1 Contrary to H_2O isostructural hydrogen sulfide (H_2S) possesses lower bond dissociation energy. Therefore, anodic sulfide oxidation reaction (SOR) will be more energy-efficient than OER. Presently, the Claus process is the most popular industrial technology for removing H_2S, but energy wasted in the form of steam. Therefore, electrochemical conversion of environment pollutant H_2S into H_2 and S provide a way to remove pollutant H2S and also emerges as new energy source.2 However, the industrialization of such energy-efficient technology never meets the expectation in reality in the absence of cost-effective and robust electrocatalyst. Herein we have designed $CoFeS_2$ based catalyst that exhibited lower onset potential of 0.23 V vs. RHE towards SOR, which is 1.25 V lower than OER. Notably, only a 1.2 V commercial battery easily derives H_2S electrolysis, which is impossible for H_2O splitting demonstrating the tremendous future prospective of H_2S for cheaper hydrogen production for a sustainable economy.

References:

1. Zhang, M.; Guan, J.; Tu, Y.; Chen, S.; Wang, Y.; Wang, S.; Yu, L.; Ma, C.; Deng, D.; Bao, X., *Energy Environ. Sci.*, **2020**, *13 (1)*, 119-126.
2. Kumar, M.; Tharamani, C. Nagaiah, *J. Mat. Chem. A*, **2022**, *10*, 7048 – 7057.

Dr. Tharamani C. Nagaiah

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Dr. Tharamani is an Associate Professor and Head, Department of Chemistry at Indian Institute of Technology (IIT) Ropar. She holds a PhD degree from Bangalore University. Prior joining IIT Ropar, she spent four years in Germany as senior scientist and postdoctoral fellow at Ruhr University Bochum and a year at University of Saskatchewan, Canada. Her research interests include design and development of various carbonaceous materials, nanomaterials, molecular catalyst with focus on energy conversion and storage, Biosensors. In-depth fundamental analysis of the newly designed electrocatalysts towards fuel cells and batteries by various electrochemical, spectroscopic, microscopic and scanning probe techniques (SECM). Her scientific output resulted in eighty-five (85) publications and three patents at international refereed journals like, Chemistry of Materials, Journal of Materials Chemistry A (16), Energy Storage Materials, Analytical Chemistry, Journal of Physical Chemistry C, ACS Applied Material and Interface, Chemical Communications, etc.

Awards and Honours:

- Member of the Editorial Board in Journal 'Electrocatalysis', Springer Nature (2022-2024). Alexander von Humboldt Renewed Research Stay Fellowship (June 2022 – July 2022)
- Fellow of Royal Society of Chemistry 2021 (Invited under Leaders in the field scheme). Fellow of Indian Chemical Society 2021 (Invited)
- Co-opted Member of Program Advisory Committee on Inorganic and Physical Chemistry, SERB, Department of Science and Technology, Govt. of India
- Alexander von Humboldt Renewed Research stay Fellowship (June 2017 – July 2017)
- Invited for the 7th Indo-German Frontiers of Engineering Symposium (INDOGFOE 2015)
- Alexander von Humboldt Renewed Research stay Fellowship (June 2014 – July 2014)
- Ramanujan Fellowship, Department of Science and Technology, India 2013.
- Alexander von Humboldt Fellowship, Alexander von Humboldt Foundation, Germany (Jan. 2009 – Mar. 2011).

CRSI Medal Lecture

Chemically Processed Functional Ceramics for Energy and Health Applications

Prof. Sanjay Mathur
University of Cologne, Germany

Chemical processing of functional ceramics has played a key role in converging disciplines, which is especially true for their bridge-building role in integrating the concepts of inorganic materials synthesis with biomedical applications. Out of a vast variety of metal and metal oxide nanoparticles that have been developed for medicinal purposes, iron oxides are one of a few materials that made it through clinical trials. Due to their high biocompatibility, stability and the abundance of iron in our environment, which results in low costs of iron-based materials, diverse iron oxide nanoparticles have been prepared for biomedical applications. Examples will include application of superparamagnetic iron oxide nanoparticles for magnetic resonance imaging (MRI) and drug delivery applications. In addition, metal oxide nanostructures with hetero-contacts and phase boundaries offer unique platform for designing materials architectures for energy harvesting applications. As viable alternative to water electrolysis, photoelectrochemical (PEC) water splitting has emerged as a competitive technology being capable of converting solar energy directly into chemical energy using stable and efficient photocatalysts for solar hydrogen production. Hematite films grown from iron precursors showed pronounced changes in crystallographic textures depending upon whether CVD was performed with or without external magnetic field. Finally, the current challenges of integration of nanomaterials in existing device concepts will be discussed.

Prof. Sanjay Mathur

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Sanjay Mathur is a Chair Professor and Director of the Institute of Inorganic Chemistry at the University of Cologne in Germany. He is also the Director of the Institute of Renewable Energy Sources at the Xian Jiao Tong University, Xian, China and a World Class University Professor at the Chonbuk University in Korea. He is a Visiting Professor in the Institute of Global Innovation Research at TUAT, Japan and a SPARC Faculty at IIT Madras, India. His research interests focus on application of nanomaterials and advanced ceramics for energy technologies. He holds 11 patents and has authored/ co-authored over 500 original research publications (h index, 67) and has edited several books. He serves as the Editor for Journal of Electro ceramics, and for Nano Energy. He is an Academician of the World Academy of Ceramics and Fellow of the American Ceramic Society and ASM International. He was awarded the Honorary Doctorate of the Vilnius University in 2016. He chaired the Academic Affairs Committee of the Materials Research Society and currently serves on the Executive Council of the European Materials Research Society. He was awarded the R. C. Mehrotra Lifetime Achievement Award of Indian Science Congress Association in January 2020. He was elected Fellow of the European Academy of Science in 2020 and as Foreign Fellow of National Academy of Science, India in 2021. He was awarded the Woody White Award of the Materials Research Society (MRS) in 2021 and had received the Medal of the Chemical Research Society of India (2022). He is also the recipient of the Materials Frontiers Award (2022) of the International Union of Materials Research Society (IUMRS, 2022). He is the current President of the American Ceramic Society (ACerS, 2022-23), USA. He was recognized by the Orton Jr. Lecture (2022/23) of the ACerS.

CRSI-RSC Lectures

Nutrition's dark matter: beyond traditional nutrients

Dr Ana Rodriguez-Mateos
Reader (Associate Professor) in Nutritional Sciences
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Most of the research conducted over the last decades investigating the effects of diet and dietary components on health has focused on 5 key nutrients: fat, carbohydrates, proteins, vitamins and minerals. However, we now know that there are thousands and thousands of chemical compounds present in foods, and we know very little about how they may affect our health. Among this "nutritional dark matter", a group of compounds present in plant foods are receiving increased interest due to their potential health benefits. Phytochemicals are secondary plant metabolites comprising a very large number of compounds with diverse structure and biological activities. They are very abundant in our diet, particularly in fruits, vegetables, wholegrains, nuts, seeds, legumes, and popular drinks such as coffee and tea. Accumulating evidence from epidemiological, clinical and pre-clinical studies indicates that some of these compounds may exert beneficial effects against non-communicable diseases, with the evidence being particularly strong for the protection against cardiometabolic diseases. However, to elucidate their health benefits and provide adequate dietary recommendations, a better understanding of their estimated content in foods and estimated intake and exposure among the general public is needed, using accurate analytical methods such as ultra-high performance liquid chromatography coupled with mass spectrometry. This lecture will discuss the latest advances and challenges on the detection and quantification of phytochemicals in foods and biological samples, and the importance of nutritional metabolomics in elucidating how food affects our health.

Dr Ana Rodriguez-Mateos

Reader (Associate Professor) in Nutritional Sciences
Department of Nutritional Sciences, King's College London
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Dr Ana Rodriguez-Mateos studied Chemistry as her first degree at the University of ACoruña, Spain, before moving to the UK to undertake a PhD in Food Chemistry at the School of Food Biosciences of the University of Reading. There she discovered her passion for the field of nutrition and she continued her postdoctoral studies investigating the metabolic fate of dietary phytochemicals and their effects on human health. Her interest in the link between diet and health led her to her first position as Research Group Leader at the Division of Cardiology, Pulmonology and Vascular Medicine of the University of Dusseldorf in Germany, where she spent 4 years investigating the bioavailability and metabolism of polyphenols and their effects on cardiometabolic health. She came back to the UK in 2016 as a Lecturer in the Department of Nutritional Sciences of King's College London. She now leads a large research group and is also the Programme Director of the BSc in Nutritional Sciences, an Associate Editor for the RSC Journal Food and Function, member of the Editorial Board of Nutrition and Healthy Aging, Fellow of the Royal Society of Chemistry and member of the UK and American Nutrition Societies. She has published >100 manuscripts that have attracted 9610 citations (h-index=42).

Research Interests:

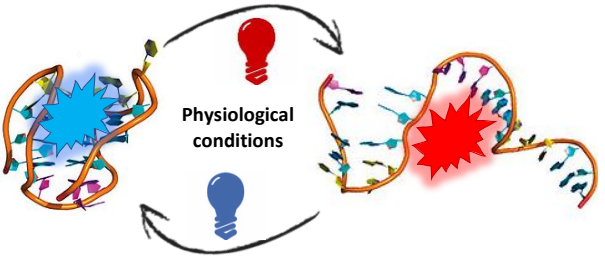
- To investigate the health benefits of plant foods and phytochemicals
- To investigate the bioavailability and bioaccesibility of dietary phytochemicals
- To investigate the interplay between diet, gut microbiota and health
- To develop novel methods for the analysis of foods and biological samples using analytical techniques such as liquid chromatography and mass spectrometry and to discover and validate new biomarkers of food and dietary intake

Awards and Honours:

- Fellow of the Royal Society of Chemistry (FRSC, since 2020)
- Fellow of the Higher Education Academy (FHEA, since 2018)
- Registered Nutritionist by the Association for Nutrition (RNutr, since 2018)
- American Aging Association Jim Joseph Memorial Award (2014)
- Young Investigator Award for Scientific Excellence, International Conference on Polyphenols and Health, Buenos Aires, Argentina (2013)
-

Photoresponsive Ligands to modulate G-quadruplex DNA

Prof. M. Carmen Galan
School of Chemistry
Cantock's Close, University of Bristol, United Kingdom
Email: m.c.galan@bristol.ac.uk



G-quadruplexes oligonucleotides (G4) are a fascinating class of nucleic acid structures formed from the self-association of guanine-rich sequences. This kind of four-stranded structures have potential applicactions in biological chemistry and responsive nanotechnology that may be exploited for therapeutic effect. While many examples of ligands that are able to stabilize G4 sequence are reported in the literature, those ligands do not induce reversible and controlable structural perturbations such as the re-folding of the G4 to an alternative topology or the unfolding of the G4 structure through binding modes at physiological pH. In this sense, light offers high spatiotemporal precision for the regulation of oligonucleotide structure.[1] During this lecture I will describe recent examples of photoresponsive ligands for G4 DNA regulations developed within our research group. From stiff-stilbene ligands which are capable of unfolding G4 DNA in physiological conditions in a reversible manner[2] to dithienylethene chromophores with inherently superior photoresponsive properties for the study of G4-binding properties which can be used for the photo-reversible control of ligand bindi ng mode and oligonucleotide folding employing exclusively red and blue visible light.[3]

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Prof. M. Carmen Galan

School of Chemistry, Cantock's Close
University of Bristol, Bristol BS8 1TS, United Kingdom
Email: m.c.galan@bristol.ac.uk

M. Carmen Galan is a Professor of Organic and Biological Chemistry in the School of Chemistry at the University of Bristol. In 2017, she was awarded the RSC Dextra Carbohydrate Chemistry award in recognition of her research into new synthetic methodologies for oligosaccharide synthesis and the development of novel glycoconjugate probes. In 2021 she received the RSC Jeremy Knowles award for the development of bioinspired synthetic probes for the targeting and regulation of cellular processes and in 2022 she was awarded the SRUK Merit award for her contributions to science and the impact of her work to the wider community. Carmen received her Ph.D. in Organic Chemistry from the Complex Carbohydrate Research Center at The University of Georgia, USA, under the supervision of Prof. Geert-Jan Boons. She then moved to California to pursue post-doctoral research with Prof. Chi-Huey Wong at The Scripps Research Institute and M.I.T with Prof. Sarah O'Connor before moving to the UK in 2006 as a Lecturer.

Research Interests:

- Carbohydrate chemistry and glycobiology
- Medicinal chemistry
- Nanotechnology

Awards and Honours:

- 2022 SRUK-CERU Merit Award
- 2021 RSC Jeremy Knowles award
- 2017 RSC Carbohydrate Chemistry award
- 2017 Visiting Professorship Université d'Orleans
- 2015 ERC Consolidator Award
- 2012 EPSRC Career acceleration Fellowship
- 2012 Visiting Professorship Université Joseph Fourier
- 2011 Hoffmann-La Roche award at the European Young Investigator Workshop in Lyon
- 2008 RS Dorothy Hodgkin Fellowship
- 2007 The Welcome Trust Value in People Award.

Developing drugs for India: Opportunities and Challenges

Dr. Radha Rangarajan
Director, CSIR-Central Drug Research Institute, India
Email: director@cdri.res.in

Research and development for new drugs in India has gone through multiple phases. The first phase was led largely by academia, with institutes like CDRI taking the lead. Notable successes from this period include the contraceptive Centchroman and anti-malarial drug, a/B arteether. In the second phase, a number of companies such as Ranbaxy, DRL and others entered the fray with dedicated R&D centres. Some had early successes; several closed their R&D operations and others pivoted to services. Interestingly this phase saw a broad expansion of the CRO industry. Beyond chemistry, India started to offer services in other segments such as biology, toxicology and formulation development. Alongside, a small number of pharmaceutical companies and a clutch of start-ups also entered the discovery space. Fast forward to 2022, it appears that drug discovery in India is entering a third phase. India's capabilities in academia, start-ups and industry have expanded. Moreover, there is demonstration of these stakeholders being able to work together effectively. Products that were taken to market in public-private partnerships (PPP) during the Covid-19 pandemic are examples. Building upon and expanding the synergies of PPP models holds the promise of India being able to develop drugs for India. I will provide examples from the pipeline of CDRI and other CSIR Institutes as illustrations of the opportunities and challenges ahead.

Dr Radha Rangarajan

Director
CSIR-Central Drug Research Institute, India
Email: director@cdri.res.in

Dr Radha Rangarajan has been actively involved in translational research and product development in the public health arena for the last two decades. Working closely at the interface between academia, start-ups and industry, her experiences span the drug discovery, diagnostics and medical devices sectors. Her core research interests are in basic and translational aspects of antibiotic resistance including novel approaches to diagnosing and treating drug resistant infections.

Between 2003 and 2009, Dr Rangarajan worked in the Drug Discovery division of Dr Reddy's Laboratories in Hyderabad. She served in multiple roles, successfully developing early-stage molecules for various therapeutic areas such as anti-infectives, diabetes and cardiovascular disease. Thereafter, she co-founded Vitas Pharma, a drug discovery and development company focused on novel therapies to treat highly resistant infections. She leveraged public-private partnerships to build a highly efficient innovation platform delivering multiple lead optimized candidates, granted patents and companion diagnostics. In 2020, she took on the role of Chief Technology Officer at Health Cubed, a medical devices company focused on affordable diagnostics, where she was responsible for product development, clinical validation, manufacturing and regulatory affairs. Dr Rangarajan is a member of the Steering Council of the MedTech Incubator, International Institute of Information Technology, Hyderabad (IIIT-H), member of the Scientific Program Committee of IHub-Data, IIIT-H, member of the Selection Committee of the NIDHI-Seed Support System at the Atal Incubation Centre-CCMB and member of the Selection Committee for DST INSPIRE Faculty Fellows.

Dr Rangarajan received the Federation of Indian Chambers of Commerce and Industries (FICCI) Award of Excellence: Women in R&D in 2019. She was selected for the "Champions of Change" initiative of Prime Minister Modi, recognizing India's emerging entrepreneurs in 2017. She led the Vitas Pharma team that received the Discovery Award of the Longitude Prize Committee, UK in 2016 and was a finalist in the Economic Times Start up Awards (Woman Ahead Category) in 2016.

Dr Rangarajan obtained her Bachelor of Science in Biology from Stanford University, Master of Science from the University of Michigan, Ann Arbor, and Ph.D. from Rockefeller University. She was a postdoctoral fellow at the Harvard School of Public Health.

Fostering Biotech Innovations and Bioeconomy

Dr. Rajesh S. Gokhale
Secretary, Department of Biotechnology (DBT)
Ministry of Science and Technology
Email: rajesh.gokhale@iiserpune.ac.in

Dr. Rajesh S. Gokhale

Secretary, Department of Biotechnology (DBT)
Ministry of Science and Technology
Government of India
Email: rajesh.gokhale@iiserpune.ac.in

Rajesh Sudhir Gokhale (born 1967) is currently the Secretary for Department of Biotechnology (DBT), Government of India. He joined National Institute of immunology after conducting his postdoctoral training at Stanford University, He was the director of Institute of Genomics and Integrative Biology from 2009 to 2016. He is known for his studies on the metabolic diversity of pathogens. He is credited with the discovery of a family of Long-chain Fatty acyl-AMP ligases (FAAL) and his studies assisted in the elucidation of *biochemical crosstalk* between fatty acid synthases and polyketide synthases in Mycobacterium tuberculosis. He holds US and Indian patents for his invention of *Method to Modulate Pigmentation Process in the Melanocytes of Skin*. An alumnus of the Indian Institute of Science, he is an elected fellow of the Indian Academy of Sciences (2007) and the Indian National Science Academy (2014). The Council of Scientific and Industrial Research, the apex agency of the Government of India for scientific research, awarded him the Shanti Swarup Bhatnagar Prize for Science and Technology, one of the highest Indian science awards, in 2006, for his contributions to biological sciences. He received the National Bioscience Award for Career Development of the Department of Biotechnology in 2009.

Correcting Genes with Precision: An Indigenous Approach

Souvik Maiti
CSIR-Institute of Genomics and Integrative Biology, Delhi
CSIR-National Chemical Laboratory, Pune
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CRISPR based genetic correction has moved rapidly into therapeutics with multiple clinical trials currently underway for predominantly monogenic disorders. One of the limitations of first generation CRISPR proteins derived from Streptococcus pyogenes (SpCas9) is the rampant off-targeting caused by high propensity to binding genetic loci with some degree of homology to the target. At the biophysical level, this can be explained by the nature of amino acid and nucleobase contacts that the domains of the Cas9 makes with a substrate. In order to make such a Cas protein more specific in targeting the desired gene, several groups have attempted to engineer SpCas9 by reducing possible contacts in the DNA backbone inevitably leading to more specific but less efficient editors that impacts the eventual therapeutic benefit. We have approached this problem from a different route by exploiting the high specificity of an orthogonal Cas protein from Francisella novicida (FnCas9). Although this protein has a very high mismatch dissociation ability, its inherent activity on cellular targets was low. To circumvent this, we have engineered residues in the PAM interacting domains of FnCas9 and developed engineered versions of the protein that uniquely combines high specificity and efficiency. We are currently taking this ahead for clinical trials for the genetic correction of hematological and ocular diseases. This talk will feature how such an engineering was done and the eventual outcome on target binding and off-target discrimination.

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Dr. Souvik Maiti

Scientist, CSIR-Institute of Genomics and Integrative Biology
Adjunct Professor, IISER-Mohali
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Souvik Maiti completed his B. Sc. (1993) And M. Sc (1995) in Chemistry from Jadavpur University, Kolkata, and PhD (1999) in synthetic polymer chemistry from the CSR-Indian Institute of Chemical Technology, Hyderabad, India. After post-doctoral training from College of Pharmacy, UNMC, Omaha, USA and Department of Physics, Curie Institute, Paris, France, he joined as a research faculty CSIR-Institute of Genomics and Integrative Biology, Delhi, in 2003. He is also adjunct research faculty in CSIR-National Chemical Laboratory, Pune and adjunct professor in the Indian Institute of Science Education and Research (IISER) Mohali. He works in the interface of Chemistry and Biology and focuses on the chemical biology of nucleic acids to address questions of importance in biology and medicine. Currently his research group is engaged in developing potent Indigenous CRISPR-Cas9 based tools for point-of care diagnostics and for the cheaper treatment of genetic diseases. Recently he is part of a team that has initiated a 5-year clinical trial to evaluate the indigenously developed CRISPR/Cas9 gene editing tool as a potential cure for sickle cell disease.

Chemical Approaches to Targeting and Imaging Tumour Hypoxia

Prof. Stuart Conway
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Tumor hypoxia (low oxygen levels) is associated with resistance to all therapeutic approaches and poor patient prognosis. Hypoxia-activated prodrugs, designed to selectively release a bioactive compound in oxygen-deficient cells, while sparing healthy tissue, represent a promising therapeutic strategy for treatment of cancers.[1,2] NI-Pano (CH-03) is a novel hypoxia-activated version of the clinically approved lysine deacetylase inhibitor, panobinostat. We have demonstrated the pre-clinical efficacy of NI-Pano, showing that it is stable in normoxic (21% oxygen) conditions but undergoes NADPH-CYP-mediated enzymatic bioreduction to release panobinostat selectively in hypoxia (<0.1% oxygen).. Importantly, NI-Pano exhibited growth delay effects as a single agent in mouse tumor xenografts. Pharmacokinetic analysis confirmed the presence of effective concentrations of panobinostat in hypoxic mouse xenografts, but not in circulating plasma, or kidneys. Our preclinical results provide a strong mechanistic rationale for the clinical development of NI-Pano and other hypoxia-activated prodrugs, for the selective targeting of hypoxic tumors.[3] To this end, we have shown that azide pro-fluorophores are reduced by cytochrome P450 enzymes, which represents a novel approach to imaging cellular hypoxia.[4] We have also recently developed a suite of hypoxia-activated fluorophores, based on the indole quinone redox trigger, that image a range of oxygen concentrations in different colours, visualising gradients of hypoxia for the first time.

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2. O'Connor, L. J.; Cazares-Körner, C.; Saha, J.; Evans, C. N. G.; Stratford, M. R. L.; Hammond, E. M.; Conway, S. J. *Nat. Protoc.* **2016**, *11*, 781–794.
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Prof. Stuart Conway

Department of Chemistry
University of Oxford
Email: stuart.conway@chem.ox.ac.uk

Stuart Conway is a Professor of Organic Chemistry at the University of Oxford, and the E. P. Abraham Cephalosporin Fellow in Organic Chemistry at St Hugh's College, Oxford. He studied Chemistry with Medicinal Chemistry at the University of Warwick before undertaking PhD studies with Professor David Jane and Professor Jeff Watkins FRS in the Department of Pharmacology at the University of Bristol. Stuart completed post-doctoral studies with Professor Andrew Holmes FRS at the University of Cambridge working on the synthesis of phosphatidylinositol polyphosphates and inositol phosphates second messengers. In 2003, he was appointed as a Lecturer in Bioorganic Chemistry at the University of St Andrews, in 2008 was appointed as an Associate Professor at Oxford, and in October 2014 he was promoted to Full Professor. Between March and August 2013 Stuart was a Visiting Associate at the California Institute of Technology, hosted by Professor Bob Grubbs and Professor Dianne Newman. Stuart is an Associate Editor for the *Journal of Medicinal Chemistry* and *ACS Bio & Med Chem* Au. He is the Immediate Past President of the RSC Organic Division, the Director of the Wellcome Trust Chemistry in Cells PhD Programme, and the Director of the EPSRC redOX⇌KCL Programme Grant. His research focuses on the development of molecular tools to enable the study of biological systems, with particular interests in epigenetics and hypoxia. This work has been recognised by the award of the 2012 Prize for a Young Medicinal Chemist in Academia by the European Federation for Medicinal Chemistry, and the 2016 Lectureship of the Biological and Medicinal Chemistry Section of the RSC.

Research Interests:

- Chemical biology and medicinal chemistry of epigenetics processes
- The development of small molecules to target and image hypoxia and cellular redox

Awards and Honours:

- Lectureship of the Biological and Medicinal Chemistry Section of the RSC (2016)
- Elected as a Fellow of the Royal Society of Chemistry (2014)
- European Federation for Medicinal Chemistry Prize for a Young Medicinal Chemist in Academia (2012)

Drug Discovery Processes and Challenges – Role of Chemist Through a Case Study

Dr. Vidya Ramadas
Director, Medicinal Chemistry, Enveda Biosciences
Email: Director @ Enveda Biosciences

Advancement in medical research led to development of treatment for many diseases over several decades. Since 2000, more than 600 new medicines have been approved by the FDA. However, there is still a huge unmet need due to adverse effects, moderate response or development of resistance to existing drugs or a rare disease for which no medicine. There is also increase in new diseases due to change in life style and environment. Although drug discovery and development are an expensive, time consuming and a high-risk endeavor, it is vitally important to discover new efficacious and safer drugs to improve patient's health and save lives. The talk will cover brief overview of the processes and challenges involved in novel drug discovery and the role of a chemist in discovering new drugs will be explained with a case study from own work. It may also enable you to appreciate how truly drug discovery is a marathon relay race of multi-disciplinary teams.

Vidya Ramadas
Director
Medicinal Chemistry
Enveda Biosciences
Email: Director @ Enveda Biosciences

Vidya has twenty years of post-PhD experience in Medicinal Chemistry and Novel Drug Discovery. She obtained her PhD in synthetic organic chemistry from Univ of Hyderabad with Prof. Goverdhan Mehta and gained her post-doctoral experience at Univ of Kansas, USA with Prof. Gunda I Georg. After her post-doctoral research, she worked in the drug discovery set-up of three different Indian pharmaceutical companies, Dr. Reddy's Laboratories, TATA-Advinus Therapeutics and Lupin Ltd. She worked on different disease targets under various therapeutic areas such as metabolic disorder, anti-inflammation, pain, anti-viral and oncology and delivered several pre-clinical candidates suitable for clinical development as a medicinal chemistry project leader. Over the years she has developed skills in novel drug design, structure-activity relationship studies, lead optimization, patent analysis and IP generation. She is a co-author to 19 publications and a co-inventor in 16 WO patents and ten are granted in US. Although, she enjoyed her teaching experience in academic set up for 18 months at IIT Jammu, she decided to come back to industry to pursue her passion for drug discovery. Currently, she is working as director in medicinal chemistry at Enveda Biosciences, Hyderabad.

Virucidal Antivirals - Preparing for the next pandemic

Dr. Samuel Jones
Lecturer
Department of Materials, University of Manchester
Email: samuel.jones-4@manchester.ac.uk

Current response options for viral outbreaks leave us vulnerable to the catastrophic impacts of future pandemics. Virus specific vaccines, antibodies and drugs, which are being developed for current epi- and pandemics, provide no protection against future viral outbreaks. Additionally, each takes too long to implement, allowing diseases to spread. Despite global action plans to contain viral outbreaks there is still a lack of rapid response options. Current rapid response options for viral outbreaks include, closing boarders, quarantine, and data sharing and yet these options alone are not enough to stop global spread, as we have seen. We urgently need a first response drug, equivalent to broad-spectrum antibiotics, to help control viral outbreaks.

On account of the COVID-19 pandemic, everyone is acutely aware of most of the approaches used to deal with viral infections. This talk will introduce a new concept of biocompatible extracellular antivirals that have a virucidal mode of action. A range of materials will be discussed with a specific focus on the use of polymers as antivirals. We will explore the properties that lead to the most potent antivirals and present data that shows efficacious use against several viruses using both in-vitro and in-vivo models.

Dr. Samuel Jones

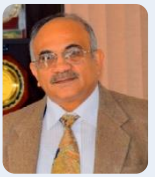
Lecturer
Department of Materials
University of Manchester
Email: samuel.jones-4@manchester.ac.uk

Dr. Samuel Jones is a Lecturer in the Department of Materials at the University of Manchester. He heads up the Jones Lab which focuses on understanding material/virus interactions. Sam completed his masters in Chemistry, from the University of Warwick, under the direction of Prof. Stefan A. F. Bon in 2009. His work at the time focused on hydrogen bonding interactions for gold nanorod assembly. During his studies he also undertook a research project at the University of Tasmania in the group of Dr. Adrian Blackman. For his Ph.D. Sam moved to the University of Cambridge where he worked in the Melville Laboratory for Polymer Synthesis under Prof. Oren A. Scherman, on the supramolecular assembly of nanomaterials via cucurbit[*n*]uril. Upon completion of his Ph.D. in 2013, Sam moved to the École Polytechnique Fédérale de Lausanne (EPFL) where he worked alongside Prof. Francesco Stellacci. His research focused on the synthesis of novel virucidal materials and the synthesis of Janus nanoparticles for targeted delivery. In 2017, Sam started his independent research career as a Dame Kathleen Ollerenshaw Fellow at the University of Manchester, before becoming lecturer in 2022.

BRIEF BIOSKETCHES OF CHAIRPERSONS

Prof. A. K. Ganguli

Department of Materials Science and Engineering,
IIT-Delhi,Hauz Khas, New Delhi-110016, India
Email: ashok@chemistry.iitd.ac.in



Prof Ganguli studied chemistry from University of Delhi and PhD from IISc Bangalore in 1990. He then was a visiting scientist at Dupont Company, USA and Ames Lab, Iowa and then he joined IIT Delhi in 1995 where he is currently Prof N K Jha Chair Professor of Chemistry and also Professor of Materials Science & Engineering. His main interest is in the area of design of materials, especially nanomaterials and superconducting materials. He has published over 350 papers and has filed five patents (two granted). He is a recipient of several awards and is a fellow of the Indian Academy of Sciences and the National Academy of Sciences, India. Dr. Ganguli is also a keen speaker for science in the rural & remote areas and has interacted with more than 320 schools/colleges in last seven years. Dr Ganguli coordinated the initiation of the Delhi S&T Cluster supported by the office of the PSA, Govt of India.

Research Interests:

- Design and synthesis of materials including nanomaterials
- Photoelectrochemical, magnetic and superconducting properties

Awards and Honours:

- DST National Award of Nanoscience7 Technology 2015
- Distinguished materials scientist of India 2021,
- CRSI silver Medal, CRSI_CNR Rao National Award

Positions Held:

- Deputy Director, IIT Delhi
- Director, INST Mohali

Dr. BVNBS Sarma

Sr Vice President
Discovery Services at Sai Life Sciences Ltd
Email: sarma.b@sailife.com

Education:

- Post-Doctoral Fellow at Steacie Institute for Molecular Sciences, Ottawa, Canada
- PhD at CSIR-Indian Institute of Chemical Technology, Hyderabad
- Osmania University

Research Interests:

- Drug Discovery and Development

Work:

- Scientist at Saiadvantium
- Sr Vice President - Discovery Services at Sai Life Sciences Ltd
- Vice President-Discovery at Sai Life Sciences Ltd

Prof. Chinmay K. Mukhopadhyay
Special Centre for Molecular Medicine
JNU, New Delhi 110 067, India.
E-mail: ckm2300@mail.jnu.ac.in

Prof Mukhopadhyay studied Bio-chemistry and obtained Ph. D in the year 1995 from the Department of Biochemistry, University of Calcutta. He received postdoctoral training from the Lerner Research Institute, Cleveland Clinic Foundation, USA. Prof. Mukhopadhyay joined at Special Centre for Molecular Medicine, JNU in the year 2001.

Research Interests:

- Role of Reactive Oxygen Species (ROS) in neurodegenerative diseases.
- Role of iron in intracellular infection, inflammation and metabolic diseases.

Awards and Honours:

- INSA-Young Scientist Award
- Senior Research Fellow, The Wellcome Trust, UK
- Member of Guha Research Conference
- Fellow of The National Academy of Sciences, India

Positions Held:

- Associate Professor, SCMM, JNU, 2001-2008
- Professor, SCMM, JNU from 2008
- Chairperson, SCMM, JNU (2005-2007 and 2013-2015)

Prof. D Srinivasa Reddy

CSIR-IICT
Indian Institute of Chemical Technology, Hyderabad
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Dr. Srinivasa Reddy has more than 20 years of research experience in the synthesis of natural products/medicinal chemistry/drug discovery. Dr. Reddy is best known for his application oriented organic synthesis towards human wellbeing. He is also known for the application of "Silicon-switch approach" in medicinal chemistry. In addition, the work carried out by his group on crop protection is worth highlighting. He is an author of ~120 publications and an inventor in ~35 patents.

- Accomplished total synthesis of ~50 natural products of biological importance.
- One of the molecules (Licogliflozin) discovered by his team in industry is currently in human clinical trials (Phase-II), where he was a project leader.
- Acquired skills in designing novel small molecules and lead optimization.
- Experienced in planning and execution of projects (Govt. and Industry).
- Discovered an anti-diabetic lead molecule (along with Shantani Pvt Ltd, Pune).
- Identified Silinezolid with high brain:plasma ratio with a potential to treat brain infections.
- Identified of an antibiotic lead compound for treating food infections.
- Identified novel Insect Repellents – Further work is in progress.
- Identified of novel Cladologs towards potent anti-malarial drug discovery.
- Dr. Reddy received several recognitions including the prestigious Shanti Swarup Bhatnagar Award (SSB) in Chemical Sciences and J. C. Bose National Fellowship by DST-SERB, Govt of India. He is also an editor of Bioorganic & Medicinal Chemistry Letters (BMCL), an Elsevier journal.

Research Interests:

- Total Synthesis of Natural Products Using Scalable Routes**.**

Positions Held:

- 2020- Present Director, CSIR- Indian Institute of Integrative Medicine, Canal Road, Jammu, India
- 2018- 2020 Senior Principal Scientist, CSIR-National Chemical Laboratory, Pune, India.
- 2014- 2018 Principal Scientist, CSIR-National Chemical Laboratory, Pune, India.
- 2010- 2014 Senior Scientist, CSIR-National Chemical Laboratory, Pune, India.

Prof. Diwan Singh Rawat

Department of Chemistry
University of Delhi
Email: dsrawat@chemistry.du.ac.in

Professor Diwan S Rawat, is a Senior Professor of Chemistry at University of Delhi. He did his Ph.D. in Medicinal Chemistry from Central Drug Research Institute, Lucknow in 1998. After completing his PhD, he worked two years in a Pharmaceutical Industry and did postdoctoral work at Indiana University (1999-2001) and Purdue University, USA (2001-2002). He was an Assistant Professor (2002-2003) of Medicinal Chemistry at National Institute of Pharmaceutical Education and Research (NIPER), Mohali and joined Delhi University in 2003, and he was promoted to Full Professor in 2010. Prof. Rawat has published 162 research papers, authored a book (book was reviewed by JACS), five book chapters, and seven patents to his credit. His work has been cited over 6270 times with h–index of 45 and i-10 index 126. One of his compounds has licensed to NurrOn Pharamaceuticals, Boston, USA for the development as a drug for the treatment of Parkinson`s disease. Prof Rawat was elected President of Chemical Sciences Section of Indian Science Congress for the year 2019-20 and he is also a Visiting Professor at Japan Advanced Institute of Science and Technology (JAIST), Japan. Professor Rawat has supervised 26 PhD students.

Research Interests:

- Medicinal Chemistry and Catalysis

Awards and Honours:

- ISCB Excellence Award in Drug Research (2022)
- Elected as a Fellow of National Academy of Sciences (FNASc, 2021)
- Vasvik research award (2021)
- Special Appreciation Award for Exemplary Services, University of Delhi (2021)
- Platinum Jubilee Lecture Award, Indian Science Congress (2021)
- Professor SP Hiremath Memorial Award, Indian Council of Chemist (2016)
- Professor RC Shah Memorial Lecture Award, Indian Science Congress (2015)
- CRSI young scientist award (2007)
- Prof. D. P. Chakraborty 60th Birth Anniversary Commemoration Award, Indian Chemical Society (2007).
- Associate Editor of Scientific Reports (Nature Research Journal), RSC Advances (Royal Society of Chemistry).

Prof. Gobardhan Das
Special Centre for Molecular Medicine
JNU, New Delhi-110067 India
Email: gobardhan.das07@gmail.com

Prof. Gobardhan Das studied chemistry and did his specialization in Immunology. He has a vast experience in the area of vaccine development and works on Tuberculosis. He is a part of many scientific committees and has received prestigious awards. His outstanding publication record serves as documentary evidence for his great work.

Research Interests:

- Biochemistry
- Molecular biology
- Immunology

Awards and Honours:

- Fellow of **"Indian Academy of Sciences",** Bangalore (FASC) 2018.
- Fellow of **"The National Academy of Sciences",** Allahabad (FNASc) 2011.
- Fellow of **"West Bengal Academy of Sciences and Technology"**, 2014.
- Fellow of **"Welcome Trust-DBT Senior Fellowship"**, 2009.
- Fellow of **"Ramalingaswami Fellowship"**, 2008.
- Fellow of **"National Research Foundation**" Govt. of South Africa, 2013.
- BD-Bioscience-TCS award, 2011.

Positions Held:

- **02, 2014-till date** Professor Jawaharlal Nehru University, New Delhi, India.
- **02, 2012-02, 2014** Professor University of KwaZulu-Natal, Durban, South Africa.
- **08, 2007- 01, 2013** Senior Scientist (Professor Grade), ICGEB, New Delhi, India.
- **07, 2002- 07, 2007** Senior Scientist, Aventis Pharmaceuticals, Bridgewater, NJ, US
- **Adjunct Professor,** Houston Methodist Hospital, Houston, USA.
- **Adjunct Professor**, Shoochow University, Suzhou, China.

Prof. G. Mugesh
Chemical Sciences Bldg.,
Indian Institute of Science, Bangalore - 560 012
Email: mugesh@iisc.ac.in

Prof. G. Mugesh completed his graduate studies in chemistry at the University of Madras in 1990 and after obtaining a master's degree from Bharathidasan University in 1993, he enrolled for his doctoral degree at the Indian Institute of Technology, Mumbai under the guidance of H. B. Singh to secure a PhD in 1998.[9] Remaining at the institute, he did his post-doctoral studies there till 2000 and moved to continue his studies at the laboratories of de: Wolf-Walther du Mont of Brunswick University of Technology and de: Helmut Sies of University of Düsseldorf on an Alexander von Humboldt fellowship till 2001. Subsequently, obtaining a Skaggs Postdoctoral Fellowship, he moved to the US to work with K. C. Nicolaou at Scripps Research Institute. Prof. G. Mugesh is known for his studies on mechanism of thyroid hormone action and is an elected fellow of the Indian Academy of Sciences, Indian National Science Academy, Royal Society of Chemistry and the National Academy of Sciences, India. The Council of Scientific and Industrial Research, the apex agency of the Government of India for scientific research, awarded him the Shanti Swarup Bhatnagar Prize for Science and Technology, one of the highest Indian science awards, in 2012, for his contributions to chemical sciences. In 2019, he was awarded the Infosys Prize in Physical Sciences for his seminal work in the chemical synthesis of small molecules and nanomaterials for biomedical applications.His recent efforts are directed toward understanding the antioxidant activity of synthetic compounds in mammalian cells, the thyroid hormone metabolism and thyroid related disorders, development of molecular probes for the detection and quantification of reactive oxygen species in the cells and oxidative stress biomarkers.

Research Interests:

- Small molecule-based Glutathione Peroxidase (GPx) Mimetics
- Nanozymes for Biomedical Applications
- Chemistry of the Thyroid Hormone Metabolism
- Halogen bond-mediated Cell Membrane Transport
- Expanding the Genetic Code by Unnatural Amino Acids

Prof. Hiriyakkanavar Ila
Organic Synthetic Laboratory
JNCASR, Bengaluru- 560064, Karnataka, India
Email: hila@jncasr.ac.in

Prof. Hiriyakkanavar Ila received her MSc from DAV College, Kanpur in 1964 and was the first woman to receive the Ph.D. in 1968 from IIT Kanpur. She did postdoctoral work at Purdue University, Lafayette in 1969 and was Alexander von Humboldt Fellow at Ludwig Maximilian University, Munich (1984-85). She was a scientist at Medicinal Chemistry Division, Central Drug Research Institute, Lucknow (1970-76) and then moved to Northern Eastern Hill University, Shillong (1977) as a founding faculty member and continued there for nearly 18 years. She was responsible for building the Chemistry Department at newly established Northern- Eastern Hill University, Shillong with state-of-art laboratory, instrumental and library facilities. She moved to IIT Kanpur as Professor (1995) and continued there till her superannuation (2006). She was a Marie- Curie Visiting Fellow at University of Cambridge (1995) and a Visiting Professor at Locker Hydrocarbon Research Institute, USC, Los Angeles (2002), at Institut de Investigacuiones, Sovilla, Span, and at Kuwait University (2007). Currently, she is an honorary chair professor at JNCASR.

Research Interests:

Prof. Ila has made prolific contributions in heterocyclic chemistry developing novel general and efficient methods for biologically important heterocyclic scaffolds utilizing polarized ketene S, S- and N, S- acetals as versatile building block.

Awards and Honours:

- Fellow, Indian Academy of Sciences, Bangalore (F.A.Sc., 1991)
- AV Rama Rao Prize, 2001.
- Fellow, Indian National Science Academy, New Delhi (FNA, 2002)
- CRSI Silver Medal, 2002.
- PC Datta Memorial Lectureship of Indian Association for the Cultivation of Sciences, Kolkata (2006).
- Chemical research Society of India (CRSI), Life time Achievement award (gold medal), 2019.

Prof. Hirendra Nath Ghosh
Radiation & Photochemistry Division
BARC, Trombay, Mumbai- 400085, India
E-mail: hnghosh2004@gmail.com

Prof. Hirendra N. Ghosh is currently serving as Senior Professor at Bhabha Atomic Research Centre (BARC), Mumbai and adjunct faculty at Institute of Nanoscience and Technology (INST) Mohali. Prof. Ghosh has obtained his M.Sc. degree I Physical Chemistry from IIT Kharagpur in 1989 and PhD degree from University of Mumbai in 1996. He has developed multiple state of the art ultrafast spectroscopic techniques which include Femtosecond broad band pump-probe spectroscopy and time-resolved tetra hertz spectroscopy.

Research Interest:

- Ultrafast interfacial electron transfer and charge carrier relaxation dynamics in semiconductor nanoparticles.
- Hybrid nano-structures.
- Plasmonic and 2D materials.

Awards and Honors:

- INSA young scientist medal (1998)
- A. K. Bose memorial award (2000)
- APA- Prize for young scientist (2004)
- Homi Bhabha Science & Technology Award (2010)
- CRSI Bronze Medal (2011)
- CRSI Silver Medal (2014)
- C.N.R. Rao National Prize for Chemical Research (2014)
- Fellow of National Academy of Sciences (F.N.A.Sc.)
- Fellow of Academy of Sciences (F.A.Sc.)
- Fellow of Indian National Science Academy (F.N.A.).

Prof. Javed Iqbal
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Hyderabad
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Prof Iqbal graduated from Delhi University and worked as a scientist at Ranbaxy Laboratories, New Delhi and subsequently worked as a SERC post-doctoral fellow at Cambridge University in the research group of Prof Ian Fleming, FRS. He later moved to Oxford University and worked as a research fellow with Prof J. E. Baldwin, FRS. He was a Professor at IIT Kanpur during 1984-99 and later moved to Dr Reddy's Laboratories Ltd (DRL), Hyderabad where he served as Distinguished Research Scientist and Global Head, Discovery Chemistry and subsequently as Director, Dr Reddy's Institute of Life sciences (2000-2013). He has also served as Director of National Institute for Interdisciplinary Science and Technology (NIIST) Council of Scientific and Industrial Research (CSIR) Trivandrum during 2002. He was visiting fellow at University of Notre Dame, USA, University of Montpellier, France and University of Okayama, Japan. Javed has also taught at New Mexico State University, Las Cruces, USA in the summer semesters during 1997-99. He was William Evans Fellow in the Department of Chemistry, University of Otago, New Zealand during March-April 2016. He was a visiting Professor at Department of Chemistry, University of Regensburg Germany in May 2019. He is currently an Adjunct Professor at Department of Chemistry, IIT-ISM, Dhanbad and Department of Molecular Science, LaTrobe University, Melbourne, Australia.

Research Interests:

- Synthetic Organic Chemistry and Medicinal Chemistry
- Chemical Biology and Drug Discovery

Awards and Honours:

- Fellow of Indian Academy of Sciences, Bangalore
- Fellow of Indian National Science Academy, New Delhi

Positions Held:

- Professor, Department of Chemistry, IIT Kanpur
- Director, CSIR-NIIST, Trivandrum
- Global Head and Distinguished Research Scientist, Dr Reddy's Laboratories Ltd.

Prof. Jitendra K Bera
Professor and Head, Department of Chemistry
Indian Institute of Technology Kanpur,
Email: jbera@iitk.ac.in

Jitendra Bera received Ph. D. from Indian IISc, Bangalore in 1999. After a couple of postdoctoral stints, he joined the faculty at IIT Kanpur in 2003, where he is currently serving as Chair Professor and head of the department. He is elected fellows of three National Science Academies (FASc, FNASc, FNA) and recipient of J C Bose National Fellowship. His research in the field of Organometallic Chemistry has earned him several awards and recognitions including Outstanding Investigator Award by DAE, Swarna Jayanti fellowship (2009) by DST and Silver medal (2020) and bronze medal (2012) by Chemical Research Society of India (CRSI). He received C. N. R. Rao National Prize (2018) in Chemical Sciences. He is currently serving as an Associate Editor, Applied Organometallic Chemistry (Wiley), Member: Editorial Advisory Board of Organometallics (ACS), Dalton Transactions (RSC). Bera's research interests span synthetic, structural and mechanistic organometallic chemistry and addresses energy, environmental and sustainability aspects of chemical synthesis.

Prof. Kamal K. Kapoor
Professor and Head, Department of Chemistry,
University of Jammu, Jammu-180 006 India
Email: kamalkka@gmail.com

Kamal K. Kapoor received his Ph.D. degree (1996) from IIT, Kanpur, India. Joined University of Jammu as Lecturer in December 1995, where he is Professor and Head at present. He has served as advisory consultant to Curadev Pharma Pvt Ltd, Noida and also as Adjunct Professor at the Central University of Jammu. He has authored more than 80 publications with his students and collaborators and is one of the inventors in six US patents. Several scholars have got their Ph.D (25) and M. Phil (14) degrees with his guidance and seven scholars are presently registered with him. He has received funding DST and UGC to support his research endeavours.

Research Interests:

- Heterocyclic Chemistry
- Chemo-sensors

Awards and Honours:

- Platinum Jublee Lecture 2020 at 107th Indian Science Congress, Bangalore
- DST-BOYSCAST and INSA-Royal Society and DFG Germany fellowships

Positions Held:

- Director, Medicinal Chemistry, Sphaera Phrama Pvt Ltd, IMT Manesar (Haryana)
- Lead Scientist, Oncology Division, Dabur Research Foundation, Sahibabad (Utter Pardesh).

Prof. Krishna N. Ganesh
Director, IISER, Tirupati
Tirupati -517507, Andhra Pradesh,
Email: kn.ganesh@iiserpune.ac.in

Krishna N Ganesh obtained his M.Sc. (1972) degree in Chemistry from Bangalore University and did his Ph.D. (1976) in Chemistry at Delhi University and another PhD degree in 1980 University of Cambridge, UK. He joined the Centre for Cellular and Molecular Biology (CSIR) at Hyderabad in 1981 and in 1987, he relocated to the National Chemical Laboratory (NCL-CSIR) where he became the Head of the Organic Chemistry Division in 1994. He was chosen as the First Director of the newly founded Indian Institute of Science Education and Research (www.iiserpune.ac.in) in Pune in 2006. He is internationally recognised for his original and creative contributions to the design of Peptide Nucleic Acid (PNA) analogues for effective cell permeation. He has more than 170 publications in reputed international journals, and 2 international patents and guided 45 students to their doctoral degrees.

Research Interests:

- Chemistry and Biology of Nucleic Acids
- Structural Biology of Collagen peptides
- DNA nanotechnology

Awards and Honours:

- Prof Ganesh is a Fellow of all the 3 Science Academies in India and a Fellow of The World Academy of Sciences (TWAS).
- Shanti Swarup Bhatnagar award
- SASTRA-CNR Rao Award of SASTRA University (2015), H K Firodia Vijnan Bhushan Award (2015) and National Researcher Award in Nanoscience and Technology (2016).

Positions Held:

- First and Founding Director of IISER Pune (June 2006-October 2017)
- Director IISER Tirupati (November 2017 onwards)

Prof. N. Sathyamurthy
Founding Director,
Indian Institute of Science Education and Research,
Mohali, Punjab, India
Email: nsath@iitk.ac.in

Prof. N. Sathyamurthy completed his B.Sc. and M.Sc. degrees from Annamalai University. He moved to the United States where he obtained his Ph.D degree working with L.M.Raff at Oklahoma State University in 1975. He further carried out postdoctoral research in nobel laureate J.C.Polanyi's laboratory. After that he joined the Indian Institute of Technology Kanpur as a lecturer in 1978. He became a professor in 1985.

Research Interests:

- Atomic and molecular clusters
- gas hydrates
- Nonadiabatic interactions
- symmetry and pattern formation in flowers
- chemical dynamics

Awards and Honours:

- Young Scientist Medal, Indian National Science Academy, New Delhi 1980
- Rev. Yedanapalli Memorial Award, Indian Chemical Society 1989
- S.S. Bhatnagar Prize in Chemical Sciences, Council of Scientific & Industrial Research, New Delhi 1990
- Fellow, Indian Academy of Sciences, Bangalore 1990
- Fellow, Indian National Science Academy, New Delhi 1992
- Sir C.V. Raman Award, Hari Om Ashram Trust, University Grants Commission, New Delhi 1997
- FICCI Award, New Delhi 2001
- Silver Medal, Chemical Research Society of India, Bangalore 2001
- Professor Navneetha Rao Best Teacher Award, Andhra Pradesh Academy of Sciences, Hyderabad 2003
- Fellow, Third World Academy of Sciences, Trieste, Italy 2005
- J. C. Bose National Fellow, Department of Science and Technology, New Delhi, 2006
- Founding Director, Indian Institute of Science Education and Research, Mohali, 2007-2017

Dr. Prabhakar Jadav
Enveda Biosciences,1880 S Flatiron Ct Ste K,
Boulder, CO 80301, United States
Email: pk.jadhav@envedabio.com

Dr. Prabhakar K Jadhav graduated with B.Sc. in Chemistry and MSc in Organic Chemistry from Bombay University. He joined National Chemical Laboratory as Junior Research Fellow to pursue PhD with Dr. U. R. Nayak. After completing PhD in 1978, Dr. Jadhav joined the Laboratory of Late Professor Herbert C Brown. In 1984, he accepted a position of staff scientist with E. I. du Pont de Nemours & Company in Wilmington, Delaware and worked in the area of medicinal chemistry and drug discovery for 16 years. While at DuPont he was promoted multiple times and reached the rank of Director of Medicinal Chemistry in 1998. In 2001 he moved to Indianapolis, Indiana to join Eli Lilly and Company as Research Fellow to continue research in medicinal chemistry and drug discovery. In 2007 he was promoted to Senior Research Fellow. To date he has authored 91 publications in peer reviewed journals and has been named inventor on more than 40 US and European patents. He has given invited talks/ lectures in over 40 International Conferences and Meetings. He has been a Leader of the teams that delivered 18 clinical candidates to the pharmaceutical industry.

After working with Eli Lilly and Company for 17 years he retired as Senior Research Fellow in December 2017 and co-founded a drug discovery company in Shanghai, China. As of August 1, 2022 he accepted a position as Senior Vice President, Discovery Chemistry at Enveda Biosciences.

Research Interests:

- Dr. Jadhav's primary interest are in the area of Organic Synthesis, Medicinal Chemistry and Discovery of New Medicines for the treatment human diseases.

Positions Held:

- Director Medicinal Chemistry - The Du Pont Pharmaceuticals Company
- Senior Research Fellow (Equivalent of Executive Director) – Eli Lilly and Company
- Co-Founder, Head of Chemistry, Senior Vice President of Medicinal Chemistry – Minghui Pharmaceutical Company – Shanghai China
- Senior Vice President, Discovery Chemistry - Enveda Bioscience

Prof. Rajiv Bhat
School of Biotechnology
Jawaharlal Nehru University, New Delhi
Email: rajivbhat@mail.jnu.ac.in

Prof. Rajiv Bhat studied chemistry at Bachelor's and Master's degree level and obtained Ph.D. degree in Biophysical Chemistry in 1986 from IIT Delhi. This was followed by Postdoctoral Associateship in the Department of Biochemistry, Brandeis University, Waltham, Massachusetts (USA) (1986-1989) and was Lecturer, Department of Biochemistry, University of Delhi (1989-1990). Assistant Professor, Centre for Biotechnology, JNU, New Delhi (1990-1998). Associate Professor, Centre for Biotechnology, JNU, New Delhi (1998-2004). Visiting Scientist, Department of Chemistry and Chemical Biology, Cornell University, Ithaca, NY, USA (2000-2001). Professor, School of Biotechnology, Jawaharlal Nehru University, New Delhi (From 2004).

Research Interests:

- Aggregation and Amyloid formation in neurodegenerative and other diseases.
- Discovery of natural products as potential inhibitors and modulators of aggregation-related diseases.
- Bimolecular Structure and Interactions; Role of water and weak interactions in protein stability and folding modulated by osmolytes.

Awards and Honours:

- National Merit Scholarship for postgraduate studies.
- Young Investigator Award of The Protein Society USA, 1988.
- Biotechnology Overseas Associate Award, DBT 2000-2001.
- Secretary, Indian Biophysical Society (2011-2015).

Positions Held:

- Dean, School of Biotechnology, JNU (2009- 2011).
- Director of Admissions, JNU (2011-2013).
- Program Coordinator, Inter-School program in the area of "Chemical and Synthetic Biology" at JNU (2012-17).
- Member INSA-IUPAB National Committee on Biophysics (2013-2018).

Dr. Vijay Pal Singh Rawat

SCMM, Jawaharlal Nehru University,
New Delhi 110067
Email: vijaypsrawat@mail.jnu.ac.in

Dr Rawat's research is focused in the fields of cancer and stem cell biology with special focus on epigenetics, molecular alteration and small non-coding RNA. His group has profound experience in the characterization of normal and malignant hematopoietic stem progenitor cells in both murine and human experimental model systems. They identify and characterize the novel oncogenes such as homeobox genes *CDX2, VENTX* and epigenetic factors *TET1-3* for leukemia, molecular mechanism, cancer stem cell population and potential drug targets for the treatment of leukemia (PNAS, Blood, Leukemia, Cancer Cell, JCI and JEM). His group is currently analyzing the functional role of epigenetic factors, miRNA and epigenetic marks in cancer initation and progression. Dr Rawat's lab has expertise in establishing syngeneic and xenograft models to study leukemic initiating cell populations, immunotherapy agents and chemical agents for cancer treatment.

Research Interests: Cancer and Stem Cell; Genetics, Epigenetics and Small non-coding RNA. Establishing in in vivo cancer models for drug screening. Gene knockdown or knockout in cancer cell lines and primary samples using lentivirus-based shRNA or CRISPR/CAS9 methods. Establishing mouse models of cancer and stem Cell

Awards and Honours:

- Young master award Annual Meeting of German/Swiss/Austrian Society of Hematology and Oncology (DGHO/SGH/ASHO), Basel, Switzerland
- Selected for Young Investigator Award, 33rd Annual Meeting of the International Society for Experimental Hematology (ISEH), New Orleans, USA
- Young investigator award 3rd International Conference on Stem cells and cancer, New Delhi, India

Positions Held:

- June, 2010 – May 2016: Assistant Professor, University of Ulm, Germany.
- July, 2016 – June 2020: Senior Scientist, at the Institute of Experimental Cancer Research, University Hospital Ulm, Ulm, Germany.
- July, 2020 – Dec 2020: Principal Scientist, at the Institute of Experimental Cancer Research, Comprehensive Cancer Center Ulm, Germany.
- Jan 2021-till date: Associate Professor, at the Special Centre for Molecular Medicine, Jawaharlal Nehru University, New Delhi-110067

Prof. Ram Vishwakarma
(Ex. Director, CSIR-IIIM, Jammu)
CSIR Distinguished Scientist, CDRI Lucknow
Email: ram@iiim.res.in

Dr Ram Vishwakarma received his post-doctoral studies from Cambridge University, England (with Sir Alan Batters by, FRS on the biosynthesis of Vitamin B12 and related corrins and porphyrins) (1991-1993). Also received Ph.D. (Medicinal Chemistry) from Central Drug Research Institute Luck now and M.Sc. (Organic Chemistry) from Bundelkhand University, India (1978-1980) Having 28 years of research experience (both in the scientific institution and pharma company) in drug discovery, medicinal chemistry, natural products chemistry, organic-synthesis, chemical-biology and glycobiology Chemical biology of Glycosylphosphatidylinositol (GPI) anchors in parasitic protozoa Molecular target-based drug discovery for cancer, diabetes, inflammation, and infections. Research and leadership experience in both academic as well as industrial settings. Specific interest in the questions related to the chemistry of small molecules in biology. He was director of CSIR - Indian Institute of Integrative Medicine, Jammu. He was also Vice-President and Head (Medicinal Chemistry) of Piramal Life Sciences (Nicholas Piramal Research Centre), Mumbai (2005-2009): Responsible for new drug discovery projects in the areas of inflammation, cancer, diabetes, and drug-resistant infections. He has over 350 original research papers and 75 patents to his credit.

Research Interest:

- Drug discovery, medicinal chemistry, natural products chemistry, organic synthesis, chemical-biology

Awards & Honours:

- He is an elected fellow of the National Academy of Sciences and was awarded Sun Pharma (Ranbaxy) Research Award (2014) in the Pharmaceutical Sciences

Prof. Ranjana Aggarwal
Director
CSIR-NIScPR
Email: director@niscpr.res.in

Prof. Ranjana Aggarwal is the founder Director of CSIR-National Institute of Science Communication and Policy Research (CSIR-NIScPR), a constituent Institute of Council of Scientific & Industrial Research, under the aegis of Ministry of Science & Technology, Government of India. The new Institute was formally announced on 14 January 2021 by then Hon'ble Minister for Science & Technology and Earth Sciences Dr Harsh Vardhan by merging the two very well recognized institutes namely CSIR-National Institute of Science Communication and Information Resources (CSIR-NISCAIR) and CSIR-National Institute of Science Technology and Development Studies (CSIR-NISTADS). Earlier Prof. Aggarwal held the position of Director of erstwhile CSIR-NISTADS (since June 2019) with the additional charge of Director of erstwhile CSIR-NISCAIR (since Nov. 2019).

Dr Aggarwal is on lien from Kurukshetra University, Kurukshetra where she served as Professor of Chemistry and Director, Women's Studies Research Centre. She received her BSc, MSc and PhD degrees from Kurukshetra University and then after carrying out two years postdoctoral research on erythromycin biosynthesis at Cambridge University, UK she joined her Alma mater in 1995. Subsequently she worked in many well-known European Labs at University of Trieste, Italy, again at Cambridge University and Trinity College Dublin, Ireland. She is actively collaborating with scientists of USA, UK, Spain and Ireland.

Her research interests consist of design and synthesis of azaheterocycles, involving green reagents, of therapeutic interest as anticancer, anti-inflammatory, antimicrobial and photodynamic agents, computational studies and 2D NMR spectroscopy. Her research contributions have been acknowledged in the form of awards and honours notably Commonwealth Fellowship by the Association of Commonwealth Universities, UK (2003), Dr.Basudev Banerji Memorial Award (2014) by Indian Chemical Society, Prof. S. S. Katiyar Endowment Award (2015) by Indian Science Congress and President, Chemical Sciences Section, Indian Science Congress (2020). As an accomplished academician she has been nominated as Member of National Monitoring Committee for Minorities Education by MHRD, New Delhi. She is visitor's Nominee for Delhi University, Delhi, Central University Assam, Silchar and Indian Institute of Technology, Delhi; and Chancellor's Nominee for many Haryana State Universities.

Prof. Sandeep Verma
Department of Chemistry
IIT Kanpur, Kanpur 208 016
Email: sverma@iitk.ac.in

Prof Sandeep Verma has been associated with IIT Kanpur since 1997. He served as Secretary, Science and Engineering Research Board, Ministry of Science and Technology (2019-2022). His research interests include chemical neuroscience, stem cell engineering, and new antibiotics. With over 225 publications and several patents to his credit, his work has been recognized by the Shanti Swarup Bhatnagar Prize, Distinguished Alumnus Award of Banaras Hindu University, Goyal Prize in Chemical Sciences, Society of Materials Chemistry (BARC) Gold Medal, CRSI Silver Medal, and Swarna Jayanti Fellowship, to name a few. He is an Associate Editor of Chemical Communications (RSC, UK) and serves on the Editorial Advisory Board of ChemBioChem (Wiley).

Prof Verma was a Member, PMO Constituted Vaccine Task Force for SARS-Cov-2; Member, Empowered Group-1 on Emergency Management Plan and Strategy for COVID-19; and Chairperson, DST Committee on Coronavirus Diagnostics, and Chairperson, Working Group in R&D and Innovation in Energy Requirements and Renewable Energy, IMAC, Ministry of Petroleum and Natural Gas, among other responsibilities.

Research Interests:

- His research interests include programmable soft matter for neuronal regeneration, bioinspired nanomaterials, novel antimicrobials, and small molecule-stem cell modulation.

Awards and Honours:

- He is an elected Fellow of the Indian National Science Academy (INSA), Indian Academy of Sciences (FASc), National Academy of Sciences (FNASc), and Indian National Academy of Engineering.
- His work has been recognized by the Goyal Prize (2019),
- J C Bose Fellowship (2015),
- Shanti Swarup Bhatnagar Prize (2010), DAE-SRC Outstanding Investigator Award (2010), Swarnajayanti Fellowship (2005), B M Birla Science Prize (2004), to name a few.

Dr. Sanjay Kumar Mishra
Scientist – H/Department of Biotechnology
Ministry of Science and Technology
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Dr Sanjay K Mishra studied Biomedical Engineering and held the prestigious Commonwealth Scholarship for his doctoral studies at University of Oxford. He worked as a tutor at University of Oxford while pursuing his PhD studies from 1996 to 1999.He, subsequently joined The Cleveland Clinic Foundation, OH, USA as a Post-doctoral research fellow (2001-2002). He has also received Ramalinga Swamy fellowship by Dept of Biotechnology to utilize his expertise in Indian academics. Since then, he has served as a faculty member and HOD at various Indian and International universities like Institute of Engineering & Technology, India; Queensland University of Technology, Australia and Shiv Nadar University, India.

Research Interests:

Dr Mishra's research interests include Bone fracture healing and Finite Element Modelling. He has been very passionate about Engineering education and has held significant positions in academic institutions in India and abroad. He has more than two dozen research publications to his credit.

Awards and Honours (Selected):

Dr. Mishra is a recipient of several national and international awards and recognitions including

- Young Scientist Award, 2000, UP State government
- Sharda Chandra Gold Medal of the Palaeontological Society of India for the joint research paper
- Vice Chancellor's Performance Fund at QUT Australia in 2009
- Publication Award at Queensland University of Technology, Brisbane Australia
- Radhakrishnan Memorial Bequest at University of Oxford, 1999

Positions Held:

- Advisor - Department of Science & Technology (DST) from 2012 to 2021
- Professor - Mechanical Engineering at Shiv Nadar University
- Senior Lecturer - Queensland University of Technology, Brisbane, Australia

Prof. Sourav Pal
Head, Department of Chemistry,
Ashoka University, Haryana
Email: sourav.pal@ashoka.edu.in

Prof. S. Pal obtained his master's degree from the Indian Institute of Technology (Kanpur) in 1977, and his doctorate from the University of Calcutta, working at the Indian Association for the Cultivation of Science (IACS), supervised by Debasis Mukherjee. He was subsequently a post-doctoral researcher at the University of Florida with Rodney J. Barlett in 1986. He was a Scientist at CSIR- National Chemical Laboratory, Pune from December 1982 to May 2015. He was the Head of the Physical and Materials Laboratory Pune, from December 2010 till May 2015. Then, he was a professor of chemistry in IIT Bombay, and an adjunct professor at the Indian Institute of Science Education and Research Pune. He was a distinguished visiting professor at the Indian Institute of Technology, Kharagpur for five years from 2016. Currently, he is head Department of Chemistry, at Ashoka University, Sonipat, Haryana.

Research Interest: Theoretical investigation on Hard- Soft Acid- Base relation, Study of electron-molecule scattering, Development and Application of Molecular Dynamics, Density functional response approach for molecular properties, Magnetic properties Application to the problem of chemical physics, Computational Material Science.

Awards and Honours:

- SASTRA-CNR Rao Award in Chemistry & Materials Science from CSIR (2014).
- Executive Council Member Federation of Asian Chemical Societies (FACS). (2010)
- JC Bose National Fellowship from DST (2008).
- Fellow of the Indian National Science Academy from 2003.
- Shanti Swarup Bhatnagar from CSIR (2000).
- Fellow of the National Academy of Sciences from 1998.
- Fellow of the Indian Academy of Sciences from 1996.

Prof. S. Chandrasekaran
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Indian Institute of Science Bangalore
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Professor Srinivasan Chandrasekaran is working as INSA Senior Scientist at the Department of Organic Chemistry, Indian Institute of Science, Bangalore, India. He has done his MSc and PhD from the University of Madras in 1967 and 1972 respectively. He has also been a Research Associate at Harvard University (with Professor E.J.Corey) and Syntex Research, USA. Among his many teaching stints he has been a Lecturer, Department of Chemistry, Indian Institute of Technology, Kanpur, (1978-80), Assistant Professor, Department of Chemistry, IIT, Kanpur, India (1981-85), Professor, Department of Chemistry, IIT, Kanpur , India (1985-1989) and Professor, Dept. of Organic Chemistry, Indian Institute of Science, Bangalore,(1989-2011).He served as the Chairman of the Department, Chairman , Division of Chemical Sciences and Dean Faculty of Science at IISc, Bangalore.

He served as National Convener, Kishore Vaigyanik Protsahan Yojana (KVPY) of the Department of Science and Technology, Govt. of India, the President of the Chemical Research Society of India (CRSI), the Chairman of the National Organic Symposium Trust (NOST) and as the Editor in Chief of the journal, Tetrahedron Letters published by Elsevier.

Research Interests:

- Development of New Synthetic Methods
- Synthesis of Natural Products, Catalysis

Awards and Honours:

- S S Bhatnagar Prize, CSIR
- Fellow, Indian National Science Academy
- Fellow, Indian Academy of Sciences
- Fellow, The World Academy of Sciences

Positions Held:

- Honorary Professor, J C Bose National Fellow
- SERB Distinguished Fellow, INSA Distinguished Professor

Prof. Srivari Chandrasekhar
Secretary,
Department of Science & Technology
Government of India
Email: srivaric@iict.res.in

Dr. Srivari Chandrasekhar, born in 1964, completed all his primary and higher education in Hyderabad and Joined CSIR, IICT for a Ph. D Programme. After completing his Ph. D (1991) with the then director Dr. A. V. Rama Rao, he moved to USA for a post-doctoral position with Prof. J. R. Falck (1991-94). He joined CSIR-IICT as Scientist C in 1994 and grew up to the level of director in 2015. He has made significant contributions in diverse areas of organic chemistry with a special emphasis on chiral chemistry, total synthesis of biologically active natural products, and pharmaceutical products. He introduced polyethylene glycol (PEG) as a novel, environmentally benign solvent medium. He has developed technologies for the synthesis of the latest anti-tuberculosis drug, bedaquiline; anti-tumor and abortive drug, misoprostol; anti-platelet molecule, beraprost; antidepressive compound, sertraline, and drug for the treatment of schizophrenia, asenapine. He has more than 285 publications with 7600 citations. 80 students have been already awarded Ph. D. degree under his able guidance and 20 post-doctoral associates have worked in his group. Presently, he is Secretary to the Government of India, Department of Science and Technology.

Research Interests:

- Synthesis of Natural Products, Catalysis
- Drug Development

Awards and Honours:

- He is a fellow of all three Indian Science academies, National Academy of Sciences (FNASc), Indian Academy of Sciences (FASc) and the Indian National Science Academy (INSA). He is also an Alexander von Humboldt fellow.
- He has received several accolades including Eminent Scientist Award for contributions in the field of Chemistry from Telangana State Government in 2017, CNR Rao National Prize for Chemical Research 2012, CSIR Technology award 2014 and Infosys prize in Chemical sciences 2014.

Prof. Rakesh K. Tyagi
Special Centre for Molecular Medicine,
Jawaharlal Nehru University
Email: rktyagi@yahoo.com

Prof. Rakesh K Tyagi obtained his Master's degree from Visva Bharati University, Santi Niketan, and PhD in Biochemistry from Jawaharlal Nehru University, New Delhi. Subsequently, during his post-doctoral career, he worked in some of the frontier areas of 'Molecular Endocrinology' at the Weizmann Institute of Science, Israel; INSERM, Paris, France, and the University of Texas Health Science Centre, USA. Presently, in addition to other assignments, he is serving as a Professor at the Special Centre for Molecular, Jawaharlal Nehru University. He has published more than 75 papers and mentored more than 20 Ph.D. students.

Research Interests:

- Molecular and Cellular Endocrinology
- Nuclear receptors in health and disease

Awards and Honours:

- Fellow, National Academy of Science, India
- Feinberg fellowship of the Weizmann Institute of Science
- INSERM International Fellowship, Paris, France
- Gold medal by the 'Society for Reproductive Endocrinology and Comparative Endocrinology'.

Positions Held:

- Professor and Chairperson of 'Special Centre for Molecular Medicine'
- Honorary Director, Advanced Instrument Research Facility (AIRF), JNU.
- Member of the Executive Council of Visva Bharati University, Santi Niketan
- Associate Editor, *Journal of Endocrinology and Reproduction*

Prof. Tharmalingam Punniyamurthy
Department of Chemistry
Indian Institute of Technology Guwahati
Email: tpunni@iitg.ac.in

Prof. Punniyamurthy completed graduate studies in Chemistry at Bharathidasan University and Ph.D. in Chemistry at the Indian Institute of Technology Kanpur under the supervision of Prof. Javed Iqbal. He pursued postdoctoral research at North Dakota State University (Prof. M P Sibi), Kyshu University (Prof. T Katsuki), and National School of Chemistry Montpellier (Prof. J E Moreau and Prof. A Vioux). He joined the Indian Institute of Technology Guwahati in July 2001 and his research focuses on the Development of Synthetic Methods for Sustainable Organic Chemistry covering C-H Functionalization, Cascade Carbon-Carbon/Heteroatom Bond Formation and Stereoselective Synthesis. He produced 7 postdocs; 25 Ph.D. Scholars and 39 M.Sc. students have 172 publications and 9700 citations. He served as the Head, Department of Chemistry, Chairman JAM. He is visiting Professor at the Scripps Research Institute, San Diego, Oxford University, and Kyushu University. He edited a book having two volumes along with a co-editor on *Transition-Metal-Catalysed C-H Functionalization of Heterocycles*. He is a Guest Editor of Synthesis along with a co-editor for a Special Issue on *C-H Bond Functionalization*. He is also the Advisory Board Member of SynOpen.

Research Interests:

- Organic Synthesis

Awards and Honours:

- Fellow of Science Academies (FASc, FNASc and INSA)
- Fellow of the Royal Society of Chemistry
- Fulbright Fellowship
- JSPS Invitation Fellowship
- Alumni Award Bharathidasan University

Prof. Uday Maitra
Department of Organic Chemistry,
Indian Institute of Science, Bangalore
Email: maitra@iisc.ac.in

Prof. Maitra obtained his M.Sc. from IIT Kanpur in the year 1981 and Ph.D. in 1986 from Columbia University, working under the guidance of Ronald Breslow, and did his post-doctoral studies at the laboratory of Paul A. Bartlett of the University of California, Berkeley. He has published more than 145 research papers and, supervised more than twenty Ph.D. students. He is involved in the popularization of chemistry. He is a member of the editorial board of the Asian Journal of Organic Chemistry and a member of various funding agencies (SERB, CSIR, DBT).

Research Interests:

- Photoluminescent metallogels
- Paper-based sensing of biomolecules
- Chemistry of Bile acids
- Soft hybrid materials

Awards and Honours:

- National Best Chemistry Teacher Award, JNCASR, 2015
- Silver Medal, Chemical Research Society of India, 2012
- Materials Research Society of India Medal, 2009
- Fellow of the Indian National Science Academy, 2009
- J.C. Bose National Fellowship, 2008
- A.V. Rama Rao Foundation Prize Lecture, JNCASR, 2007
- S.S. Bhatnagar Prize in Chemical Sciences, 2001
- Bronze medal, Chemical Research Society of India, 2000
- Millennium medal (Indian Science Congress Association), 2000
- Fellow of the Indian Academy of Sciences, 1998
- Young Associate, Indian Academy of Sciences, 1989-1992

Prof. Vinod K. Singh
Department of Chemistry
Indian Institute of Technology, Kanpur
Email: vinodks@iitk.ac.in

Prof. Singh obtained M.Sc. in Chemistry from B.H.U. (1980) and Ph.D. in the year 1986 under the guidance of Dr. Sukh Dev from Malti-Chem Research Center from M.S. University Baroda. Professor Singh spent 2 years for his postdoctoral work in Canada (1985-1987) at the University of Calgary and the University of British Columbia. He subsequently moved to the U.S.A. for another postdoctoral work (1987-1990) at Harvard University with Professor E. J. Corey, a Nobel Laureate. After a brief stint as a Senior Scientist at Neurogen Corporation, CT, USA, Vinod Singh joined IIT Kanpur in 1990 as an Assistant Professor and rose to the rank of Professor. He is the Founding Director of IISER Bhopal and served there for more than 10 years (2008-2018). He is also Director's Chair Professor at IISER Bhopal & adjunct Professor at NIPER Hyderabad. He is currently President of the Chemical Research Society of India (CRSI) and the Chairperson of Governing Council of IACS Kolkata. Prof. Singh has made significant contributions to the management of higher educational institutes, science education, science policy, and planning.

Research Interests:

- Asymmetric synthesis

Awards and Honours:

- TWAS-CASAREP Award for Building Scientific Institutions (2020)
- Padma Shri (2014)
- CRSI Silver Medal (2014)
- Elected Fellow of the Indian National Science Academy (FNA), Indian Academy of Sciences (FASc), National Academy of Sciences (FNASc), and The World Academy of Sciences (FTWAS).
- Vigyan Ratna Award of U.P. (2006-2007)
- Shanti Swarup Bhatnagar Award (2004)
- Rajib Goyal Prize (2002)

Presentation by DRDO and BARC Delegate

Unravelling the Role of Nanofillers to Polymer Matrix Interactions in Conductive Inks for Printable Electronics

Dr. Debmalya Roy
Nanoscience & Coating Division
DMSRDE, Defense Research & Development Organizations, Kanpur
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The elastic conductors enable the physiological sensors to be printed on any arbitrary locations and any geometry of the substrate. This is an important step toward producing intelligent surfaces for human-machine interfaces. The design of functional nanomaterials to tailor the interfacial interaction with hydrophilic and hydrophobic polymer matrix is important to develop stretchable sensors for next-generation wearable electronic applications. The printable physiological sensors on human skin or textile surface have huge applications in healthcare, energy and strategic area and has been an intense research topic across the world. The conducting nanofillers generate interpenetrating network structures to make the elastomer matrix conducting where the chemistry of nanomaterials decides the cyclic stabilities of conduction channels in multiple stretching/bending. The challenges and opportunities for printable, skin-mountable and wearable strain sensors based on flexible nanocomposites will be discussed.

Dr. Debmalya Roy
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Dr. Debmalya Roy is currently leading a group of scientists and technical staff to develop various hybrid materials at different length scales where multifunctionalities were generated to obtain heterogeneous performance objectives in a single material system. He published more than a hundred peer-reviewed research papers/book chapters and national/international patents. Dr. Roy is educated in Chemistry from Visva Bharati University, Santiniketan, and obtained Ph. D. from the University of Delhi. He worked as a Guest Scientist at Leibniz Institute of New Materials, Saarbrucken, Germany under a DAAD Research Fellowship.

Research Interests:

- Nanomaterials
- Polymers
- Composites

Awards and Honours:

- He is the recipient of the 11th National Petrochemical Award of the Ministry of Chemical & Fertilizers and the commendation certificates & medals for the National Science Day & National Technology Day Orations.
- He was awarded the Scientist of The Year Award and twice the Technology Group Awards by DMSRDE, DRDO, Kanpur
- He is a fellow of the Royal Society of Chemistry

Cucurbituril-based Supramolecular Assemblies: Prospective Applications

Dr. Jyotirmayee Mohanty
Radiation & Photochemistry Division, BARC Mumbai
Email: jyotim@barc.gov.in

Supramolecular assemblies based on noncovalent host-guest interactions have attracted immense research interests owing to their potential applications in catalysis, fluorescent sensors, drug delivery, adsorbents, etc.[1] Our group has demonstrated the modulation of molecular properties of some of the technologically and biologically important guest molecules through supramolecular assembly formation using various macrocyclic hosts such as cyclodextrins, calixarenes and cucurbiturils. Among them, cucurbiturils, a relatively young, popular class of macrocyclic receptors, display interaction in a highly selective manner with certain types of guest molecules such as metal ions, protonated alkyl and aryl amines, cationic dyes and surfactants through ion-dipole and hydrophobic interactions and also with polyanions through peripheral binding/interaction. The presentation will discuss some of the recent work on the cucurbituril-assisted functional assemblies of nitrogen-based hydride, fluoroquinolone drugs and polyoxometalate and their respective applications toward the H_2 generation, antibacterial agents and ^{99m}Tc radionuclide separation.[1-3]

References and Notes:

1. Ruz, P.; Banerjee, S.; Khurana, R.; Barooah, N.; Sudarsan, V.; Bhasikuttan, A. C.; Mohanty, J.; Author, B.; *ACS Appl. Mater. Interfaces*, **2021**, *13*, 16218-16226.
2. El-Sheshtawy, H. S.; Chatterjee, S.; Assaf, K. I.; Shinde, M. N.; Nau, W. M.; Mohanty, J.; *Scientific Reports*, **2018**, *8*, 13925.
3. Goel, T.; Barooah, N.; Mallia, M. B., Bhasikuttan, A. C.; Mohanty, J.; *Chem. Commun*., **2016**, *52*, 7306-7309.

Dr. Jyotirmayee Mohanty
Head, Nano & Reactor Chemistry Section
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Dr. Jyotirmayee Mohanty obtained her M. Sc. in Chemistry from Utkal University, Odisha in 1992 and joined Bhabha Atomic Research Centre, Mumbai, India, as Scientific Officer in 1994 after a one-year advanced orientation course conducted by the institute. After her Ph.D. from the University of Mumbai in 2002, she carried out her postdoctoral research at Max-Planck Institute for Biophysical Chemistry (MPIBPC), Göttingen and Jacobs University Bremen (JUB), Bremen, Germany, 2002-2004. She visited Jacobs University Bremen as visiting Scientist under AvH Fellowship during Nov. 2013-Jan 2014. Dr. J. Mohanty has about 110 publications in high impact International Journals e.g., J. Am. Chem. Soc., Angew. Chem. Int. Ed., ACS Appl. Mater. Interfaces, Chem. Commun., etc. including two Patents and six Book Chapters which have attracted more than 5025 citations with h-index of 37 (Google Scholar).

Research Interests:

- Supramolecular Host-Guest Chemistry
- Molecular Photochemistry
- Nanochemistry

Awards and Honours:

- SERB POWER Fellowship, SERB, DST, 2022
- Fellow of the Royal Society of Chemistry (FRSc), 2022
- Homi Bhabha Science & Technology Award-2019 from DAE, 2021
- CRSI Bronze Medal-2017
- Fellow of the National Academy of Sciences (FNASc, 2014)
- Humboldt Fellowship for Experienced Researchers, Alexander von Humboldt Foundation, 2013
- The ‘APA Prize for Young Scientist-2010’, Asian and Oceanian Photochemistry Association (APA), 2010
- The ‘Distinguished Lectureship Award’, The Chemical Society of Japan,

Cyclotron Produced Innovative Radionuclides for Theranostic Applications

Dr. Puja Panwar Hazari[a]

Institute of Nuclear Medicine and Allied Sciences, Brig SK Mazumdar Road, Delhi

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In nuclear medicine imaging and therapy, radiopharmaceuticals are essential for the diagnosis and/or therapy of specific pathological ailments. Radioisotopes are administered to various organs for diagnostic, therapeutic, or theranostic purposes. Positron emission tomography (PET) and single photon emission computed tomography (SPECT) are the two most used diagnostic procedures which are heavily dependent on the exogenous radiolabeled biomarkers. Non-Metallic and metallic radionuclides have a wide range of half-lives, emission types, energy, and branching ratios, making them useful diagnostic and therapeutic agents. With the rise of theranostics, studies into radioisotopes like $^{123/124}$I, $^{67/68}$Ga, ^{44}Sc, ^{89}Zr, and $^{67/64}$Cu are becoming more popular. ^{64}Cu is gaining popularity due to its ability to emit both positron and beta particles, making it suited for the theranostic application. The demand for ^{64}Cu in PET studies began to evolve, due to the establishment of its production on medical cyclotrons. Due to the shutdown of major reactors, radioisotope production with reactors is decreasing. Currently, cyclotrons are considered a reliable and commercially available alternative to reactors. Medical cyclotrons are expected to become the primary source of radioisotopes in nuclear medicine. Cyclotron at INMAS with its 16.5 MeV capacity and is equipped with liquid, gas, and solid target with an external beam transfer line, which is an excellent example of a state-of-the-art facility for the production of medical radioisotopes for theranostic applications, After the successful productions on liquid and gas targets we are now focusing on the production of non-conventional innovative medical radioisotopes which are not readily available for clinical use. Scandium is an interesting radioisotope since ^{43}Sc/^{47}Sc and ^{44}Sc/^{47}Sc represent promising theranostic pairs. The chemistry continues to be developed because the original cages could not hold the copper in place in vivo. In addition, there is interest in using ^{64}Cu as a potential radiotherapeutic isotope because of its dual beta decay. The development of innovative radionuclides can benefit greatly from the use of PET and SPECT imaging techniques, and these studies also present an ideal opportunity to create outstanding new diagnostic and therapeutic radiopharmaceuticals through Cyclotron.

Dr. Puja Panwar Hazari
Scientist F, Head DCRS
Institute of Nuclear Medicine and Allied Sciences, DRDO
Email: puja.inmas@gov.in

Dr. Puja Panwar Hazari is currently working as a Biomedical Scientist, and Heading the Division of cyclotron and radiopharmaceutical Sciences, INMAS. She completed her Ph.D. in Biomedical Sciences from ACBR, Delhi University, India in 2006. She is the recipient of national fellowships awarded by the research organizations like the 'Catch them Young' Scholarship CSIR, ICMR, and has national and international awards to her credit in conferences of high repute. As a Scientist, she has taken a keen interest in the development of radiopharmaceuticals for SPECT and PET imaging and translated basic research successfully in clinics.

She has demonstrated expertise in developing new PET radiolabelling towards small molecules with carbon-11 and fluorine-18. More recently, she has focused on and implemented fluorine-18-based labelling techniques that can readily be extended to peptides and nucleic acids for specific targeting in neuro/onco diseases and small animal imaging. Developed methodologies via Prosthetic Group to radiolabel Dimeric Radioligands. C-11 Based Molecular Imaging Probes: Organic Synthesis, Radiochemistry, and Application in Oncology and Neuroscience.

Research Interests:

- Bioconjugate Chemistry
- Radioisotope Production
- Radiopharmaceutical
- Preclinical Imaging

Awards and Honours:

- 2001-2002: 'Catch them Young" Scholarship (Masters in Biomedical Sciences)
- 2001: Best paper presentation award Society of Nuclear Medicine, India
- 2004: Best paper award CBISNF, Delhi University, India
- 2009: Laboratory Technology Group Award
- 2010: Best paper presentation award Society of Nuclear Medicine, India
- 2013: Best paper presentation award 'Second World Congress on Galium…'
- 2013-2014: Laboratory scientist of the year, DRDO
- 2017: Best paper award SNMICON.

Poster Presentations

Chairpersons (Poster Presentation)

Prof. Bijoy Kumar Kuanr
School of Physical Science
Jawaharlal Nehru University,
New Delhi

Dr. Debendra K Mohapatra
CSIR-Indian Institute of Chemical
Technology, Hyderabad

Dr. Pijus Kumar Sasmal
School of Physical Science
Jawaharlal Nehru University,
New Delhi

Prof. Parthasarathi Das
Head of the Department
Indian Institute of Technology
(ISM) Dhanbad

Dr. Jaideep Saha
Centre of Biomedical Research
(CBMR), Lucknow, India

Dr. Manoj Munde
School of Physical Science
Jawaharlal Nehru University,
New Delhi

Prof. G. Sekar
Indian Institute of Technology
Madras, Chennai

Dr. Dinabandhu Das
School of Physical Science
Jawaharlal Nehru University,
New Delhi

Dr. Raja Angamuthu
Indian Institute of
Technology , Kanpur

Prof. Ravi P. Singh
Indian Institute of Technology, Delhi
New Delhi

Dr. Poonam Mehta
School of Physical Science
Jawaharlal Nehru University, New Delhi

Dr. Arnab Bhattacharjee
School of Computational and Integrative Sciences, JNU

Dr. Neel Sarovar Bhavesh
International Centre for Genetic Engineering and Biotechnology (ICGEB)

Prof. Anil Kumar
Department of Chemistry
BITS, Pilani

Prof. Sarabani Taraphder
Indian Institute of Technology, Kharagpur

Dr. Ankita Rai
School of Physical Science
Jawaharlal Nehru University, New Delhi

Dr. Supriya Sabbaani
School of Physical Science
Jawaharlal Nehru University, New Delhi

Dr. Vijay Goel
School of Physical Science
Jawaharlal Nehru University, New Delhi

Poster Presentations @ 30th CRSI-NSC

Poster Presentations-I (Feb. 03, 2023, Friday): Poster Nos. P001-P130

Poster Presentations-II (Feb. 04, 2023, Saturday): Poster Nos. P130-P262

Poster No.	Name	Affiliation	Title of the Poster
P-1	**Aashish**	Department of Chemistry, University of Delhi, Delhi, India	Cross-Coupling and Oxidation Reactions Mediated by the Visible Light
P-2	**Aastha Palta**	School of Chemistry and Biochemistry, Thapar Institute of Engineering and Technology, Patiala	ICT efficient "turn-on" fluorescent probe for selective Al^{3+} and HSO_4^- ions: Real-time application in water samples and molecular keypad lock
P-3	**Abhijeet Singh**	Indian Institute Technology Delhi, Hauz Khas, New Delhi, Delhi	Regioselective Direct C-H Phosphorylation of Benzofulvenes
P-4	**Aishwarya Chauhan**	Indian Institute of Technology Delhi, India	Synthesis and structural features of Alkaline earth metal phosphite-/phosphonate- complexes.
P-5	**Ajay Gupta**	School of Physical Sciences, JNU, New Delhi	Mitochondria Targeted Heterobimetallic Iridium(III)-Platinum (IV) Conjugate as Potent Anticancer Theranostic Agent
P-6	**Ajijur Rahaman**	CSIR - Central Salt and Marine Chemicals Research Institute, Bhavnagar and AcSIR, Ghaziabad	Catalytic Methylene Insertion between Amines and Terminal Alkynes via C–N Bond Cleavage of N, N-Dimethylacetamide: A Unique Access to Propargylic Amines
P-7	**Akankasha Yadav**	Centre of Advanced Study, Department of Chemistry, University of Rajasthan, Jaipur, India	Study of Structural Profiles of Multi-target Binding of Cytotoxic Alkaloid Vinblastine

P-8	**Akanksha Singh Baghel**	Department of Chemistry, Indian Institute of Technology Patna, India	One-pot Multiple C-C bond Formation via Pd(II)-Catalyzed reaction: En route Synthesis of Succinimide-fused Dihydrophenanthrenes
P-9	**Akhil Patter**	Department of Chemistry, Indian Institute of Technology Roorkee, Roorkee 247667, India	Polymer supported dioxidovanadium(V) complex based heterogeneous catalyst for the multicomponent Biginelli reaction producing biologically active 3,4-dihydropyrimidin-2-(1H)-ones.
P-10	**Alka Ambali**	Department of Chemistry, Indian Institute of Technology Bombay, Mumbai, India.	Regioselective synthesis of meso-tetraaryl Bromo [14]Triphyrins (2.1.1) and Their Effects on Structural, Spectral and Redox Properties
P-11	**Amar Diliprao Uike**	Department of Chemistry, Indian Institute of Technology, Kanpur	Ruthenium-Catalyzed Oxidative Cross-Coupling Reaction of Activated Olefins with Vinyl Boronates for the Synthesis of (E, E)-1,3-Dienes
P-12	**Amarish Kumar**	Department of chemistry, Indian Institute of Technology, Kanpur-208016	Nickel (II) borohydride catalyst for Hydrodehalogenation reactions for Chlorinated pollutant
P-13	**Amita Saini**	Department of Chemistry, Punjab Agricultural University, Ludhiana, Punjab-141004	Structural elaboration of Xanthine and its evaluation as potent agrochemicals
P-14	**Anjali Giri**	School of Chemistry and Biochemistry, Thapar Institute of Engineering and Technology, Thapar Technology Campus, Patiala, Punjab, India	Understanding Structural Changes During Salt-induced Ovalbumin Amyloid Aggregation
P-15	**Anjali Tripathi**	School of Physical Sciences, Jawaharlal Nehru University, New Delhi-110067, India	Sustainable Oxidation of Sulfides with Peroxide Catalysed by Efficient & Reusable Transition Metal Based Preyssler System
P-16	**Ansalin Gnana**	Centre for Human and Organizational Resources	Study of Inorganic flame retardants for leather applications.

	Sowndarya A	Development (CHORD), CSIR-Central Leather Research Institute, Chennai, India. AcSIR, Ghaziabad, India.	
P-17	**Antra**	Special Centre for Molecular Medicine, Jawaharlal Nehru University, New Delhi	Radiosensitizing role of Pixantrone in KRAS mutated cancer cells via suppression of radiation induced pro-survival pathways
P-18	**Anubha Rajput**	Indian Institute of Technology Delhi, Delhi	Intrinsic Lability of $NiMoO_4$ to Excel the Oxygen Evolution Reaction
P-19	**Aparna Tyagi**	Department of Chemistry, Indian Institute of Technology Delhi	Catalyst Switchable Divergent Synthesis of Bis(indolyl)alkanes and 3-Alkylated Indoles from Styrene Oxides
P-20	**Apoorva Malik**	Department of Chemistry, Indian Institute of Technology Jodhpur, Jodhpur, India.	Experimental and Computational Studies on Cinchona Anchored Calixarene Catalysed Asymmetric Michael Addition Reaction
P-21	**Archana**	Jawaharlal Nehru University, New Delhi; National Institute of Immunology, New Delhi, India	Fabrication of Molecularly Imprinted Polymer based Electrochemical Sensor for Gut Microbiota Derived Metabolites Detection
P-22	**Archana Kumari Pattnaik**	Indian Institute of Technology Bhubaneswar	Study of Organophosphorous Acid Coordinated Assemblies with Ethylene and Azo Bridging Ligands
P-23	**Arijit De**	Centre of Biomedical Research, SGPGIMS, Lucknow, 226014, India.	One-Pot Multi-Enzymatic Cascade Synthesis of Natural Naphthalenones via Reduction of Unactivated Alkenone
P-24	**Arsheed Ahmad Bhat**	Department of Chemistry, Indian Institute of Technology Kanpur	Cp*Co(III)-Catalyzed Ketone-Directed ortho-C−H Activation for the Synthesis of Indene Derivatives
P-25	**Arvind Singh**	Indian institute of technology Delhi 110016, India	Understanding Mixed Crowding Through Enzyme Activity and Dynamics

P-26	**Aryan Gautam**	School of Physical Sciences, JNU, and Department of Physics, IIT-Delhi	Visible and NIR-Light Photoactivatable o-Hydroxycinnamate System for Efficient Drug Release with Fluorescence Monitoring
P-27	**Atikur Hassan**	Department of Chemistry, IIT-Patna; Department of Chemistry, IISER-Pune	Ordered Macro/Microporous Ionic Organic Framework for Efficient Separation of Toxic Pollutants from Water
P-28	**Atul Kumar**	Department of Chemistry, IIT-Bombay, Powai, Mumbai 400 076	Total Synthesis of (+)-Dihydroitomanallene B and Formal Synthesis of (-)-Kumausallene
P-29	**Awadhesh Kumar Verma**	Special Centre for Nanoscience, Jawaharlal Nehru University, New Delhi - 110067, India.	Polymer functionalized zinc oxide quantum dots as a selective probe for specific detection of antibiotics
P-30	**Ayushi Chaudhary**	Department of Chemistry, Indian Institute of Technology Kanpur, 208016, Uttar Pradesh	Ligands Inspired by HDAC Inhibitors: Source for Anticancer and Antimicrobial Agents
P-31	**Ayushi Kaushik**	Department of Chemistry, Indian Institute of Science Education and Research, Bhopal	A bisperylenediimide-conjugated macrocycle: Supramolecular, conformational, photophysical and electrochemical studies
P-32	**Bhanu Priya**	Discipline of Biological Engineering, IIT Gandhinagar; and Discipline of Chemistry, Indian IIT Gandhinagar, Gujarat, India.	Exploring SPK98 for selective killing of ATM- or P53-deficient cancer cell
P-33	**Bharath Govind G S**	Amity Institute of Applied Sciences, Amity University, U.P.	Imidazolium and Pyridinium Functionalized Polyethylene Membrane through Microwave Assisted Grafting as Alkaline Anion Exchanger
P-34	**Bharath M**	Department of Chemistry, Ashoka University, Sonipat, Haryana-131029, India	Bis-Chelated Mono-Centric Hexa Coordinated Fe(III) Complex Showing Ligand Centered Hydrogen Evolution Reaction

P-35	**Bharti yadav**	Department of Chemistry, Indian Institute of Technology, Powai, Mumbai 400076, India	Synthesis and Studies of PAHs Based Expanded Porphyrinoids
P-36	**Bhawna joshi**	Department of Applied Sciences, National Institute of Technology Delhi, New Delhi- 110036	Metal-Functionalized Ordered Mesoporous Silicas (OMs) and Their Catalytic Applications in the Aminolyis, Suzuki–Miyaura and Heck Coupling Reaction
P-37	**Bhuvnesh Singh**	Indian Institute of Technology, New Delhi	A Chiral Silver Phosphate Catalyzed Asymmetric Synthesis of Tetrasubstituted β-Amino Indenones
P-38	**Bisma Rasool**	Natural Product Chemistry & Bioorganic Chemistry Division, IIIM, Jammu, 180001, INDIA	One pot Domino transformation of Glycals into pyrano cis fused heterocycles via Nickel Catalysis
P-39	**Chandani Mathur**	Chemistry Department, IIS, Jaipur	Imidazo[1,2-a]pyridines-Tetracyanoethylene Donor-Acceptor Complexes as Potential Organic Semiconductors
P-40	**Chandini Pradhan**	Organometallic Synthesis and Catalysis Group, Organic Chemistry Division, CSIR−National Chemical Laboratory (CSIR−NCL), Pune 411 008, Maharashtra, India	Iron-Catalysed Regioselective Addition of C─H Bond in Indoles to Alkenes via Weak Chelation Assistance
P-41	**Daksh Singh Davas**	IIT Delhi, Hauz Khas, 110016	Ru-Catalyzed Benzannulation of Vinyl Sulfoxonium Ylide with Electron-Deficient Alkynes and Alkenes
P-42	**Danish Ali**	Department of Chemistry, Indian Institute of Technology Patna, Bihta, Patna-801106, India	Hydrogen Peroxide-Mediated Rapid Room Temperature Metal Free C (sp^2)-H Thiocyanation of Amino Pyrazoles, Amino Uracils, and Enamines.
P-43	**Darshna Hirpara**	Applied Chemistry Department, The Maharaja	Solubilization of Curcumin and its Precursor (CurcumaLongin) Conventional and Deep Eutectic

		Sayajirao University of Baroda, Vadodara	Solvents with and without Ionic Surfactants
P-44	**Deep Chowdhury**	Department of Chemistry, IITBhilai, GEC Campus, Chhattisgarh, India.	A Metal-free Approach Towards Reductive Amination of Carbonyl Compounds
P-45	**Deepa Bhardwaj**	Department of Chemistry, IITD, Hauz Khas, New Delhi-110016, India	Functional Activities of UO_2(VI) Ion On Interaction with (O, N) and (O, N, S/Se) Based Acyclic and Cyclic Donor Bases
P-46	**Deepika Singla**	School of Chemistry and Biochemistry, Thapar Institute of Engineering and Technology, Thapar Technology Campus, Patiala, Punjab, INDIA	Salt-induced Inhibition and Disaggregation of Protein Amorphous Aggregates
P-47	**Deepika Thakur**	Department of Chemistry, University of Delhi, Delhi-110007, India	Unveiling the Three-component Phosphonylation on Alkynylaldehydes: Toolbox Towards Fluorescent Molecules
P-48	**Devesh Kumar Mishra**	Department of Applied Sciences, National Institute of Technology Delhi, New Delhi-110036	BODIPY immobilized MCM-41 based Solid Optical Sensors for Heavy Metal Ions Detection and Removal from Aqueous Medium
P-49	**Dhananjay Chaudhary**	CSIR-CDRI, Lucknow 226031	Palladium-catalyzed N-Protecting Group controlled Regiodivergent cascade cyclization/alkoxylation of Allenamides.
P-50	**Dharmendra Kumar**	Medicinal and Process Chemistry Division, CSIR-CDRI, Lucknow 226031, India. And Academy of Scientific and Innovative Research (AcSIR), Ghaziabad, 201002, India	Domino reaction of tryptamines and diazo compounds to access hexahydropyrroloindoline derivatives under Cu-catalysis
P-51	**Dipika Sharma**	Complex Systems Group, Department of Chemistry,	Enhanced photoelectrochemical response of reduced graphene

		University of Delhi, Delhi, India	oxide covered inexpensive TiO_2-$BiFeO_3$ composite photoanodes
P-52	**Dnyaneshwar Ambadas Gorve**	Department of Chemistry, IIT-Bombay, Powai, Mumbai 400 076, Maharashtra India.	Protecting-Group-Directed Stereodivergent Tsuji-Trost Cyclization: Total Synthesis of (+)-Petromyroxol
P-53	**Dolly Chandel**	Department of Chemistry, Indian Institute of Technology Kanpur, Kanpur-208016	Modulation of Supramolecular Chirality by Stepwise Axial Coordination in a Nano Size Zn(II)porphyrin Trimer
P-54	**Dr Uttama Mukherjee**	Department of Chemistry and Centre for Energy Science, Indian Institute of Science Education and Research, Pune, Maharashtra, India	Quantum Chemical Investigation of Post Combustion CO_2 Capture Using N-Heterocyclic Systems
P-55	**Dr. Ekta Jakhar**	Indian Institute of Technology Delhi	Insight into the High Proton Conductivity of One-/Two-Dimensional Cadmium Phosphites
P-56	**Ekta Chauhan**	Department of Inorganic and Physical Chemistry, Indian Institute of Science, Bangalore	Chalcogen Bond-mediated Cellular Uptake of Fluorescent Compounds
P-57	**Fatimah Ali Hussein**	Department of Chemistry, University of Delhi, Delhi 110007 India	Schiff Base Ligand Based Complexes as Electro Catalysts for Proton Reduction
P-58	**Gargi Dey**	Department of Sciences & Humanities, Rajiv Gandhi Institute of Petroleum Technology, Jais, Amethi, Uttar Pradesh, 229304, India	Heterogenization of non-precious homogeneous catalysts within MOF pores for borrowing hydrogen catalysis
P-59	**Ghanshyam Mali**	Indian Institute of Technology Jodhpur	Development of Green Multicomponent Approach to Synthesize Biologically Active 2,3-Dihydrofurans and 2,3-Dihydrofuro[3,2-c] Coumarins
P-60	**Gokul S Londhe**	Department of Chemistry, Indian Institute of Science Education and Research, Pune, India	Fe-catalyzed Sequential Oxidative Cleavage and Nucleophilic Addition of Peroxyoxindole Towards the Spiro[indoline-3,4'-

			pyran]-2-ones, 2-(2-oxoindolin-3-ylidene) Malononitriles and Spiro [dibenzo[c,h]xanthene-7,3'-indolin]-2'-ones.
P-61	**Gouranga Naskar**	Department of Chemistry, Indian Institute of Technology Madras, Chennai-600036, Tamil Nadu	Ligand-Enabled Pd (II)-catalyzed [3+2] Annulation via C(sp^3)-H and C(sp^2)-H Bond Activation
P-62	**Gulenur Nesha Khatun**	Department of Chemistry, Indian Institute of Technology Bombay, Mumbai, India	New Directions in Diene Functionalization: Oxidative Cleavage and Hydroalkoxylation
P-63	**Gulista Bano**	Indian Institute of Science (IISc)	Boron Based Dual emissive Single Fluorescent Probe for Differentiating Autophagy and Apoptotic Cells/Tissue
P-64	**Harendra Sheshma**	School of Physical Sciences, Jawaharlal Nehru University	Graphitic Carbon Nitride as Responsive Photocatalyst for Expeditious C-H activation /Oxidative Dearomatization in Organic Synthesis
P-65	**Harish Kumar Harit**	Indian Institute of Technology, New Delhi	Synthesis of 2-Quinolinone Derived -Quinone Methide via Ring Expansion of Isatins using 1,2-Phospha-Brook Rearrangement
P-66	**Haritha D.**	Discipline of Chemistry, Indian Institute of Technology Gandhinagar, Gujarat.	Evaluating the in vitro potential of novel benzimidazole derivatives as Helicobacter pylori IMPDH inhibitors
P-67	**Harpal**	Department of Chemistry, Indian Institute of Science Education and Research, Bhopal	Transition from innocent to non-innocent character by changing the meso- substitution on corrole
P-68	**Hemant Kumar**	Indian Institute of Technology Delhi	Germyliumylidene catalyzed hydrosilylation of aldehydes and ketones

P-69	**Hungharla Hungyo**	Special Centre for Molecular Medicine, JNU, New Delhi	Prochlorperazine targeting mutant KRAS and its response in non-small cell lung carcinoma
P-70	**Ibrahim Annan**	Department of Chemistry, University of Delhi, Delhi-110007, India	Detection of Assorted Analytes by Coumarin-Based Chemosensors
P-71	**Ida Angel Priya S**	Chemistry Division, Vellore Institute of Technology Chennai campus, Vandalur, Tamil Nadu	Greener and Efficient Transamidation Protocol for Weakly Nucleophilic Aromatic Amines with N-Acyl-2-Piperidinones
P-72	**Ishaniya W**	Department of Chemistry, SRM Institute of Science and Technology, Tamil Nadu	Nano-encapsulation of melatonin into polydiacetylene-phospholipid assembly for sustained-release and enhanced bone formation in zebrafish
P-73	**Jaipriya Khatri**	Department of Chemistry/School of Natural Sciences/Shiv Nadar Institute of Eminence	C-H Bond Chlorination by Ni(II)-Biguanide Complexes
P-74	**Jaspreet Kaur**	School of Chemistry and Biochemistry, Thapar Institute of Engineering and Technology, Thapar Technology Campus, Patiala-147004, Punjab, INDIA	Insights into calcium-induced aggregation of milk proteins using spectroscopic tools
P-75	**Jayendra Kumar Himanshu**	[a]Special Centre for Nanoscience, JNU, New Delhi; [b]Department of Biotechnology, Mahatma Gandhi Central University, Motihari, Bihar	Carbon Quantum Dots embedded Screen-Printing Electrodes electrochemical Aptasensor development for Chlorpyrifos detection
P-76	**Juhi**	Department of Chemistry, [2]Department of Biological Sciences and Bioengineering,	Cytotoxic Photoactive Ruthenium (II) Polypyridyl Oxalate Complexes: Synthesis, Characterization, Biological Interaction, and their Anticancer Activity against HepG2 Cells

		IIT-Kanpur, Kanpur-208016, India	
P-77	**Juhi Pal**	Department of Chemistry, Indian Institute of Technology Bombay, Mumbai, India	Stereoselective Synthesis of Isoxazolidine via Alkyne–Oximium Cyclization
P-78	**Junaid Shafi Banday**	Natural Products and Medicinal Chemistry Division, CSIR-IIIM Jammu	Iodine Catalysed Tandem Stereoselective Acetalation-Glycosylation of Reducing Sugars Using Acetals/Ketals: Application in the Synthesis of EIDD Molecules
P-79	**Kajal Chaudhary**	Department of Chemistry, Indian Institute of Technology Kanpur	Derivatives of NNO based pincer type ligands as an Inorganic Antibiotics
P-80	**Kanika Devi**	School Of Physical Sciences/Jawaharlal Nehru University, New Delhi-110067	Design and Synthesis of a Library of Short Peptide Sequences and In-silico Screening Against pf-DHFR for Antimalarial Chemotherapy
P-81	**Kapil Mohan Saini**	Department of Chemistry, Kalindi College, University of Delhi-110008	Unconventional Ag-Catalyzed Cycloaromatiza- tion and Au-Catalyzed Double C–H Activation: Synthesis of Polyaromatic Biaryls
P-82	**Kavita Choudhary**	Department of Chemistry, Indian Institute of Technology, Kanpur, India	Kinetic Resolution of Electron Deficient Bromohydrins via Cu (II) Catalysed C-C Bond Cleavage
P-83	**Kavita Singh**	Glyco-chemistry Laboratory, School of Physical Sciences, Jawaharlal Nehru University, New Delhi	Organo-catalyzed synthesis of α, β-unsaturated carbohydrate enals (Perlin's aldehyde)
P-84	**Kirandeep Bhagat**	Department of Chemistry, IIT Delhi; Department of Materials Science & Engin., IIT Delhi	Microemulsion route-based synthesis of lanthanum oxides-based nanomaterials and to study their magnetic and photoelectrochemical properties
P-85	**Krishanu Bera**	Department of Chemistry, Indian Institute of	Manganese Catalyst for α Alkylation of Nitriles with Alcohols

		Technology Bhilai, Raipur 492015 Chhattisgarh, India	
P-86	**Krishanu Mondal**	Department of Chemistry and Chemical Biology, Indian Institute of Technology (Indian School of Mines)Dhanbad	Exploiting the Versatility of 7-Azaindole for Mechanistic Study of Chan-Lam Type Coupling
P-87	**Krishna Biswas**	Department of Chemistry, IIT-Kharagpur, Kharagpur - 721302, West Bengal	Organophosphorus Catalyzed Stereoselective Borylative Ring-Opening of Vinylcyclopropanes: A Route of -Valerolactones
P-88	**Krishna Kumar M S**	Jawaharlal Nehru University, New Delhi.	Electrochemically synthesized highly stable double zwitterionic Naphthalenediimide from ultra-electron deficient molecule
P-89	**Kundan Singh Mehra**	Indian Institute of Science Education and Research Bhopal	Deep LUMO based Terrylene Diimide with NIR emission
P-90	**Kusaji Raul**	Indian Institute of Science Bengaluru, India	Photoinduced apoptosis by Mitochondria targeting Pyrene-mercaptobenzimidazole conjugate due to mitochondrial cardiolipin disruption
P-91	**Kush Kaushik**	School of Chemical Sciences, IIT Mandi	Controlling the fluorescence intermittency of water-soluble BSA-conjugated Quantum Dots with Super resolution of Lysosomes
P-92	**Lalit Mohan Kabadwal**	Indian Institute of technology Roorkee, Roorkee, 247667	Iron-catalysed alkylation of 2-methyl and 4-methyl azaarenes with alcohols via C-H bond activation
P-93	**Lalropuia**	Department of Industrial Chemistry, School of Physical Sciences, Mizoram University, Mizoram	Drug design, Green Synthesis, Hirshfeld Analysis and anticancer activity of dihydropyriminidone analogs
P-94	**Laxmi**	SPS biophysical lab JNU, Munirika, New Delhi, Delhi 110067	Thermodynamic Studies of interaction between basic ligands and DNA

P-95	**Mahanthi Sankarrao**	Department of Chemistry, Indian Institute of Technology Madras, Chennai – 600036, India	UV-Light Promoted Oxidative Cleavage of 2,5-Diarylphenanthreno-[c]-thiophenes to 9,10-Diaroylphenanthrenes
P-96	**Manajit Mandal**	Department of Chemistry, Indian Institute of Technology Kanpur, Uttar Pradesh	Circular Polarised Light Directed study in Chirality Regulation of Amino Acid Capped Nickel Nanoparticles
P-97	**Manav Chauhan**	Department of Chemistry, Indian Institute of Technology, New Delhi, India	Metal-Organic Framework Encaged Monomeric Cobalt(III)-Hydroperoxides Enable Chemoselective Methane Oxidation to Methanol
P-98	**Manisha**	Natural Product laboratory, Department of Chemistry, University of Rajasthan, Jaipur (India)	Phytochemical profiling and GC-MS analysis of Nigella sativa (black cumin) seeds.
P-99	**Manisha Sisodia**	Department of Chemistry, IIS (Deemed to be University), Jaipur	tert-Butyl nitrite mediated azo coupling reactions of imidazole derivatives and sulphur containing amino compounds
P-100	**Mitrali Biswas**	Department of Chemistry, Indian Institute of Technology Bombay, Powai, Mumbai, 400076	Redox Induced Diverse Functionalization of Bis (aldiimine) Ligands on Electron Rich Ru-Platform
P-101	**Mohammad Yaqoob Bhat**	Natural Product and Medicinal Chemistry Division, CSIR-IIIM, Jammu; AcSIR, Ghaziabad, India	Sulfonyl Promoted Michaelis-Arbuzov Type Reaction: An Approach to S/Se-P bonds.
P-102	**Mohan Ilakiyalakshmi**	Department of Chemistry, Vellore Institute of Technology University, Vellore.	Furan Appended Benzothiazole Based Schiff Bases For a Highly Selective Visual and Fluorimetric Detection of Cu 2+ ion with Density Functional Theory Studies and its Application For Real-life Samples.

P-103	**Mohd Shakir**	Department of Biosciences, Jamia Millia Islamia, Jamia Nagar, New Delhi, 110025	Synthesis and mechanistic studies of Isatin-pyrazole hydrazones as bacterial MetAP Inhibitors
P-104	**Mohit**	Department of Chemistry, University of Delhi, Delhi-110007, India	Evolution of IBX based oxidation: Transformation of alcohols into corresponding aldehydes and Ketones
P-105	**Monika**	School of Physical Sciences, JNU, Delhi	Vanadium-based Mixed Metal Oxides for effective removal of Toxic Pollutants
P-106	**Monika**	Department of Chemistry/School of Natural Sciences/Shiv Nadar Institute of Eminence	Aromatic C-H Activation by Bioinspired Cu(II)- complexes
P-107	**Mostofa Ataur Rohman**	Spectroscopy Laboratory, School of Physical Sciences, JNU, New Delhi	Effect of Dehydrating Agent on the Kinetics of Ligand/G-quadruplex DNA Interaction
P-108	**MS. Lalita Kumari**	Department of chemistry, University of Rajasthan, Jaipur	Phytochemical study of Petroleum Ether Extract of Seeds of Psoralea Corylifolia by GC-MS
P-109	**Muskan**	Department of Chemistry, University of Delhi, Delhi-110007, India	Stereoselective Synthesis of Densely Functionalized Indenes via Regioselective Cascade Iodoalkylation of Alkyne
P-110	**Naved Akhtar**	Department of Chemistry, Indian Institute of Technology, New Delhi, India	Chiral iron(II)-catalysts within valinol-grafted metal-organic frameworks for enantioselective reduction of ketones
P-111	**Naveen**	Department of Chemistry, Indian Institute of Technology Delhi, New Delhi, 110016, India	Brookhart's Acid-Catalyzed Switchable Regioselective N-Alkylation of Arylamines/Heterocyclic Amines with Cyclopropylcarbinols by Temperature Regulation
P-112	**Naveen Kumar**	Indian Institute of Technology Roorkee	Mononuclear/Binuclear [VIVO]/[VVO2] Complexes Derived from 1,3-Diaminoguanidine and Their Catalytic Application for the

			Oxidation of Benzoin via Oxygen Atom Transfer
P-113	**Naveen Sihag**	Department of Chemistry, IIT Delhi, New Delhi, India	Photo-Induced Decarboxylative Radical Cascade for Synthesis of Quaternary-CF3 Containing Oxindoles and Indoline-Alkaloids
P-114	**Neelakshi**	Indian Institute of Technology Kanpur	Bolaamphiphilic Surfactants Derived From L-Lysine and L-Glutamic Acid
P-115	**Neerathilinga M N**	Department of Organic chemistry, University of Madras, Chennai, India	Substituent-controlled selective synthesis of 1,2-diketones and internal alkynes from terminal alkynes and arylboronic acids via α-stilbene radicals obtained from heteroleptic Cu(I) complexes under visible light
P-116	**Neha Dagar**	Indian Institute of Technology, Delhi	Diastereoselective Decarboxylative Alkylation of Coumarins via Dual Synergistic Role of Cerium in Ligand-to-Metal Charge Transfer and Lewis Acid Catalysis
P-117	**Neha Jha**	Department of Chemistry, Indian Institute of Science Education and Research Bhopal	Regiocontrol via electronics: Ru/Cu co-catalyzed site-selective alkylation of isoquinolones by C-C bond activation of cyclopropanols
P-118	**Neha Singh**	Department of Chemistry, Indian Institute of Technology Kanpur, Kanpur-208016, India.	Giant electron transport properties of functionalized superparamagnetic nanoparticle
P-119	**Neha Yadav**	Complex System Group, Department of chemistry, University of Delhi, Delhi, 110007	Theoretical and Experimental Investigation of Influence of Solvents and Electrode Roughness on Potential of Zero Charge
P-120	**Nidhi Kumari**	Indian Institute of Technology Delhi	Anchoring of Phosphine on Metal-oxide Nanostructure for Heterogeneous Catalysis.
P-121	**Nitika Garg**	Department of Chemistry, Indian Institute of	Crystal facet-engineered NaNbO3/Ag2S stable inks for

		Technology Delhi, Hauz Khas, New Delhi-110016	visible light photoelectrochemical water splitting
P-122	**Nitin Kumar Tyagi**	Department of Chemistry, School of Natural Sciences, Shiv Nadar Institute of Eminence, Dadri	Surface Modulated Free-standing Copper Electrodes for Nitrate to Ammonia Synthesis
P-123	**Rajdeep Tyagi**	Glyco-chemistry Laboratory, School of Physical Sciences, Jawaharlal Nehru University New Delhi-110067	Efficient Synthesis of Triazole Bridged Indole-based Glycohybrids
P-124	**Nivedita Rana**	Indian Institute of Technology-Roorkee, Roorkee, Uttarakhand-247667, India	Power of Protons on Porphyrin Macrocycle
P-125	**Norein Sakander**	Natural Product and Medicinal Chemistry Division, IIIM, Jammu	Reactivity Switch for Selective Nucleoside Formation from 2-Acetoxy Methyl Glycals: Synthesis of C-2 Methylene and C-2-Functionalized Nucleoside Mimetics
P-126	**Om Prakash Joshi**	Department of Chemistry, School of Chemical Sciences and Pharmacy, Central University of Rajasthan	Synthesis of Benzofuran and Indole Scaffolds via One-Pot Domino Sonogashira Coupling/Cyclization using Abnormal NHC based Pd-PEPPSI Complexes
P-127	**Padma Sharma**	National Institute of Technology, Patna	Enhance antioxidant and cytotoxic activity of ferrocenyl- substituted curcumin via stabilization of promoter c-MYC silencer element
P-128	**Palani Purushothaman**	Department of Chemistry, School of Advanced Science, VIT University, Tamil Nadu, India	Ultrasensitive fluorogenic detection of Hydrargyrum in Industrial Effluent and Utilization of Conjugated Thiophene Carboxaldehyde in Forensic Fingerprint Imaging with DFT Calculation

P-129	**Pallabi Halder**	Department of Chemistry and Chemical Biology, Indian Institute of Technology, Dhanbad, India	Chloroform-COware Chemistry: An Emerging Tool for Palladium-Catalyzed Aminocarbonylation
P-130	**Pallavi Malhotra**	Department of Chemistry, University of Delhi, Delhi; School of Pharmacy, University of Mississippi, USA	An investigation of 4-aminoquinoline-quinazoline (AQ-QN) molecular hybrids as potent antimalarial agents
P-131	**Pankaj Kumar**	Ashoka University, Rajiv Gandhi Education City, Sonipat	Electrocatalytic Hydrogen Evolution Reaction by μ-Oxo Iron Complex bearing thiazolinium moiety as proton relay
P-132	**Papita Behera**	Department of Chemistry, Berhampur University	Oxygen-bridged $CuMoO_4$ catalyst for Csp^2-Se cross-coupling
P-133	**Partha Pratim Sen**	Indian Institute of Technology Delhi	When Organic Lewis Acid Turn out to be a Photooxidant to Build a New Avenue for Azolation of Unactivated Arenes
P-134	**Parvez Alam**	Spectroscopy Laboratory, School of Physical Sciences, Jawaharlal Nehru University, New Delhi	Molecular Crowders Modulate Ligand Binding Affinity to G-Quadruplex DNA by Decelerating Ligand Association
P-135	**Pooja Negi**	School of physical sciences, Jawaharlal Nehru University, New Delhi -110067, India.	A comprehensive Biophysical analysis of the effect of ss DNA binding on the fluorescence intensity of metal nanoclusters.
P-136	**Pooja Soam**	School of Chemistry and Biochemistry, Thapar Institute of Engineering and Technology, Patiala	Synthesis of 3-alkenyl-oxindole derivatives using Pd-catalyzed multicomponent reaction
P-137	**Pooja Yadav**	Indian Institute of Science Education and Research, Tirupati	Sustainable synthesis of diverse molecular scaffolds via photoredox catalysis and electro-organic Synthesis
P-138	**Poonam Rani**	Indian Instituite of Science Bangalore-560012	Design and Development of small molecule activators to treat neurodegenerative diseases

P-139	**Poonam Saini**	School of Physical Science, JNU, New Delhi, 110067, India	Synthesis of Stable Perylenediimide-based Neutral Radicals with Switchable States
P-140	**Poornima U S**	Department of Chemistry, Shiv Nadar Institute of Eminence, Delhi NCR, India	Natural herbs (Neem, Curry and Mint) - based Extracellular Vesicles hold potential in delivery applications.
P-141	**Prabhat Majumdar**	Indian Association for the Cultivation of Science, Kolkata	Aza[7]Helicene: Overcoming the Synthetic Bottleneck, Chiral Resolution and Modulating the Chiroptical properties.
P-142	**Prachi Bhatia**	Department of chemistry, Indian Institute of Technology, Roorkee-247667, India	Exploring 4-hydroxy-3,5-dinitropyrazole as a precursor for the synthesis of N-methylene-C bridged insensitive energetic materials
P-143	**Prachi Varshney**	Indian Institute of Science Education and Research, Bhopal	Copper Corrole Immobilized onto Reduced Graphene Oxide: An Efficient Catalyst for Hydrogen Evolution Reaction (HER)
P-144	**Pradeep sachan**	IIT Kanpur, India	Coordination-driven Opto-electroactive molecular thin films in electronic circuits
P-145	**Pradyota Kumar Behera**	Department of Chemistry, Berhampur University	Synthesis of Cotarnine Based Scaffold for Oral Cancer
P-146	**Pragya**	Indian Institute of Technology Delhi	Metal-Free Straightforward Synthesis of β,β-Di-aryl Esters: A Cascade Strategy towards 3-Aryl-1-indanone Cores
P-147	**Prakriti Saraf**	Birla Institute of Technology and Science, Pilani campus, Rajasthan	Regioselective Synthesis of Oxadiazolyl and Triazolopyridyl BODIPYs for Sensing of Mercury Ions and pH Sensors
P-148	**Prasanth K**	University of Madras	Visible Light Catalyzed PCET of Quinazolinones/ Benzothiadiazines as Amidyl/Aminyl Radical Precursors for Controlled Cascade Cyclization

P-149	**Pratik kumar Lakhani**	Applied Chemistry Department, The Maharaja Sayajirao University of Baroda, Gujarat, India	Development of BINOL-Ru Catalyst Covalently Immobilized on MSNs and Their Application in Asymmetric Hydrogenation
P-150	**Prerna**	Complex Systems Group, Department of Chemistry University of Delhi- 110007, India	Theory and Experiment for migration-diffusion controlled reversible electron transfer reaction
P-151	**Priyanka Chakraborty**	Indian Institute of Technology Kanpur, Kanpur, Uttar Pradesh 208 016 (India).	Alcohols as the Alkylating Agent under Base Metal Catalysis: Applications and the Underlying Mechanistic Landscape
P-152	**Priyanka Choudhary**	Department of Chemistry, IIT-Bombay, Powai, Mumbai 400076, Maharashtra, India	Regioselective C-5 Halogenation of 8-Aminoquinoline by Ni-Catalyst and Co-Catalysed Chelation Assisted ortho-Iodination of Aromatic Sulfonamides with Molecular Iodine
P-153	**Priyanka Gautam**	School of Chemistry and Biochemistry, [b] Department of Chemical Engineering, [c]TIET-VT Centre of Excellence for Emerging Materials, Thapar Institute of Engineering and Technology, Patiala, India	Catalytic synthesis of energy-rich fuel additive levulinate esters from levulinic acid using modified ultra-stable zeolite Y
P-154	**Priyasha**	Jawaharlal Nehru University, New Delhi- 110067	The temperature-induced phase transition generates the thermosalient effect in an organic salt.
P-155	**Pronab Kundu**	Spectroscopy Laboratory, School of Physical Sciences, JNU, New Delhi	Dansyl Based Molecular Rulers for Probing Depth-Dependent Solvation Properties at Charged-Lipid/Water Interface
P-156	**Pushpendra**	UGC-SRF/Centre of Biomedical Research SGPGIMS-Campus Raibareli Road.	TFA-Mediated One-Pot Tandem Regioselective Synthesis of 3-Substituted-1-Aryl-1H-Pyrazolo-[3,4-b]quinolines from Anilines and Pyrazolones Using DMSO as one Carbon Source

P-157	**Rabban**	Biomimetic Supramolecular Chemistry Laboratory, Department of Chemistry, Shiv Nadar Institution of Eminence, Uttar Pradesh, India	Spontaneous self-assembly of macrocycles to extended nanostructures
P-158	**Rahul**	Department of Chemistry, University of Delhi, Delhi-110007, India.	Regioselective Carbosulfonylation of Alkynes: Metal free Approach to Access β-Carbo Vinylsulfones
P-159	**Rahul Kumar Singh**	Department of Chemistry, Indian Institute of Technology Indore, Indore 453552, India	Cationic Ruthenium(II)-CNC Pincer Complexes with Multiple NHC Ligands: Catalytic Application in Hydration of Nitriles under mild Condition
P-160	**Rahul P.**	CSIR – National Institute for Interdisciplinary Science and Technology, Thiruvananthapuram	Inverse Electron Demand Diels Alder Reaction of Aza-o-Quinone Methides and Enaminones: Accessing 3-Aroyl Quinolines and Indeno[1,2-b]quinolinones
P-161	**Rajat**	Indian Institute of Technology Delhi, Hauz Khas, New Delhi 110016	Photoredox/Palladium Dual Catalysis for Visible-Light Mediated C-H Functionalization of N-protected carbazoles
P-162	**Rajesh Kumar**	Department of Chemistry, Indian Institute of Technology Roorkee, Roorkee 247667, India	Synthesis, Spectral and Redox Properties of Barbituric Acid appended N-Confused Sn(IV) Porphyrin and its Utilization in Photodynamic Therapy
P-163	**Rajnish**	Department of Chemistry, Indian Institute of Technology Roorkee, Uttarakhand, India	Hypervalent Iodine(III) Mediated Synthesis of Isoxazoline via Oxidative of cyclization of Aldoximes
P-164	**Rakhi yadav**	Glyco-chemistry Laboratory, School of Physical Sciences, Jawaharlal Nehru University, Delhi	Recent Development Towards Green Synthesis of Anticancer Molecules

P-165	**Ravisen Rai**	Department of Chemistry, Institute of Science, Banaras Hindu University, Varanasi, UP, INDIA	A new Naphthalimide based fluorescence probe for selective detection of Picric Acid
P-166	**Rimpi Bhandari**	Department of Chemistry, Institute of Science, Banaras Hindu University, Varanasi, India.	A highly selective fluorescent sensor for Fe3+ based on covalently linked derivative of two naphthalimide unit
P-167	**Rina Mahato**	Department of Chemistry, Indian Institute of Technology Delhi, Hauz Khas, New Delhi, India	HFIP Promoted Metal-free Homodimerization of Styrene Diols: An Efficient Approach toward the Synthesis of 2-Phenylnaphthalenes
P-168	**Rinshad V A**	Department of Inorganic & Physical Chemistry, IISC Bangalore	Solvent Induced Conversion of a Self-Assembled Gyrobifastigium to a Barrel and Encapsulation of Zinc-Phthalocyanine within the Barrel for Enhanced Photodynamic Therapy
P-169	**Rohit**	Indian Institute of Technology Roorkee, Roorkee, Uttarakhand-247667, India	Ratiometric and colorimetric "naked eye" selective detection of CN^- ions by electron deficient Ni(II) porphyrins and their reversibility studies
P-170	**Rohit Kumar**	IIT Delhi, New Delhi-110016, India	Photocatalyzed Hydroxy-Arylation of Olefinic Double Bond in visible light: Synthesis of 3-Benzyl-3-Hydroxyisoindolin-1-Ones
P-171	**Rohit Kumar Maurya**	Student/Dept. of Chemistry, IIT-Kanpur	Femtosecond Laser-Induced Thermal Spectroscopy for Investigating the Molecular Interactions in Liquids
P-172	**Ruchi**	School of Physical Sciences, Jawaharlal Nehru University, New Delhi-110067	Design and Synthesis of POM-MOF Hybrid Materials
P-173	**Ardhra. Shylendran**	Department of Chemistry and Centre for Energy Science, Indian Institute of Science Education and	Molecular simulations of temperature and concentration dependence of structure and ionic

		Research Pune, Pune 411008, India	mobility in diglyme-based Sodium-Ion electrolytes
P-174	**Sadiya Tanga**	Department of Chemistry, [b]Department of Biology, Ashoka University, Sonipat, India	A Turn-Off CRISPR/Cas9 System for Precision Genome Engineering Applications
P-175	**Sahel Fajal**	Department of Chemistry, and Centre for Water Research, IISER, Pune, India.	Nanotrap Grafted Cationic Hybrid Composite Material for Effective Toxic Chemical Segregation from Water
P-176	**Saksham Mishra**	Department Of Chemistry, Indian institute of Technology, Patna, India	Arylation of Maleimide via Weakly Coordinating Acetamide Assisted Cross-dehydrogenative Coupling
P-177	**Sambit Pradhan**	Department of Inorganic and Physical Chemistry, Indian Institute of Science, C.V. Raman Avenue, Bangalore 560012, India	New Insights into Proteasome Inhibition Strategy for Enhanced Specificity and Cellular Toxicity
P-178	**Samim Sohel Rana**	Organometallics & Smart Materials Laboratory, Department of Chemistry, IISER-Bhopal	Mechanoresponsive Heptagon-Containing Non-planar Heteronanographenic Molecules
P-179	**Samina Easmin**	School of Basic Sciences, Indian Institute of Technology Bhubaneswar, Bhubaneswar, India	An Anomalous Phase Transformation of Three Different Co-crystals of Citric Acid and 1,2-bis(4-pyridyl)Ethene in Solution and Solid-State Along with [2+2] Photochemical Reactivity
P-180	**Sandhya Singh Yadav**	Department of Chemistry, IIT-Bombay, Powai, Mumbai 400076, Maharashtra, India	Anti-Markovnikov Palladium-Catalyzed Oxidative Acetalization of Activated Olefins
P-181	**Sandipan Ghorai**	Organic & Medicinal Chemistry Division, CSIR-Indian Institute of Chemical Biology, Kolkata	Anion-templated programmable Chiral Self-Sorting in Pd_2L_4 Cages and the switching between chiral and achiral isomers
P-182	**Sangeeta**	School of Physical Sciences, Jawaharlal Nehru University, New Delhi-110067	Photochemical Properties of Polyoxometalate Supported Transition Metal Complexes

P-183	**Sanjeev Kumar**	Department of Chemistry, University of Delhi, Delhi, India	Tungsten Based Tin Oxide Nanoparticles: Role of Sacrificial Agents in Degradation of Organic Toxic Dye
P-184	**Sanjeev Kushwaha**	Catalysis Group, Department of Chemistry, Indian Institute of Technology Indore, Simrol, Indore 453552, Madhya Pradesh, India	Hydrogen Production from Formic Acid over Ruthenium Catalysts in Water
P-185	**Sanju**	School of Physical Sciences, Jawaharlal Nehru University, New Delhi, India 110067	Novel Route to Synthesize 1,4-Dihydroquinoline Derivatives by Nitrene Insertion Using Five Membered Heterocyclic Rings as Diene Precursor for [4+2] Cycloaddition with Benzyne
P-186	**Sanyukta Mayuri**	National Institute of Technology, Patna	Fluorescent Copper conjugated Curcumin cystine nanoprobe for selective determination of Fe^{3+} and G-quadruplex DNA
P-187	**Satyajit Patra**	New Chemistry Unit, Jawaharlal Nehru Centre for Advanced Scientific Research (JNCASR), Jakkur P.O., Bangalore-560064	Liquid-liquid Phase Separation (LLPS) from Small Molecules and Their Fates
P-188	**Sayak Ghosh**	Department of Medicinal Chemistry, National Institute of Pharmaceutical and Educational Research (NIPER)-Ahmedabad, Palaj, Gandhinagar-382355, Gujarat, India	A micellar catalysis strategy applied to the Pd-catalyzed C–H arylation of indoles in water
P-189	**Shadab Saifi**	Rajiv Gandhi Institute of Petroleum Technology Jais Amethi U.P. – 229304, India	Coupling of Single –Ni-Atom with Ni-Co Alloy Nanoparticles for PEM Fuel Cell Application
P-190	**Shagun Sharma**	School of Chemical Sciences, Indian Institute of Technology Mandi, H.P., 175075, India	Deciphering the Role of Metal-Thiol Bond on the Excited State Relaxation Process of BSA Protected Metal Nanoclusters
P-191	**Shambhavi C N**	Department of Chemistry, Indian Institute of Technology, Madras, Tamil Nadu-600036	Ruthenium (II)-Catalyzed Redox-Neutral C−H Alkylation of Arylamides with Unactivated Olefins

P-192	**Shankhajit Mondal**	Department of Chemistry, Indian Institute of Science Education and Research, Pune, India	Continuous-flow Fe-Zeolite catalyzed temperature directed synthesis of bioactive tetraketones and xanthenes using epoxide and cyclic-1,3-diketone via Meinwald
P-193	**Shanmugapriya K**	Department of chemistry, School of Advanced Sciences, Vellore Institute of Technology, Vellore	A Protective Metal-Organic Framework with Multiple Donor Site for an Efficient Surface Coating Application Supported by Optical Spectroscopic and DFT Studies
P-194	**Shashikant Tiwari**	Department of Chemistry, University of Delhi, Delhi-110007, India.	A practical, Metal and additive free regiodivergent synthesis of polysubstituted indolizines
P-195	**Sheba Ann Babu**	Academy of Scientific and Innovative Research (AcSIR), Ghaziabad-201002, India	Pd-catalyzed site selective and Chemoselective CH functionalization towards Polyring Fused N-heterocycles
P-196	**Shishir Singh**	Department of chemistry, Indian Institute of Technology, Kanpur-208016	Aminium radical-cation catalysed SN2 type Nucleophilic Ring Opening of Activated Azetidines with Arenes and Heteroarenes: Synthetic Route to Tolterodine
P-197	**Shiva**	Department of chemistry, Banaras Hindu University, Varanasi, India.	Cadmium-metal-organic framework: Synthesis, characterization and fluorescent studies towards nitroaromatic explosives
P-198	**Shivam Abhineet Meena**	Department of Chemistry, University of Delhi, Delhi-110007, India	Stereoselective Synthesis of Functionalized Succinimides by Radical Cascade Sulfonation, Cyclization, and Concomitant Thiolation/Selenation of Aza-1,6-Enynes.
P-199	**Shivangee Jha**	Department of Chemistry, [a]Indian Institute of Science Education and Research Bhopal	Bay expanded Terrylene Diimide exhibiting Room Temperature Phosphorescence
P-200	**Shreya Juneja**	Department of Chemistry, Indian Institute of	Classifying deep eutectic solvents for polymer solvation via intramolecular dimer formation

		Technology Delhi, Hauz Khas, New Delhi, India	
P-201	**Shruti Rajput**	IIT Delhi, New Delhi-110016, India	Visible-light-driven Photoredox and Palladium dual catalysis: a route to directing group assisted decarboxylative site-selective benzoylation of N-phenyl-7-azaindoles
P-202	**Shubhangi Majumdar**	Indian Institute of Technology, Delhi	A Photophysical Insight into the Mode of Action of Polyphenols as Protein Aggregation Modulators in The Ultrafast Timescale
P-203	**Shyam Kumar Lokhande**	Department of Medicinal Chemistry, NIPER – Ahmedabad, Palaj, Gandhinagar, Gujarat, India	Water enabled, nickel-catalyzed highly chemoselective C-allylation of (NH)-indoles employing alcohols
P-204	**Smaranika Patra**	School of Physical Science, JNU, New Delhi, 110067, India	Cobalt (II)-based spin crossover materials with twisted PDI dianion
P-205	**Sonali Ghosh**	Supramolecular & Structural Chemistry Laboratory, Indian Institute of Technology Bhubaneswar, Argul, Bhubaneswar, India	Influence of C–H•••S Hydrogen Bonds on Thermal Expansion Studies in Two Concomitant Co-crystals of Ethionamide and 2-Thiobarbituric acid
P-206	**Soni Kumari**	Department of Chemistry, Indian Institute of Technology Roorkee, Roorkee-247667, India	Synthesis, Spectral and Electrochemical Studies of Dicyanovinyl Substituted Porphyrins for Excited State Charge Transfer Dynamics
P-207	**Soundraya Palanisamy**	Department of Chemistry, Indian Institute of Technology Madras, Chennai 600036, India	Cu-Catalyzed and Iodine Assisted Domino Synthesis of Thioaurones through C-S Bond Formation using Xanthate Surrogate
P-208	**Sourav Pramanik**	Centre of Biomedical Research	Hydroxamate-Directed Access to β-Kdo Glycosides
P-209	**Srashti Bhardwaj**	Department of Chemistry, Indian Institute of Technology Delhi	A Bidirectional Iterative Approach to Sequence-Defined Unsaturated Oligoesters

P-210	**Sreshtha Chaki**	Department of Chemistry, Indian Institute of Technology Kharagpur, Kharagpur	Probing the effect of glycation on the esterase activity of Human Serum Albumin: A spectroscopic study
P-211	**Sruthi S. L., and Meenakshy C. B.**	Department of Chemistry, University of Kerala, Kariavattom, India, 695581	Green Synthesis of Biologically Active Spiro Heterocyclic Compounds
P-212	**Stanzin Chuskit**	School of Phyiscal Sciences, Jawaharlal Nehru University	Effect of methyl substituent on thermal expansion in imidazolium-p-hydroxybenzoate Salt
P-213	**Subhadip Pramanik**	Department of Chemistry, Indian Institute of Technology Kanpur, Kanpur, India	Control of Spin Coupling Through Bridge in Bimetallic Porphyrin Dimer
P-214	**Subhalaxmi Panda**	Department of Chemistry, Berhampur University, Odisha-760007	Oxygen Bridged Bimetallic $BaCu_2O_3.4H_2O$ Nano Catalyst For C-O Cross-Coupling Reaction
P-215	**Suchita Dattatray Shinde**	Department of Medicinal Chemistry, NIPER, Ahmedabad, Gujarat, India	Synthesis and investigation of backbone modified squaramide dipeptide self-assembly
P-216	**Sukriti Santra**	Department of Chemistry, University of Delhi, Delhi - 110007	Regioselective synthesis of 5,6,7,8-tetrahydroindolizine via 1,1,2- trifuctionalisation of alkynes
P-217	**Suman Majee**	Amity Institute of Click Chemistry Research & Studies	Base Promoted C-3 Chalcogenylation of Indolines with Dichalcogenides
P-218	**Sumanta Let**	Department of Chemistry, Indian Institute of Science Education and Research, Pune, India	Palladium anchored N-Heterocyclic Carbene on a Porous Polymer – An Efficient Heterogeneous Composite Catalyst for Eco-Friendly Suzuki-Miyaura Coupling
P-219	**Sumit Kumar Yadav**	Department of Chemistry, Indian Institute of Technology Roorkee, Roorkee, India	Synthesis of meso-tetracyanobutadiene-Appended Porphyrin for NLO Application

P-220	**Sumithaa Chezhiyan**	SRM Institute of Science and Technology, Kattankulathur, Tamil Nadu, India	Nanoencapsulation of Ru(p-cymene) Complex Bearing Ginger-based Natural Product into Liposomal Nanoformulation to Improve Its Cellular Uptake and Antiproliferative Activity
P-221	**Sunil**	Glyco-Chemistry Laboratory, School of Physical Sciences, Jawaharlal Nehru University, Delhi	Recent Advancement in Synthesis of Organo-Catalysed Antitubercular Agents
P-222	**Supraja N**	Department of chemistry, School of Advanced Sciences, VIT, Vellore – 632014	"Naked eye" colorimetric sensing response of benzothiazole-based imine chemosensor towards copper (II) ion detection: synthesis, characterization and theoretical investigations
P-223	**Suraj Kashyap**	Department of chemistry, Indian Institute of Technology, Kanpur	Aminium Radical-Cation Catalyzed S N 2-type Ring-Opening Reactions of Aziridines with O/S/N/C-Nucleophiles: Formal Synthesis of (R)-Halostachine
P-224	**Suresh Kumar Yadav**	Department of Chemistry, Indian Institute of Technology, Madras, Tamil Nadu	Regio- and Chemoselective [4+2]-Annulation of Aromatic Sulfoxonium Ylides with 1,3-Diynes via Cp*Co(III) Catalysis
P-225	**Swati Singh**	Indian Institute of Technology, Delhi	Metal- and catalyst-free photoinduced radical cascade reactions to achieve thioalkylation of quinoxalin-2(1H)-ones: an efficient synthesis of β-heteroaryl thioethers
P-226	**Tabish Iqbal**	Indian Institute of Science	Deciphering a Membrane-bound Hydrocarbon Producing Metalloenzyme
P-227	**Tanaya Manna**	Centre of Biomedical Research, SGPGIMS Campus, Lucknow-226014, India	Biocatalytic Asymmetric Synthesis of Tetrahydro-1-Benzazepines using Imine Reductases (IRED)

P-228	**Tanya Agrawal**	Department of Chemistry, Shiv Nadar Institute of Eminence, New Delhi, India	Imperative Label-free distinctions between breast cancer and normal chromosomes
P-229	**Tapaswini Sethi**	School of Physical Sciences, Jawaharlal Nehru University, New Delhi	Tuning of Thermal Expansion Properties of Mixed-Ligand MOF by Ligand Variation
P-230	**Tazeen**	Department of Biological and Synthetic Chemistry, Centre of Biomedical Research, SGPGIMS-Campus, Lucknow, India	First NHC Catalyzed Enantioselective Cycloaddition Reactions of Enals with α-Functionalized Vinyl Ketones
P-231	**Tohasib Yusub Chaudhari**	Special Centre for Molecular Medicine, Jawaharlal Nehru University, New Delhi	A Bronsted acid-catalysed regioselective carboxamidation of 2-indolylmethanols with isonitriles
P-232	**Tushar Ashok Kharde**	Catalysis Group, Department of Chemistry, Indian Institute of Technology, Indore	Low-temperature hydrogen production from methanol
P-233	**Uma Shankar**	Glyco-Chemistry Laboratory, School of Physical Sciences, JNU, Delhi, India	Recent Synthetic Development on 2-Hydroxy-1,4-naphthoquinone (Lawsone)
P-234	**Umabharathi P S**	Department of Chemistry, School of Advanced Science, VIT University, Tamil Nadu	Detection of cyanide in mainstream smoke of tobacco products through Naked-eye colorimetric, turn-on fluorescent Schiff base sensor and its theoretical studies.
P-235	**Vaishaly Duhan**	Department of Chemistry, School of Natural Sciences, SNIoE Gautam Buddha Nagar, Uttar Pradesh, India	Effect of Hydrogen Bonding as a Latent Catalyst in Greener Substituted Benzoxazine and their Applications
P-236	**Varsha Jain**	Department of Chemical Sciences, IISER Mohali, Punjab 140306, India	Imine-based highly polar achiral unsymmetrical four-ring bent shaped liquid crystals: Design, synthesis and characterization
P-237	**Vatsala Cilamkoti**	Department of Chemistry, Indian Institute of	Studies on Photoluminescence Property of Silicon Dioxide Quantum Dots Anchored on Different Types of Carbonaceous

		Technology, Roorkee, 247667, India	matrix & their Application for Metal Ion Sensing
P-238	**Vikas Dixit**	Indian Institute of Technology, Delhi, India	Visible light mediated Direct Activation of Benzoquinone for the Generation of Quinoxaline Derivatives
P-239	**Vikas Maurya**	Special Centre for Molecular Medicine, Jawaharlal Nehru University, New Delhi-110067, India.	Unraveling topoisomerase IA gate dynamics in presence of PPEF and its preclinical evaluation against multidrug-resistant pathogens
P-240	**Vikram Singh**	Centre of Biomedical Research, Lucknow	Iodine(III) Catalyzed Unprecedented Direct Construction of (Hetero)functionalized Pyrazolines, Pyrazoles and Isoxazoles
P-241	**Vimlesh Kumar**	Department of Chemistry, Indian Institute of Technology Kanpur	Ruthenium Catalyzed Stereo- and Chemoselective Oxidative Coupling Reaction of Vinyl ketones and Acrylates: Application to Synthesis of FR252921
P-242	**Virender**	School of Physical Sciences, Jawaharlal Nehru University, New Delhi-110067	Synergistic Antimicrobial treatment by amino acid & peptide conjugated copper oxide nanoparticles.
P-243	**Vishal Jyoti Roy**	Indian Institute of Technology, Delhi	Tetrel-bonding Interaction in Action: C-N Activation Approach Towards the Synthesis of Unsymmetric Tertiary Amines and α-Amino Carbonyl Derivatives
P-244	**Vishali Pathania**	Department of Chemistry, Indian Institute of Technology Delhi, New Delhi, 110016, India.	Unveiling Phenalenyl as a Potent Photoreductant: Enabling Access to the Reductive Functionalization of Aryl Halides through Visible Light-Induced Electron Transfer Processes
P-245	**Vishnu K. Omanakutta N**	Chemical Sciences and Technology Division, CSIR-NIIST,	Palladium Catalyzed Desymmetrization of Diazabicylic Olefins with 4-Halo-1,3-dicarbonyl compounds: Accessing

		Thiruvananthapuram-695019, India.	3(2H)-Furanone Appended Cyclopentenes
P-246	**Vishwajit Chavda**	Applied Chemistry Department, The Maharaja Sayajirao University of Baroda, Vadodara	GO Driven Fluorescence Modulation of Rhodamine B in Aquoline: A Water-Based Deep Eutectic Solvent
P-247	**Writakshi Mandal**	Department of Chemistry, Indian Institute of Science Education and Research (IISER) Pune	Unfolding the Impact of Diverse Morphology of Ionic Porous Organic Polymer with Mechanistic Investigation on the Rapid and Selective Sequestration of Toxic Pollutants from Water
P-248	**Yogita Arya**	Department of Chemistry, Indian Institute of Technology Bombay, Powai, Mumbai, 400076	Redox Non-Innocence Behavior of Hinge-like Deprotonated Bis-lawsone on Ruthenium and Osmium Platforms
P-249	**Parul Mittal**	Division of Cyclotron and Radiopharmaceutical Sciences, Institute of Nuclear Medicine and Allied Sciences, Delhi	Intranasal delivery using Acetylcholinesterase Targeted Micellar nanocarrier for C-site Directed Designer Oximes for Reversible Reactivation
P-250	**Manoj Chahal**	Hindu College, University of Delhi	Binding enabled catalytic activation of SO2 by copper koneramine complexes under ambient conditions
P-251	**Dr. Soumabha Bag**	Assistant Professor, Department of Industrial Chemistry, School of Physical Sciences, Mizoram University, Aizawl, Mizoram, India	Synthesis, Characterization, and Applications of Nanoglass
P-252	**J. Shakina**	Department of Chemistry and Research Centre, Sarah Tucker College (Autonomous), Affiliated to Manonmaniam Sundaranar University, Tamil Nādu, India	Development of Novel Triazine-based Chemosensor for Cu(II) detection and DNA binding Studies.
P-253	**Premlata Kumari**	Department of Chemistry, Sardar Vallabhbhai National Institute of Technology, Surat, Gujarat	Design, Synthesis, and in silico Study of New Coumarin-Piperazine Hybrids as Potential Antibacterial and Anticancer Agents

P-254	**Sasanka Deka**	Department of Chemistry, University of Delhi, North Campus, Delhi-110007, India	Robust and promising hydrogen and oxygen evolution reaction by nanostructured bifunctional FeCoPd alloy electrocatalyst
P-255	**S. Mula**	Homi Bhabha National Institute, Anushakti Nagar, Mumbai 400094, India.	Design and Synthesis of BODIPY Helicenes as Heavy-Atom-Free Triplet Photosensitizers for Photodynamic Therapy of Cancer
P-256	**Akshi Tyagi**	Department of Chemistry, Indian Institute of Technology Delhi, New Delhi, India.	Understanding Cyclic(alkyl)(amino)carbene-Copper Complex Catalysed N-H and O-H Bond Addition to Electron Deficient Olefin
P-257	**Jyoti Dalal**	School of Physical Sciences, Jawaharlal Nehru University, New Delhi	In-silico Drug Design and Discovery using MMP (Matrix Metalloproteinases)
P-258	**Manisha Patni**	Department of Chemistry, IIS (Deemed to be University), Jaipur	Theoretical investigation of Donor-Acceptor behaviour of Nitrogen containing Heterocycles
P-259	**Nutan Sharma**	Department of Chemistry, Faculty of Science, SGT University, Gurugram-122505	Synthesis of Biologically Important sulphonamide Linked Trifluoromethylated Pyrazoles
P-260	**Raakhi Gupta**	IIS (deemed to be University), Jaipur 302020, India	Reaction of imidazo[1,2-a]pyridines with acetylenic esters: Formation of new cross-conjugated mesomeric betaines.
P-261	**Biswajit Saha**	Amity Institute of Biotechnology, Amity University, Noida Sector 125	An Atom economical Approach Metal-free C-5 Chalcogenation of 8-Aminoquinolines: under Mild Conditions
P-262	**Rashmi Prakash**	aDepartment of Chemistry, Indian Institute of Technology Delhi, Hauz Khas, New Delhi, 110016, India.	Electricity Induced Rhodium-Catalyzed Oxidative C–H/N–H Annulation of Alkynes with Dihydrophthalazinediones

P-1: Cross-Coupling and Oxidation Reactions Mediated by the Visible Light

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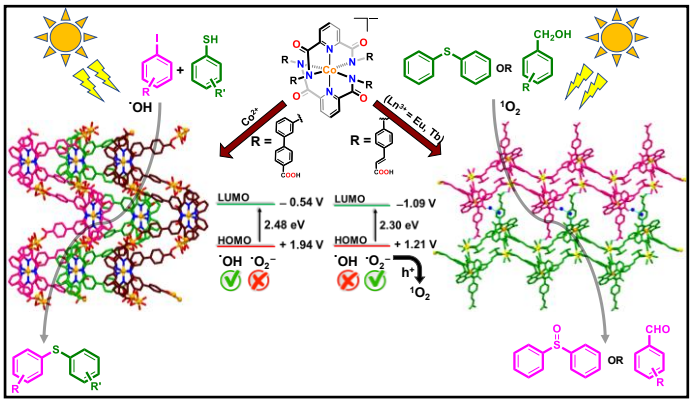

Metal-organic frameworks (MOFs) offer noteworthy structural properties including large surface area, high porosity and pore-size tunability.[1] In order to optimize the structural control of the resultant materials, metalloligand-based approach has been developed for the synthesis of various MOFs.[2] A special class of MOFs has the ability to acts as the notable photocatalysts due to their semiconductor nature. Our research group has developed a variety of MOFs utilizing a number of metalloligands.[1,2] Such metalloligand-based MOFs have been found to absorb light in the visible region, thus, allowing them to separate electrons (e^-) and holes (h^+). This charge separation allows the generation of reactive oxygen species (ROS) such as hydroxyl radical (·OH), superoxide radical ($\cdot O_2^-$) and singlet oxygen ($^1O_2$) depending on the band gap energy of the resultant MOFs. Such material can catalyze a range of photocatalytic reactions depending on the nature of ROS. In this work, we present the synthesis and characterization of various MOFs and their application in assorted photocatalytic reactions based on the generated ROS.[3]

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P-2: ICT efficient "turn-on" fluorescent probe for selective Al^{3+} and HSO_4^- ions: Real-time application in water samples and molecular keypad lock

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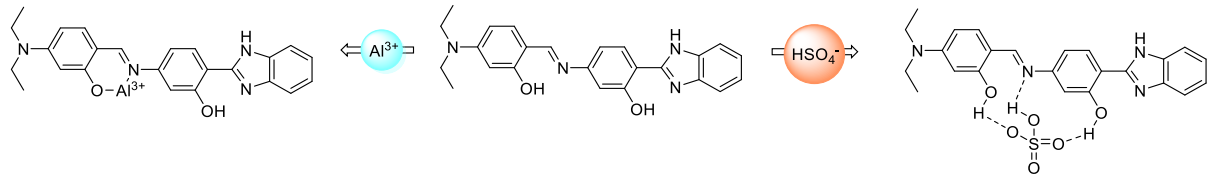

The photophysical characteristics of compounds can significantly vary as a result of the intramolecular proton transfer phenomenon [1-3]. The ESIPT compounds have been recognized with optoelectronic applications, such as laser dyes and OLEDs, molecular switches, fluorescence sensors, and so on, because of the distinctions between the two tautomeric structures in the excited state [4-7]. We designed and synthesized a Schiff base probe **1** with N,N-Diethylamino salicyladehyde group to check the effect of electron donor group. Probe **1** contains two ESIPT sites, one with imine bond (-C=N-) and hydroxyl group (-OH) and the other with benzimidazole and hydroxyl group. Probe **1** showed absorption peak at 325 nm and the emission peak at 435 nm with large stokes shift of 110 nm, which was originated from ESIPT phenomenon. The geometrical parameters and FTIR analysis favor the ESIPT process whereas potential energy curves (PECs and frontier molecular orbital analysis suggested intramolecular charge transfer (ICT) process. Probe **1** can act as donor for Al^{3+} ions and can also detect HSO_4^- ions through hydrogen bonding selectively with very low detection limit up to 39 nM and 23 nM respectively in the aqueous solution. Also, it can be used for the detection of Al^{3+} and HSO_4^- ions in real field water samples and can be used as molecular keypad lock.

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P-3: Regioselective Direct C-H Phosphorylation of Benzofulvenes

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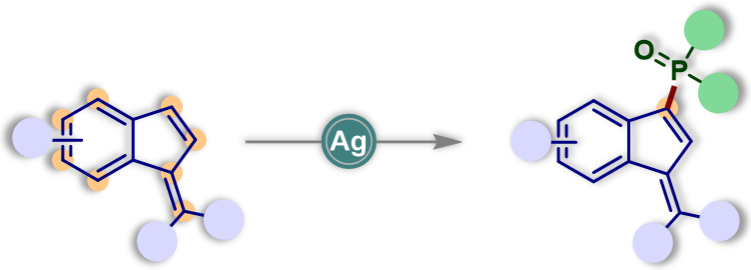

- *Regioselective Benzofulvene Phosphorylation*
- *31 examples*
- *Reversal of Polarity*
- *Excellent post synthetic applications*

A practical and straightforward protocol to access direct regioselective phosphorylation of benzofulvenes through cross-dehydrogenative coupling, employing silver salt as a promoter, is described here. Remarkably, this protocol provides a broad, structurally diverse novel phosphorylated benzofulvene. Initial mechanistic studies shed light on its radical coupling nature and reveal an avenue for oxidative coupling of two nucleophilic moieties.

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P-4: Synthesis and structural features of Alkaline earth metal phosphite-/phosphonate- complexes.

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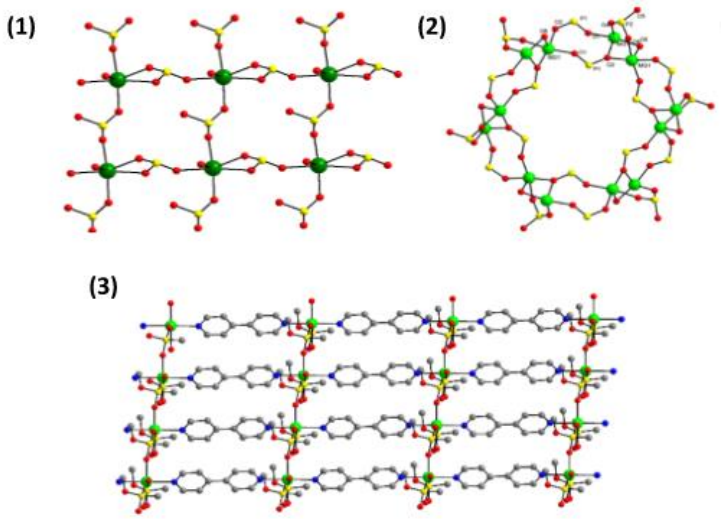

Figure 1. A perspective view of **(1)** $[Ca(HPO_3)_{0.5}H_2O]_n$. **(2)** $[Mg\{OP(O)(OH)H\}_2]\cdot H_2O$ **(3)** $[Mg\{OP(O)(OMe)Me\}_2(4,4'\text{-bipy})(H_2O)]$**.**

The anions derived from phosphite-/phosphonate esters, $RP(O)(OR)_2$ (R = H, alkyl or aryl) has been well recognized in coordination chemistry.[1] While the dianions, $[RPO_3]^{2-}$ has featured quite prominently, role of monoanions, $[RP(O)(OR)O]^-$ in the synthesis of metal organic frameworks is relative less explored. The study unfolds the synthesis of Mg(II) and Ca(II) based coordination frameworks, $[Ca(HPO_3)_{0.5}H_2O]_n$**(1)**., $[Mg\{OP(O)(OH)H\}_2]\cdot H_2O$**(2),** $[Mg\{OP(O)(OMe)Me\}_2(4,4'\text{-bipy})(H_2O)]$**(3),** by following solvo-/hydrothermal approach. X ray crystallographic studies reveal variable coordination modes of the ligands to assist two-/three dimensional frameworks with exquisite topologies.

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P-5: Mitochondria Targeted Heterobimetallic Iridium(III)-Platinum(IV) Conjugate as Potent Anticancer Theranostic Agent

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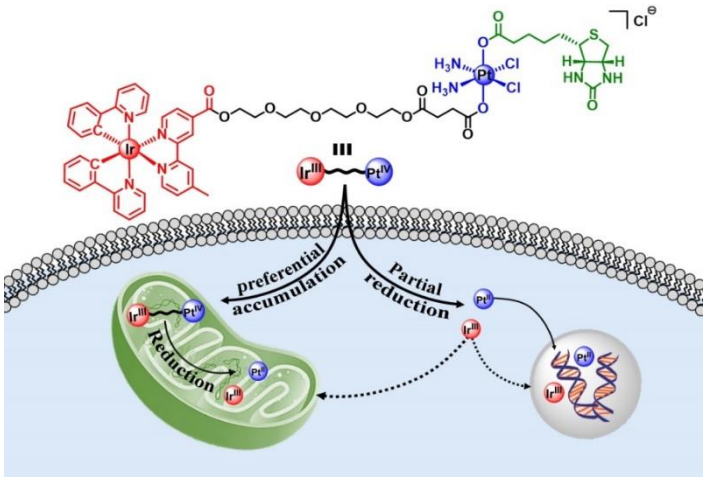

Pt(IV) prodrugs have emerged as a promising alternative to classical Pt(II) drugs such as cisplatin and its derivatives due to better selectivity, reduce side effects and overcome chemoresistance.[1,2] Recently, cyclometalated Ir(III) complexes have gained immense interest as potential chemotherapeutics because of their mitochondria targeting capabilities combining with theranostic properties.[3] In this work, we have reported **IriPlatin**, the first example of heterobimetallic Ir(III)-Pt(IV) conjugate as a multifunctional potent anticancer theranostic agent. The conjugate comprises of a Pt(IV)-prodrug as a chemotherapeutic agent, an Ir(III) complex as a mitochondria-targeting anticancer theranostic agent, and a biotin ligand as a cancer-cell targeting moiety. The conjugate preferentially accumulates within mitochondria of cancer cells and subsequently Pt(IV) is reduced to Pt(II) species that concomitantly releases both Ir(III) complex and biotin from its axial sites. The **IriPlatin** conjugate demonstrates potent cytotoxicity in the low nanomolar range in various 2D monolayer cancer cells including the drug-resistant cells and 3D multicellular tumor spheroids.

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P-6: Catalytic Methylene Insertion between Amines and Terminal Alkynes via C–N Bond Cleavage of *N, N*-Dimethylacetamide: A Unique Access to Propargylic Amines

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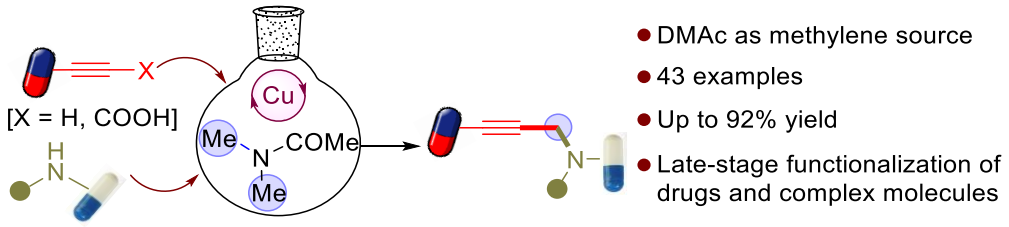

The selective installation of a C-1 unit, specifically methyl/methylene group, within an organic scaffold *via* the cleavage of a C–N bond holds paramount significance, given the predominance of alkylamines and *N*-alkylamides in natural and synthetic compounds.[1] In general, the high dissociation energy of C_{alkyl}–N bonds and stability of inactivated amines and amides make the C–N bond cleavage process inherently challenging.[2] A literature survey indicates that the C_{methyl}–N bond of *N,N*-dimethylformamide (DMF) is cleaved by a transition metal catalyst or an organocatalyst to give a C-1 unit in methylene insertion reactions.[3] It is also reported that a methylene group can be inserted between an amine and a stronger nucleophile, e.g. C≡N substituent, via the copper catalyzed cleavage of C_{methyl}–N bond of DMF and a subsequent formation of C–N bond with an amine leading to cyanomethylated amines.[3d] However, an analogous methylene insertion process between an amine and a milder nucleophile, such as terminal alkyne or its equivalent, i.e. a "C≡C" counterpart, has remained elusive. Herein, we present a copper catalyzed methylene insertion between an amine and a milder nucleophile, including a terminal alkyne counterpart, *via* C–N bond cleavage of *N,N*-dimethylacetamide.[4] The method gives an expedient access to propargylic amines in good to excellent yields.

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P-7: Study of Structural Profiles of Multi-target Binding of Cytotoxic Alkaloid Vinblastine

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Structural information about drug-receptor interactions has a critical role in drug discovery and further optimization processes, as the drugs can bind to multiple potential targets due to the presence of various functional moieties in their structures. Advanced computational tools are being used increasingly as powerful for prediction of ligand-receptor interaction events in modern drug discovery approach. Knowledge about such interactions offers possibilities for repurposing and developing potent inhibitors of disease pathways. Vinblastine (VLB) is a potent anticancer molecule known to show multiple receptor interactions with different affinities and degrees of structural perturbations. We have investigated the interaction profile of VLB with DNA and human serum albumin (HSA) using extensive experimental spectroscopic, computational quantum mechanical methods and molecular dynamics simulations in a dynamic physiological environment to evaluate the structural features, mode of binding, ligand/receptor flexibility, and energetics of complexation. Results obtained confirm that VLB prefers to bind in the major groove of DNA with some inclination toward Thymidine residue and the TR-5 binding site in HSA with its catharanthine half making important contacts with receptor sites. Conformational diversity of the VLB is observed on binding with multiple receptors. Spectroscopic investigation at different temperatures indicates that VLB binding is entropy driven representing the interaction in major groove and TR-5 binding site which is facilitated by sufficient number of vander Waals contacts and conventional H-bonds.

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P-8: One-pot Multiple C-C bond Formation *via* Pd(II)-Catalyzed reaction: En route Synthesis of Succinimide-fused Dihydrophenanthrenes

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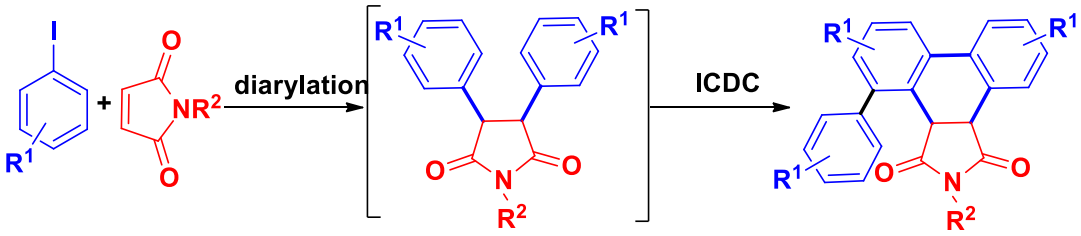

Phenanthrenes and its derivatives belong to an important class of organic compounds due to their ubiquitous presence as core structural motifs in biologically active compounds and natural products. Indeed, they also serve as a common structural scaffold in materials science-based industry owing to their high photochemical, and electroluminescent properties. On the other side, maleimide derivatives have also attracted considerable attention due to their potential application in the pharmaceutical industry and extraordinary electronic properties make venerable precursors for smart materials and are broadly used as coupling partners in C-H activation reaction for the synthesis of nitrogen-containing polyheterocyclic compounds. With these understanding and continuation of our research interest in the development of a new synthetic protocol for the synthesis of functionalized organic molecules from readily available starting materials. Herein, we report an efficient and straightforward strategy for the synthesis of succinimide-fused-unsymmetrical 9,10-dihydrophenanthrenes from aryl iodides and maleimides *via* Pd(II)-catalyzed three-fold C-H activation in one-pot fashion. Overall, 4-carbon-carbon bonds have been constructed under the optimized conditions and developed method eventually satisfy the parameters of sustainable chemistry.

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P-9: Polymer supported dioxidovanadium(V) complex based heterogeneous catalyst for the multicomponent Biginelli reaction producing biologically active 3,4-dihydropyrimidin-2-(1H)-ones

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Dioxidovanadium(V) complex [$V^{V}O_2$(sal-aebmz)] (**1**) (where Hsal-aebmz = Schiff base derived from the condensation of salicylaldehyde and 2-aminoethylbenzimidazole) has been immobilized on chloromethylated polystyrene (PS-Cl) cross-linked with divinylbenzene to obtain [$V^{V}O_2$(aebmz-sal)]@PS (**2**), a heterogeneous complex. Both complexes, after characterization, have been used as catalysts to explore a single pot multicomponent (benzaldehyde or its derivatives, urea and ethyl acetoacetate) Biginelli reaction producing biologically active 3,4-dihydropyrimidine (DHMP) based biomolecules under solvent-free conditions in the presence of H_2O_2 as a green oxidant. Various reaction conditions like amounts of catalyst and oxidant, temperature, time and solvent have been optimized to obtain maximum yield of DHMPs. The polymer immobilized complex has been found to show excellent catalytic activity, giving more than 90% yield of DHMPs under optimized reaction conditions selectively.

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P-10: Regioselective Synthesis of meso-tetraaryl Bromo[14]Triphyrins(2.1.1) and Their Structural, Spectral and Redox Properties

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meso-Tetraaryl [14]triphyrin(2.1.1) was subjected to stepwise regioselective bromination to investigate the effect of bromination on structural, spectral, photophysical and redox properties. Triphyrin(2.1.1) **1** was treated with appropriate equivalents of N-bromosuccinimide (NBS) at ambient temperatures to synthesize a series of b-monobromo to b-hexabromo triphyrins(2.1.1) **2**-**7** in good yields. The regiochemistry of bromines in these bromotriphyrins(2.1.1) was confirmed by X-ray crystallography. The X-ray crystallographic analysis showed that the effect of stepwise bromination of triphyrin(2.1.1) on structural framework was prominent in case of hexabromotriphyrin(2.1.1) **7** compared to other bromotryphyrins(2.1.1). The absorption spectroscopy showed that the substitution of bromines at b-pyrrole carbons of triphyrin(2.1.1) resulted in bathochromic shifts of absorption bands relative to triphyrin(2.1.1). Also, hexabromotriphyrin(2.1.1) showed absorption bands at longer wavelengths. The electrochemical studies showed that the bromo derivatives **2**-**7** were easier to reduce compared with triphyrin(2.1.1) and the first reduction potential wave shifted anodically with increase in number of bromines at b-pyrrole carbons of triphyrin(2.1.1) from one to six. These were also predicted by Density functional theory (DFT) calculations were carried out to predict these structural, spectral and electrochemical properties and the analysis was consistent with the experimental observations.

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P-11: Ruthenium-Catalyzed Oxidative Cross-Coupling Reaction of Activated Olefins with Vinyl Boronates for the Synthesis of (*E*,*E*)-1,3-Dienes

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An oxidative cross-coupling reaction between activated olefins and vinyl boronate derivatives has been developed for the highly stereoselective construction of synthetically useful (E, E)-1,3-dienes. The highlight of this reaction is that exclusive stereoselectivity (only E, E-isomer) was achieved from a base-free, ligand-free, and mild catalytic condition with a less expensive $[RuCl_2(p\text{-cymene})]_2$ catalyst.

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P-12: Nickel (II) borohydride catalyst for Hydrodehalogenation reactions for Chlorinated pollutant

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Persistent organic pollutants *(POP*s) are classified as chemical substances that persist in the environment, bioaccumulation through the food web, and possess a direct risk to human health.[1] Dichlorodiphenyltrichloroethane (DDT) is a highly persistent organic and toxic chlorinated pesticide.[2] Transition Metal borohydrides have been used for various chemical transformations, here we used reductive dehalogenation of organic halides.[3-4] The pyridophane based macrocyclic N4 ligand and their nickel(II)-complexes, $[L(Ni)Cl_2]$ and $[L(Ni(CH_3CN)_2](BPh_4)_2]$ were synthesized and their solid state structure were confirmed by single crystal X-ray diffraction studies. The nickel(II)-borohydride chelate$[L(Ni)(\eta^2\text{-}BH_4)]^+$ was obtained mechanochemically by using sodium borohydride with nickel(II) complex in open air, it was characterized using FT-IR Spectroscopy and powder X-ray diffraction techniques. This reactive nickel(II) borohydride was further examined for degradation of certain environmentally chlorinated pollutant, such as carbon tetrachloride and DDT.

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4 Raje S.; Angamuthu, R. *Green Chem.*, **2019**, *21*, 2752–2758.

P-13: Structural Elaboration of *Xanthine* and its evaluation as potent agrochemicals

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Xanthine (3,7-dihydropurine-2,6-dione) and its derivatives are the prominent N-heterocyclic bioisosteres due to their inherent versatility. These have been identified as true keystones in pharmaceutical and agricultural industry and act as the perfect scaffold for design and development of promising plant growth regulators, herbicides, fungicides and antibacterial agents *etc*. Structural elaboration of xanthine at N-3 and N-7 poisitions was carried out by using alkylating agents and all the synthesized derivatives were characterized through various spectral techniques. Xanthine and its derivatives were evaluated as antinemic agents against root-knot nematode, *Meloidogyne incognita*, which is a major class of plant-parasitic nematodes causing damage and high yield losses in crop producing countries. The biological screening of compounds were identified them as true drugs with remarkable activity and selectivity. Further, the compounds were subjected to *in silico* studies for structure activity relationship studies. Results showed that the maximum inhibition/killing of nematodes is due to the inhibition of the major acetyl choline esterase enzyme.

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P-14: Understanding Structural Changes During Salt-induced Ovalbumin Amyloid Aggregation

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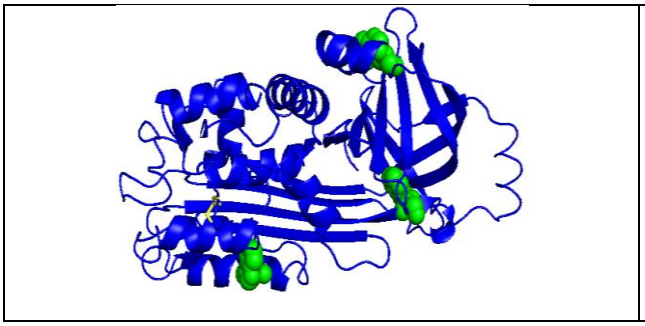

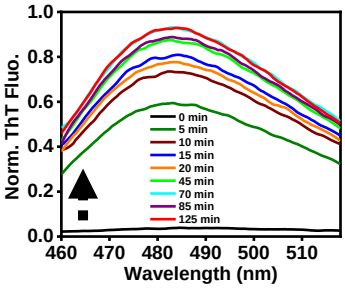

Protein conformational disorders leading to the formation of nanoscopic, ordered, cross β-sheet-rich amyloid aggregates are associated with various neurodegenerative diseases, namely, Alzheimer's disease, Parkinson's disease, prion diseases as well as localized and systemic amyloidosis. It has been demonstrated that the aggregation kinetics and the nanoscopic morphology of the amyloid fibrils are influenced by changes in solution pH, ionic strength, and temperature. However, systematic studies on effect of variable ionic strength on protein aggregation kinetics coupled with the protein structural changes during the course of self-assembly remains limited. In this work, I will describe our recent efforts in elucidating the structural changes during salt-induced ovalbumin amyloid aggregation as a function of variable ionic strength using fluorescence and Raman spectroscopy, dynamic light scattering, and transmission electron microscopy. We observed that solution ionic strength greatly affects the aggregation kinetics whereby electrostatic charge screening and hydrophobic interactions exhibit opposing effects that in turn, govern the fibril morphologies. Additionally, we gained molecular insights into protein structural changes in a residue-specific manner during salt-induced ovalbumin aggregation.

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P-15: Sustainable Oxidation of Sulfides with Peroxide Catalysed by Efficient & Reusable Transition Metal Based Preyssler System

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Polyoxometalates functionalized with transition metals are the focus of modern materials produce structurally varied metal clusters with a wide range of dimen-sionality and potential application.1-3 Especially, metal-oxo compounds have gained considerable interest in catalysis in organic chemistry. In this work, we report the synthesis of a series of metal oxide clusters composed of redox active Preyssler anion [NaP5W30O110]14- , linked by different transition metals ions (M= Cu, Co, Ni, Zn)2+. These hybrids have been successfully synthesized and well-characterized by different characterization techniques like single crystal X-ray diffraction, TGA analysis and powder X-ray diffraction, electrochemical analysis, spectroscopy (UV-Vis, FTIR). Importantly, the excellent heterogenous catalytic activity of these hybrids has been demonstrated by the atom efficient and selective oxidation of sulfides to sulfoxides and sulfones with hydrogen peroxide as an oxidant. The reaction yield and selectivity were crucially affected by different reaction time and temperature. The progress of the reaction was monitored by gas chromatography and 1H NMR spectroscopy. All the four hybrids catalysts exhibited good recyclability and reusability in consecutive reaction cycles without significant loss of catalytical activity or selectivity.

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P-16: Study of Inorganic flame retardants for leather applications.

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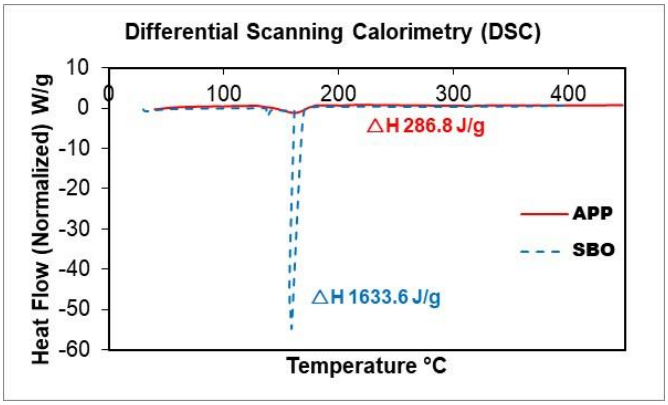

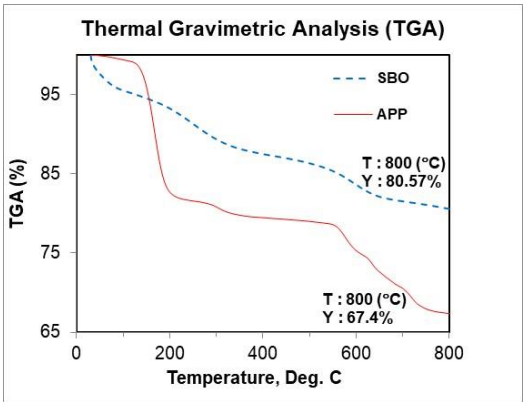

Flame Retardants (FR) are chemicals that are added to the materials to slow down the spread of fire in case of fire accidents. Halogenated, organophosphorus-based, nitrogen phosphorus-based, inorganic metal oxides/hydroxides, and composites of two or more FR chemicals are the general FR chemicals available in today's market. Leathers are natural fiber materials widely used in protective garments, fashion garments, footwear, handbags, upholstery, etc., Antimony pentoxide-Sb_2O_5(SBO), a metal oxide-based flame retardant, and ammonium polyphosphate (APP), a nitrogen-phosphorus-based inorganic flame retardant, were taken as the FR chemicals of interest and examined in detail. The selected FR chemicals were characterized by FESEM, XRD, and FT-IR. The thermal properties were studied by TGA and DSC. The flame retardant behaviour of the selected FR chemicals was tested by applying 3% of SBO/APP to leathers during the post-tanning operation and the standard leather making process was followed. The SBO/APP-treated leathers were characterized by FTIR-ATR, TGA, and DSC. The Horizontal Flame retardancy test (ISO 17074) was conducted to assess the flame-off time, smoke-off time, percentage weight loss, and flammability degree of the SBO/APP-treated leathers. SBO improved the flammability degree of leather by 13%, whereas APP improved the flammability degree of leather by 4%. The present study revealed the suitability of SBO over APP for leather application.

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P-17: Radiosensitizing role of Pixantrone in KRAS mutated cancer cells via suppression of radiation induced pro-survival pathways

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Radiation therapy is a primary treatment modality for multiple cancer types (1). However, the emergence of radioresistance against radiation therapy has raised the need for radiosensitizing drugs. KRAS mutations drives radioresistance in cancer cells. Oncogenic KRAS mutations are the single most common mutations reported in multiple cancer types (2). The present study has demonstrated the sensitization of tumor cells against radiotherapy via inhibition of KRAS activation. Using a drug repurposing approach, the *in-silico* screening identified pixantrone, an antineoplastic drug, possesses a high affinity towards KRAS mutant subtypes: G12C and G12D. Surface plasmon resonance study indicated maximum affinity of pixantrone with KRAS G12C>WT>G12D and G12S. Stable transfectants of KRAS G12C and G12D are potentially radiosensitized after pixantrone treatment. Pixantrone along with radiation causes increased dsDNA breaks, ATM expression, and late apoptosis. *In vivo* studies on NCr- fox1^{nu} xenograft mice proves inhibition of tumor growth and prolonged survival of animal after pixantrone treatment. The combination treatment of pixantrone and radiation also downregulated the effector proteins of RAS downstream pathways such as, PI3K/Akt/mTOR and MAPK pathways. Senescence marker; p21 was potentially upregulated in tumor cells after combination treatment. These findings indicate a correlation between KRAS mutation, RAS signalling, pixantrone treatment and radiation conferring cancer cell death.

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P-18: Intrinsic Lability of $NiMoO_4$ to Excel the Oxygen Evolution Reaction

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Nickel-based bimetallic oxides such as $NiMoO_4$ and $NiWO_4$, when deposited on the electrode substrate, show remarkable activity toward the electrocatalytic oxygen evolution reaction (OER). The stability of such nanostructures is nevertheless speculative, and catalytically active species have been less explored. Herein, $NiMoO_4$ nanorods and $NiWO_4$ nanoparticles are prepared via a solvothermal route and deposited on nickel foam (NF) ($NiMoO_4$/NF and $NiWO_4$/NF). After ensuring the chemical and structural integrity of the catalysts on electrodes, an OER study has been performed in the alkaline medium. After a few cyclic voltammetry (CV) cycles within the potential window of 1.0−1.9 V (vs reversible hydrogen electrode (RHE)), ex situ Raman analysis of the electrodes infers the formation of $NiO(OH)_{ED}$ (ED: electrochemically derived) from $NiMoO_4$ precatalyst, while $NiWO_4$ remains stable. A controlled study, stirring of $NiMoO_4$/NF in 1 M KOH without applied potential, confirms that $NiMoO_4$ hydrolyzes to the isolable NiO, which under a potential bias converts into $NiO(OH)_{ED}$. Perhaps the more ionic character of the Ni−O−Mo bond in the $NiMoO_4$ compared to the Ni−O−W bond in $NiWO_4$ causes the transformation of $NiMoO_4$ into $NiO(OH)_{ED}$. A comparison of the OER performance of electrochemically derived $NiO(OH)_{ED}$, $NiWO_4$, ex-situ-prepared $Ni(OH)_2$, and NiO(OH) confirmed that in-situ-prepared $NiO(OH)_{ED}$ remained superior with a substantial potential of 238 (±6) mV at 20 mA cm^{-2}. The notable electrochemical performance of $NiO(OH)_{ED}$ can be attributed to its low Tafel slope value (26 mV dec^{-1}), high double-layer capacitance (C_{dl}, 1.21 mF cm^{-2}), and a low charge-transfer resistance (Rct, 1.76 Ω). The $NiO(OH)_{ED}$/NF can further be fabricated as a durable OER anode to deliver a high current density of 25−100 mA cm^{-2}. Post-characterization of the anode proves the structural integrity of $NiO(OH)_{ED}$ even after 12 h of chronoamperometry at 1.595 V (vs reversible hydrogen electrode (RHE)). The $NiO(OH)_{ED}$/NF can be a compatible anode to construct an overall water splitting (OWS) electrolyzer that can operate at a cell potential of 1.64 V to reach a current density of 10 mA cm^{-2}. This work understandably demonstrates monoclinic $NiMoO_4$ to be an inherently unstable electro(pre)catalyst, and its structural evolution to polycrystalline $NiO(OH)_{ED}$ succeeding the NiO phase is intrinsic to its superior activity.

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P-19: Catalyst Switchable Divergent Synthesis of Bis(indolyl)alkanes and 3-Alkylated Indoles from Styrene Oxides

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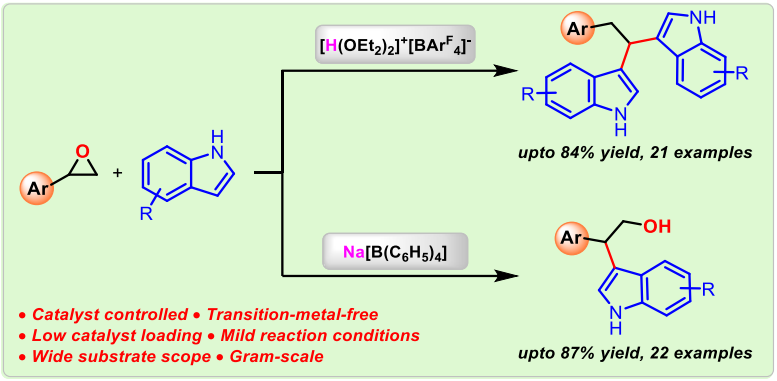

A novel and effective Brønsted acid-catalyzed chemoselective synthesis of bis(indolyl)alkanes and 3-alkyl indoles are reported. The selectivity of two significant indole derivatives is attained by allowing the same substrates to go through divergent reaction routes catalyzed by different catalysts. Furthermore, a wide range of bis(indolyl)alkanes and 3-alkyl indoles were afforded in moderate to good yields, demonstrating good substrate universality. It was concluded from control experiments and *in-situ* IR study that in the presence of Brookhart's acid, the phenyl oxirane rearranged to phenylacetaldehyde as an intermediate. Moreover, the bisindoylation reaction occurs promptly at room temperature. This reaction was found to be scalable with good efficiency.

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P-20: Experimental and Computational Studies on Cinchona Anchored Calixarene Catalysed Asymmetric Michael Addition Reaction

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Calixarene supramolecular catalysis has drawn incredible interest in the last two decades.[1] Calixarenes are considered an ideal scaffold due to their rigid shape with ease of functionalization. The synthetic flexibility of calixarenes makes them suitable candidates for a wide range of applications, including molecular recognition, sensors, catalysis, drug delivery, and separation science.[2] Interestingly, their hydrogen bond donating and noncovalent interaction ability make them active organocatalysis.[3] Upon chiral functionalization, the calixarene scaffold could serve as asymmetric organocatalysts for organic transformations. The current poster presentation will show lower-rim Cinchona anchored calix[4]arene cationic catalysts for asymmetric Michael addition of acetylacetone to β-nitrostyrenes with excellent yield (~99%) and enantioselectivity (>99% ee) for variety of Michael adduct[4] . Density functional theory investigations are carried out to understand catalyst-substrate interaction and energetics for high enantioselectivities.

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P-21: Fabrication of Molecularly Imprinted Polymer based Electrochemical Sensor for Gut Microbiota Derived Metabolites Detection

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The gut microbiota, a diverse microbial community found within the intestine of humans has a dynamic ecology [1]. It has been found that some gut microbiota-derived metabolites (GMDM) such as trimethyl amine N-Oxide (TMAO), trimethyl amine (TMA), indoxyl sulphate, polyamines, H_2S, etc. shown to have an adverse effect on the human health [2]. Therefore, it causes chronic or acute diseases such as colorectal cancer (CRC), cardiovascular disease, chronic kidney disease (CKD), hypertension, autism, etc. [2]. When the exogenous/endogenous compounds complete their metabolic pathways, these metabolites are released either in the form of the main component of the process or as a by-product. Therefore, GMDM detection are important for the prognosis, treatment, and prevention of chronic or acute diseases. Conventional techniques such as Liquid Chromatography-Mass Spectrometry (LC-MS), High-Performance Liquid Chromatography (HPLC), etc. are available for their detection in human body fluids [3]. However, these techniques are time-consuming, expensive, and have a low detection threshold. Among the presence of other detection techniques, electrochemical sensors have demonstrated remarkable potential for the detection due to their high sensitivity, specificity, broad range of detection, quick response, and low detection limit (LOD). Fabricated electrochemical sensors particularly for GMDM detection without using any antigen-antibody has found to be highly specific by the molecularly imprinted polymer (MIP) technique [4]. MIP acts as an artificial receptor which are highly specific towards the analyte due to their spatial arrangements and lock-key mechanism. MIPs are synthesized using a functional monomer, a cross-linker, and a desired template by chemical polymerization process. In the present work, MIP has been synthesized by polydopamine as polymer matrix and immobilized onto the paper-based screen-printed carbon electrode (SPCE) and characterized by Fourier Transform Infrared Spectroscopy (FT-IR) and Scanning Electron Microscopy (SEM) techniques. The fabricated MIP/SPCE has been used for the GMDM detection in the wide range of concentrations from 0.1 ng/mL to 300 ng/mL with LOD of 0.018 ng/mL. Such MIP-based electrochemical sensors can be utilized for further detection of small molecules or analytes to resolve the issues related to disease diagnosis.

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P-22: Study of Organophosphorous Acid Coordinated Assemblies with Ethylene and Azo Bridging Ligands

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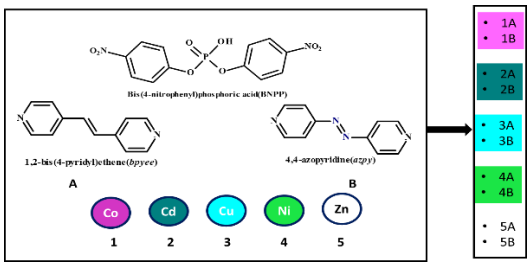

Coordination polymers are well studied in the recent literature, especially the ensembles having porosity (Metal-Organic Framework Structures), in particular, using the organic building blocks having –COOH functional groups.[1] In the domain of organic chemistry, apart from –COOH, ligands with a variety of functional groups are documented, for example, -NO_2, -CN, -NH_2, -POOH, etc. Herein, such coordination polymers involving organophosphoric acid ligands[2] are discussed, highlighting the significance of the ligands mimicking the carboxy ligands in the formation of 1D, 2D and 3D extended network solids, with promising functionalities such as sorbents, ion-exchangers, catalysts, gas storage materials *etc*.[3] In these organophosphate ligand assemblies, bis(4-nitrophenyl)phosphoric acid, BNPP, along with isoelectronic linear spacers 1,2-bis(4-pyridyl)ethane (*bpyee*) and 4,4'-azopyridine (*azpy*) are ensembled with transition metal ions, Co(II), Cd(II), Cu(II), Ni(II) and Zn(II), as illustrated in Scheme 1. To unravel the structure-property relationship of the coordinated assemblies, the topology of the frameworks and the role of coordination geometry of metal nodes have been explored. In this process, a detailed study on a series of these network solids, mainly driven by coordinate bonds and noncovalent interactions like H-bonds (O–H···O, C–H···O, C–H···N, *etc*.), π-π interactions, have been carried out to deduce structural diversity and to assess the influence of building blocks in the self-assembly process.

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P-23: One-Pot Multi-Enzymatic Cascade Synthesis of Natural Naphthalenones via Reduction of Unactivated Alkenone

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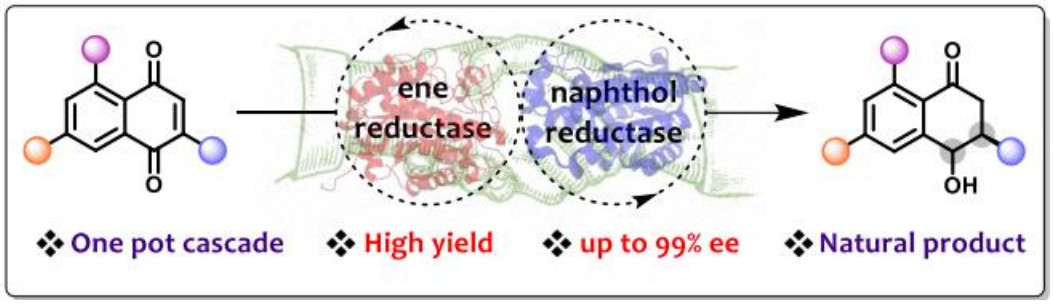

The efficient asymmetric hydrogenation of an unactivated conjugated alkene is the major challenge in synthetic chemistry. Although ene reductases (EREDs) have an ancient legacy for the asymmetric reduction of activated alkene bonds, but the reduction of unactivated C=C bond of naphthoquinones by EREDs has not been explored. [1,2] Here, we report stereoselective reduction of alkenone bond of naphthoquinone using EREDs with high turnover number. The combination of Nostoc-ER with naphthol reductase (NR) from Magnaporthe grisea in one pot enabled us to develop a multienzyme cascade for the reduction of substituted naphthoquinones to corresponding chiral alcohol containing two stereogenic centres. [3]

The one pot multienzyme cascade is being applied for the synthesis of (+)-isoshinanolone, (+)-isosclerone,(+)-shinanolone, (−)-shinanolone, teratosphaerone B and (+)-xylarenone with high yield (up to 96%) and stereoselectivity (up to >99% ee and 98:2 dr).3,4 This result exemplifies the versatility of this method and its potential for further utilization in asymmetric hydrogenation of unactivated alkenes by expanding the toolbox of currently available reductases via enzyme engineering and discovery.

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P-24: Cp*Co(III)-Catalyzed Ketone-Directed ortho-C−H Activation for the Synthesis of Indene Derivatives

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A weakly coordinating, carbonyl-assisted C−H activation of aromatic systems with α,β-unsaturated ketone and subsequent aldol condensation has been developed using a Cp*Co(CO)I_2 catalyst. The developed method is the first example of indene synthesis by cobalt catalyzed C−H activation. In addition, the reaction requires mild reaction conditions and easily accessible starting materials, and it shows excellent functional group compatibility.

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P-25: Understanding Mixed Crowding Through Enzyme Activity and Dynamics

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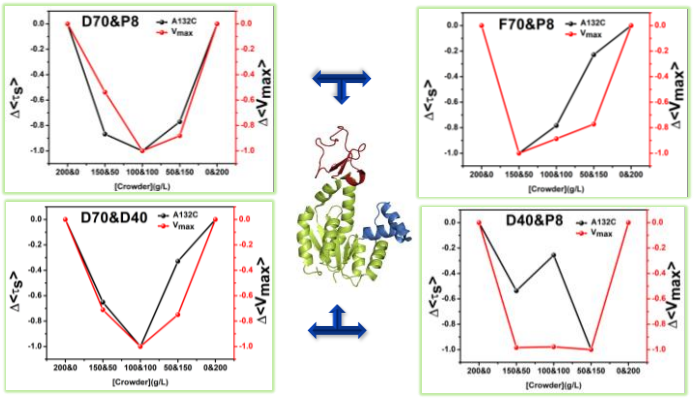

To understand the heterogeneity of the intracellular environment we have used binary mixtures of commonly used crowding agents, namely, Ficoll 70, Dextran 70, Dextran 40, and PEG 8000 and have observed their effects on the activity and dynamics of the enzyme AK3L1, an isoform of adenylate kinase.[1] Enzyme activity was carried out with the wild-type protein while for dynamics, three single mutants were made (A74C, A132C, and A209C), with the mutations spanning three strategic locations on the enzyme structure. A coumarin based solvatochromic dye was covalently ligated to the cysteine residues and solvation studies, based on time dependent Stokes shift measurements, were performed as a function of the binary crowder combinations. Analyses of the solvation and enzyme activity data, reveal that the values obtained in the mixtures (200 g/L) are lesser than that of the sum of the component crowders. The results suggest that the extent of excluded volume in the binary mixtures is reduced as compared to the individual ones with the Ficoll based mixtures showing the maximum deviation. This we have attributed to the possible segregative phase separation at the microscopic level of the individual crowders based on their incompatibility in size and structural dispositions.[2] Taken together and with further analyses, we hope to provide a comprehensive picture of the manner in which mixed crowding affect biomolecular structure and dynamics.[3]

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P-26: Visible and NIR-Light Photoactivatable o-Hydroxycinnamate System for Efficient Drug Release with Fluorescence Monitoring

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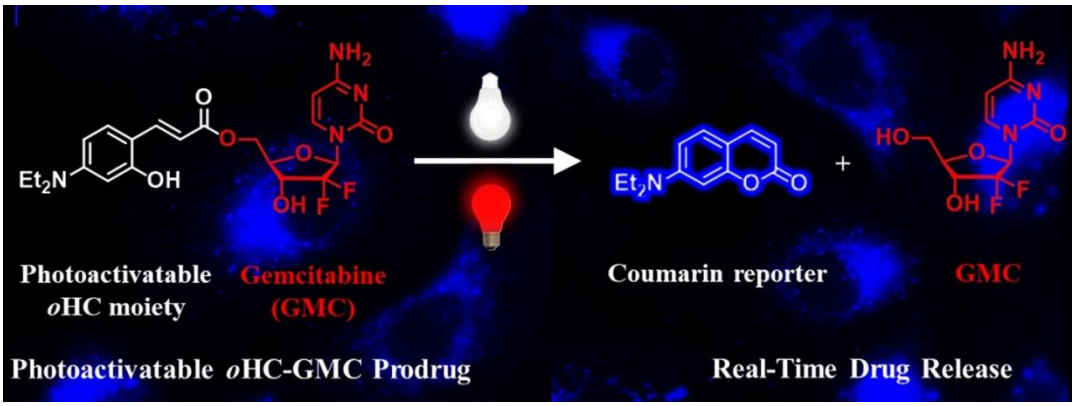

Photoactivatable protecting groups (PPGs) have become the powerful materials for controlling the activity of biologically important molecules in biomedical field.[1] However, designing PPG that can be efficiently activated by biologically benign visible and NIR light with fluorescence monitoring is still a great challenge.[2,3] Herein, we report *o*-hydroxycinnamate based PPG that can be activated both at visible (one-photon) and NIR (two-photon) light for controlled drug release with real-time monitoring. Thus, a photoremovable 7-diethylamino *o*-hydroxycinnamate group is covalently attached with an anticancer drug gemcitabine to establish a photoactivatable prodrug system. Upon excitation at visible (400-700 nm) or NIR (800 nm) light, the prodrug efficiently releases drug which is quantified by monitoring the formation of strongly fluorescent coumarin reporter. The prodrug is uptaken by the cancer cells and interestingly accumulates within mitochondria determined by FACS and fluorescence microscopy imaging. Further, the prodrug demonstrates photo-triggered temporally controlled cell death upon irradiation of both visible and NIR light. This photoactivatable system could be useful and adapted in the future for the development of advanced therapies in biomedicine.

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P-27: Ordered Macro/Microporous Ionic Organic Framework for Efficient Separation of Toxic Pollutants from Water

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In case of pollutant segregation by porous materials, fast mass diffusion is a fundamental criterion in-order to achieve improved performance. The rapid mass-transport through porous materials can be achieved by availing large open pores followed by easy and complete accessibility of functional recognition sites.[1] Inducing macroporosity into such materials could serve as ideal solution, providing access to large macropores that offer unhindered transport of analytes and full exposure to interactive sites.[2] Moreover, the challenge to configure the ionic-functionality together with macroporosity could emerge as an unparalleled avenue toward excellent environmental remediation approach, however, still not explored. Herein, we strategized a synthetic protocol for construction of a positively charged hierarchically-porous ordered, interconnected macro-structure of viologen-unit grafted organic-framework, where the size and number of macropores can easily be tuned. The ordered large macropores along with strong electrostatic interaction, synergistically demonstrated ultrafast removal efficiency toward various toxic pollutants from water.[3]

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P-28: Total Synthesis of (+)-Dihydroitomanallene B and Formal Synthesis of (–)-Kumausallene

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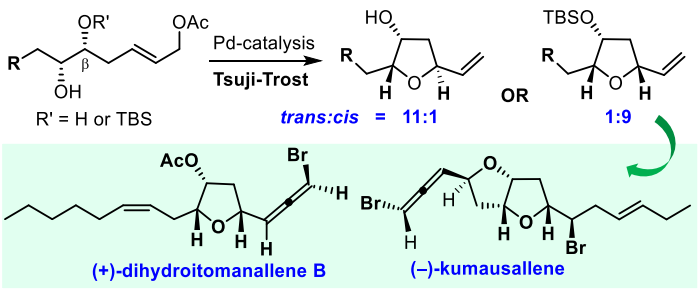

The structurally intriguing bromoallene containing natural metabolites have been reported in last few decades from various marine algae, invertebrates, plants and other organisms.[1] Extensive bio-screening of these molecules resulted in the discovery of novel antibacterial, antitumor and antiviral agents.[2] In 2012, Vairappan and coworkers[3] collected and studied six different populations of *L. nangii* from Tun Sakaran Marine Park, Sabah, Malaysia. Different halogenated non-terpene metabolites were found from these six populations and each of these showed the presence of a new bromoallene, dihydroitomanallene B along with two known molecules, itomanallene B and pannosallene. (–)-Kumausallene was first isolated by Kurosawa and his group from Japanese *Laurencia nipponica* Yamada.[4] Its structure and absolute stereochemistry is well established with a few syntheses being reported recently by different routes.[5] The first asymmetric total synthesis of (+)-dihydroitomanallene B, its two diastereomers and formal synthesis of (–)-kumausallene is reported.[6] The synthesis of former was completed in 18 steps from 1,4-butanediol (3.4% overall yield), with diastereoselective Tsuji–Trost cyclization to access *cis*-2,5-disubstituted-3-oxygenated THF scaffold and Corey–White–Posner reaction to install the bromoallene moiety as key steps. In addition, the enantioselective formal total synthesis of (–)-kumausallene involving the key Tsuji–Trost cyclization is also realized.

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P-29: Polymer functionalized zinc oxide quantum dots as a selective probe for specific detection of antibiotics

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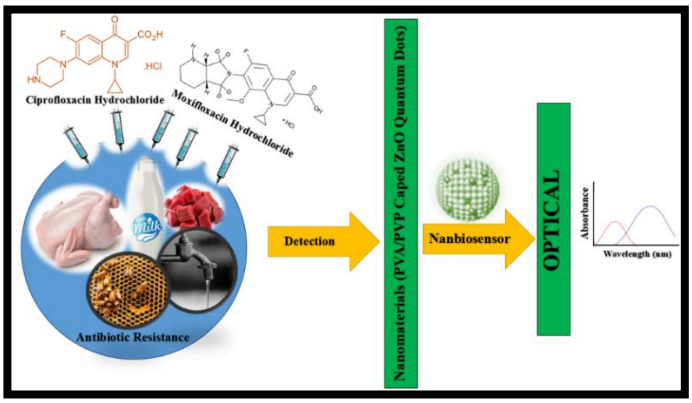

Antibiotic, a corner stone of modern medicinal industry is the drug or medicine which stops or kills the growth of microbial diseases. It is crucial to monitor the antibiotic levels in the environment like water, food products in the current scenario as the antibiotic concentration above threshold is harmful for the human health. Excess consumption of antibiotics leads to antibiotic resistance that hinders the control and cure of microbial diseases. So, these challenges motivated to devise an optical nano-bio-senor which can sense the ultra-low concentration of antibiotics. In this proposed research work, emphasis is to develop a method which is simple and selective to analyse the detection and presence of antibiotics in various samples like tape water milk etc. using fluorescent ZnO QDs based nano-sensor. For this, fluorescent and different polymers (polyvinyl alcohol – PVA and polyvinyl pyrrolidine – PVP) capped ZnO QDs were synthesized using modified sol-gel technique. These were used as fluorescent probe to monitor the presence of antibiotics. The optical characterizations of synthesized QDs were performed using UV-Visible absorption & fluorescence spectroscopic methods while structural characteristics were analysed by using Raman spectroscopy and X-Ray Diffraction spectroscopy. Charge on the synthesized QDs were obtained with the help of ZETA potential. Here ten different antibiotics were checked among, Ciprofloxacin and Moxifloxacin have shown excellent sensing and specificity with PVA-ZnO QDs and PVP-ZnO QDs respectively.

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P-30: Ligands Inspired by HDAC Inhibitors: Source for Anticancer and Antimicrobial Agents

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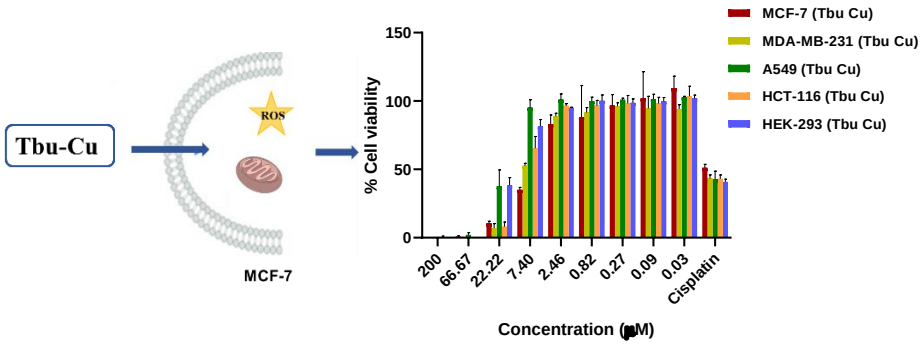

Histone deacetylase (HDAC) enzymes are a major class of molecular targets for the treatment of cancer. There are several classes of HDAC protein, out of that sirtuin is a class III NAD^+ dependent HDAC protein present in mammalian cells.[1] Sirtinol is the sirtuin inhibitor that shares characteristics of effective metal coordinating species and has been utilized in many studies aimed at establishing sirtuin as the therapeutic target for the treatment of cancer.[2] Copper ions display high redox activity that makes them highly toxic; thus, there should be strong regulation of copper ions within cells.[3] The elevated copper levels are well documented in different types of cancers viz, breast, liver, prostate, lung, and sarcoma.[4] Herein, we have designed a library of HDAC inhibitor (Sirtinol)-derived ligands and their Cu (II) complexes. All compounds were characterized by spectroscopic methods (^{1}H and ^{13}C NMR, UV−vis, IR) and electrospray ionization (ESI) mass spectrometry, while some of the ligands and their metal complexes, in addition, by X-ray crystallography. The compound Tbu and Tbu-Cu displayed high antiproliferative activity on all the above-mentioned cancer cell lines and displayed the highest cytotoxicity on the breast cancer cell line MCF-7. The generation of ROS and disruption of mitochondrial membrane potential was also observed by treating Tbu-Cu on MCF-7. The low cytotoxicity of Tbu-Cu on the primary embryonic human kidney cell line 'HEK-293' and less % hemolysis on human blood makes it a promising drug candidate for the treatment of cancer.

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P-31: A bisperylenediimide-conjugated macrocycle: Supramolecular, conformational, photophysical and electrochemical studies

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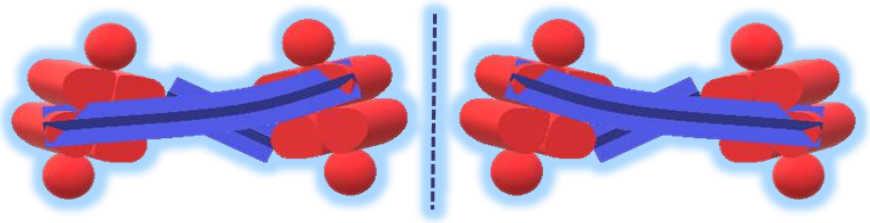

Supramolecular studies for the recognition of cations and neutral molecules using macrocycles have always been fascinating for scientists for many decades.[1] These macrocycles have applications as molecular sensors, in supramolecular catalysis and optoelectronics.[2] Herein, we present a novel bisperylenediimide-conjugated strained macrocycle that incorporates two different chromophores with an −A−D−A−D− pattern, where A is the acceptor, which is the perylene diimide unit and D is the donor. The macrocycle formed shows strong π-π stacking between the π-faces of the perylene diimide units. The strength of this π-π stacking decides the size of the cavity. We aim to utilize this macrocycle for sensing different ions and molecules. The behavior of this macrocycle is compared with an open-bisperylenediimide molecule. The perylene diimide subunits were connected through their bay positions which imparts chirality to the macrocycle and provides a high interconversion barrier between the stereoisomers. We are also interested in separating the stereoisomers using chiral high-performance liquid chromatography and studying their interconversion barriers. The macrocycle is deep blue with an absorption spectrum that covers the entire UV-visible range. The open-molecule shows H-type aggregation, whereas the closed-macrocycle shows J-type aggregation as observed from photophysical studies. Electrochemical measurements reveal the electron-deficient nature of the macrocycle due to the strong π-π stacking of the PBI units. The temperature-dependent and solvent-dependent studies were carried out to check the conformational changes. Further density functional theory calculations reveal a photoinduced-electron-transfer from the donor to the acceptor unit (perylene diimide) in both molecules.

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P-32: Exploring SPK98 for selective killing of ATM- or p53-deficient cancer cell

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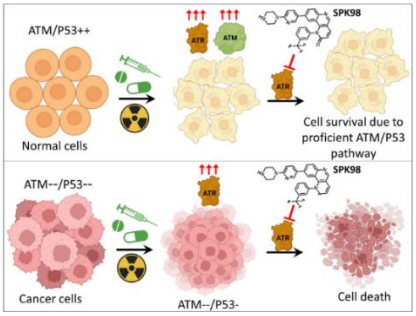

DNA damage response (DDR) pathway is one of the fundamental cellular processes that maintain the integrity of our genome. It encompasses cellular networks involved in DNA repair and cell cycle checkpoints[1]. DDR pathway proteins are also responsible for limiting the effectiveness associated with various modes of the genotoxic agent. Due to proficient DNA repair mechanisms, cancer cells overturn the induced damage resulting in Chemo and radio-resistance, making it an appealing target. Ataxia-telangiectasia mutated (ATM) and Ataxia-telangiectasia and Rad3 related (ATR) kinase are the major sensors in theDDR pathway[2]. Both recognizes DNA strand breaks and activated downstream protein involved in cell cycle arrest and DNA repair. Frequent mutation in the ATM/P53 pathway has been documented in many human cancers, which makes them reliant on functional ATR protein for survival. This has encouraged research in developing ATR inhibitors for the selective sensitization of P53/ATM-deficient cancer cells, but no therapeutic success has been attained to date3. This study explores the therapeutic potential of SPK98, an analogue of Torin2 and potent ATP competitive inhibitor of ATR and mTOR in P53- and ATM-deficient cancer cells[4-5]. Furthermore, the prospect of improving the therapeutic outcome of the genotoxic agent was also explored. SPK98 was shown to inhibit full-length human ATR protein purified from HEK293T cells. Taken together, our findings suggest that SPK98 is a promising therapeutic molecule for P53- or ATM-deficient malignancy that merits additional preclinical investigation.

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P-33: Imidazolium and Pyridinium Functionalized Polyethylene Membrane through Microwave Assisted Grafting as Alkaline Anion Exchanger

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Anionic exchange membranes have revolutionized the alkaline-based fuel cell industry by replacing older liquid electrolyte alkaline fuel cells (AFCs). Recent years have seen a significant uptick in the study on membrane technology with improved properties. However, scalable alkaline anion exchange membranes, a key component of Hydroxide Exchange Membrane Fuel Cells (HEMFCs), with desired properties are currently unavailable, which presents a major barrier to the development of HEMFCs. Here we designed a hydroxide exchange membrane based on Polyethylene-Linear Low Density Polyethylene (LLDPE) containing imidazolium and pyridinium cationic moieties via Microwave-assisted Chemical Graft Copolymerization in a novel glycerol-water solvent system. The prepared membrane possesses adequate ionic conductivity, chemical stability, mechanical robustness, ion exchange capacity and water uptake. These properties originate from the combination of the imidazolium-pyridinium cationic moieties and the polyethylene backbone.

P-34: Bis-Chelated Mono-Centric Hexa Coordinated Fe(III) Complex Showing Ligand Centreed Hydrogen Evolution Reaction

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In the present study, we report the synthesis and electrocatalytic activity of hexa-coordinated Fe (II) complex $Fe[L^1]_2$ towards hydrogen evolution reaction (HER). $Fe[L^1]_2$ displayed different mechanisms in presence of acids with different pK_a in DMF. In presence of strong acid CF_3COOH, a ligand-assisted metal-centred mechanism was followed which resulted in the rupture of the hexa-coordinate complex. Degraded species adsorbed to the electrode as a Fe-containing film. Whereas in presence of weaker acids like NEt_3.HCl and CH_3COOH complex displayed a metal-assisted ligand-centred mechanism with better acid stability. Maximum faradaic efficiency of 88% was observed for $Fe[L^1]_2$ with TON 21 when titrated with AcOH. Using DFT studies we calculated the electronic and geometric properties of the Fe catalyst. The geometry optimization of different intermediates helped in understanding the mechanism of HER. The probable sites for protonation and reductions were evaluated by calculating the equilibrium constants and reduction potentials. Accuracy in comparison between the computational and experimental data confirms the mechanism for HER.

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P-35: Synthesis and Studies of Polyaromatic Embedded Expanded Porphyrinoids

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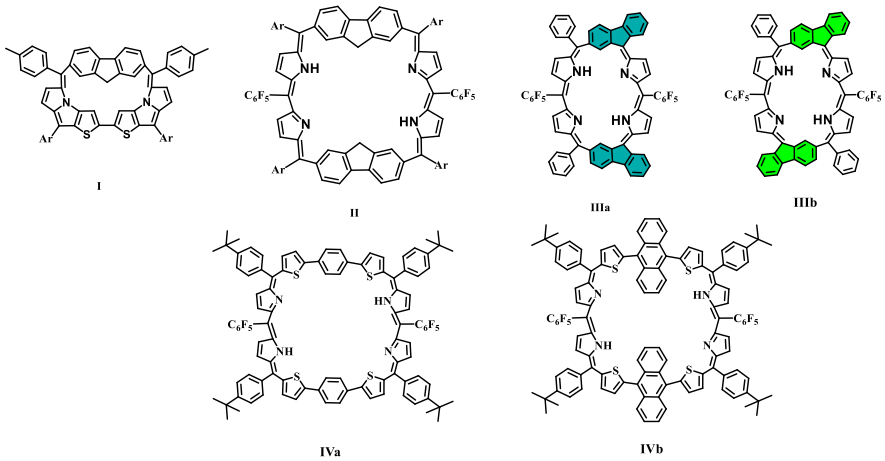

Polyaromatic hydrocarbons/heterocycles (PAHs) embedded porphyrinoids have drawn significant attention in the recent past in the light of their tremendous applications as fluorescent sensors and NIR dyes. The altered π-conjugation in the macrocyclic framework of PAH embedded porphyrinoids leads to interesting coordination and physico-chemical properties. PAH embedded porphyrinoids are relatively new ligands in the literature where the polyaromatic hydrocarbon moiety may or may not participate in the macrocyclic ring π-delocalization. These porphyrinoids have been explored for cation/anion sensing and as photosensitizers in photodynamic therapy but the reports on fused expanded PAH embedded porphyrinoids are very few. Our group has recently reported the synthesis of several PAH embedded expanded porphyrinoids **I (Chart)**. In this poster, we present the synthesis and studies of *bis*-(fluorene) embedded hexaphyrin **II**, the structural isomers of *meso*-fused hexaphyrins **IIIa/IIIb** and benzene/anthracene based decaphyrins **IVa/IVb (Chart)**. The structural, spectral, electrochemical and computational studies of these macrocycles will be discussed.

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P-36: Metal-Functionalized Ordered Mesoporous Silicas (OMs) and Their Catalytic Applications in the Aminolyis, Suzuki–Miyaura and Heck Coupling Reaction

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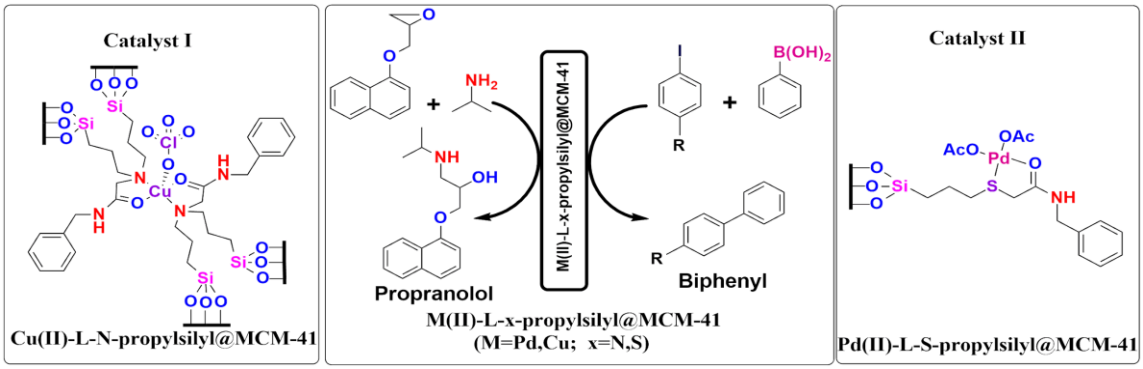

Considerable efforts have been devoted to employing heterogeneous catalysis in the chemical reaction due to their easy recovery and reusability.[1] Mesoporous material such as MCM-41 is extensively investigated in heterogeneous catalysis because of their large surface area, adjustable pore size (2-50 nm), and uniform arrangement of pores on the surface. Generally, these heterogeneous catalysts can be synthesized by post-functionalization of MCM-41 with suitable catalytically active metal ions. The present work demonstrates the immobilization of catalytically important metal ions such as Cu(II) and Pd(II) on MCM-41 and explores the catalytic application in the various organic transformation reactions. The solid Lewis acid catalysts Cu(II)L-propylsilyl@MCM-41 and Pd(II)L-propylsilyl@MCM-41 were prepared by the immobilization of Cu(II) and Pd(II), respectively, on MCM-41 with the support of organosilica precursor.[2,3] Synthesized Cu(II)L-propylsilyl@MCM-41 shows higher catalytic efficiency in the aminolysis reactions with high regioselectivity and stereoselectivity. On the other hand, the Pd(II)L-propylsilyl@MCM-41 was explored to catalyze Suzuki Miyaura and Heck coupling reactions. Both catalysts can be recovered and reused up to ten catalytic cycles without significantly losing their catalytic efficiency and with high product yield. Synthesized catalysts were characterized by various spectroscopic techniques and analyses such as Powder X-ray diffraction, N_2 adsorption-desorption isotherm, TEM, TGA, X-ray photoelectron spectroscopy (XPS), and EPR.

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P-37: A Chiral Silver Phosphate Catalyzed Asymmetric Synthesis of Tetrasubstituted β-Amino Indenones

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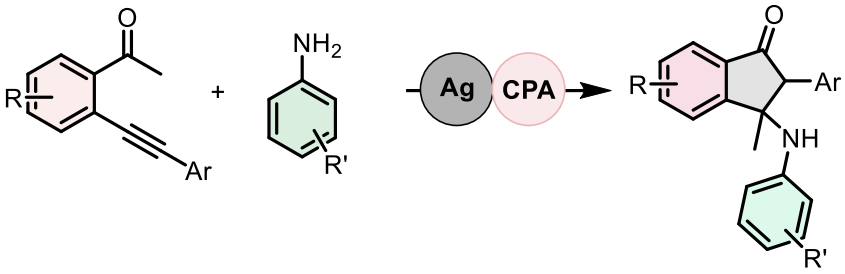

Herein, we report an efficient enantio- and diastereoselective approach for the synthesis of β-amino indenones by utilizing α-alknynl acetophenones and anilines, in moderate to good yields with excellent diastereoselectivity (>20:1) and enantioselectivity (up to 98% ee). The *in-situ* generation of a silver and chiral phosphoric acid (CPA) complex gives access to a variety of tetrasubstituted β-amino indenones. It is proposed that the reaction's mechanism is a domino effect that includes the hydrolysis of the ynone motif, a Knoevenagel condensation, and an aza-Michael addition. Thus, this protocol demonstrates the formation of both C-C and C-N bonds in one pot.

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P-38: One pot Domino transformation of Glycals into pyrano cis fused heterocycles via Nickel Catalysis

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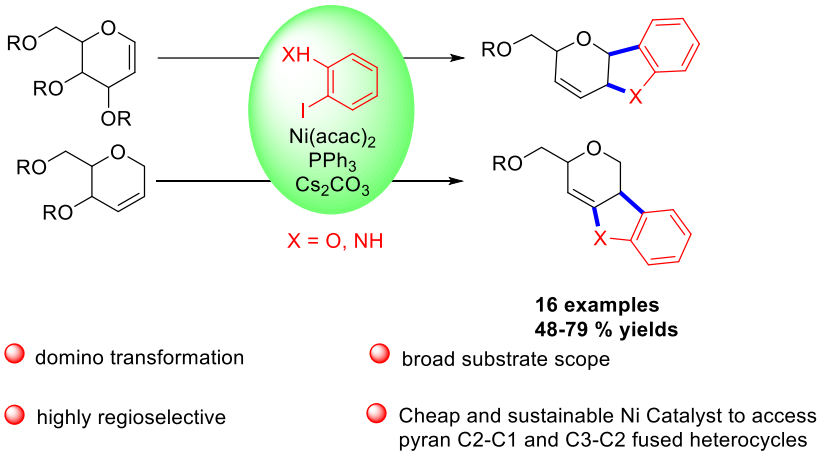

A direct access to various pyrano *cis* fused dihydro benzofurans and indoles from unsaturated enopyranoses and *o-iodo* phenols/anilines via the Ni catalysis is developed. Domino synthesis of pyrano C2-C1 and C3-C2 *cis* fused heteroarynes were achieved both from glycals and pseudo glycals in which heteroatoms are linked at C2 and C3 positions respectively with excellent chemo-selectivity. This newly developed general one pot strategy possesses significant potential towards the synthesis of various natural product and pharmaceutically active molecules.[1]

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P-39: Imidazo[1,2-*a*]pyridines-Tetracyanoethylene Donor-Acceptor Complexes as Potential Organic Semiconductors

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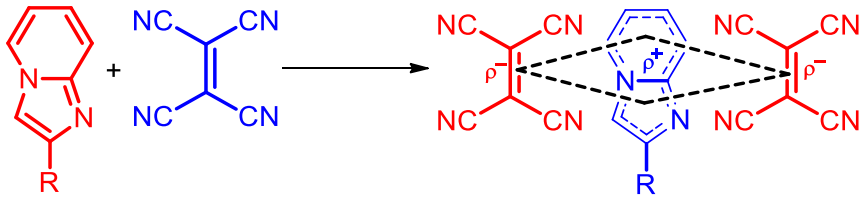

R= H, C_6H_5, *p*-$H_3COC_6H_4$, *p*-$O_2NC_6H_4$

Organic Donor Acceptor (DA) complexes have emerged in recent years as materials of choice for the organic binary electronics.[1] In recent decades, organic solar cells have attracted much attention due to their potential for developing low cost, light weight, ultrathin, flexible plastic modules.[2] Imidazo[1,2-*a*]pyridines react with tetracyanoethylene (TCNE) in 1:2 molar ratio to afford four new DA complexes.

The structures were unambiguously established on the basis of IR, ^{1}H, ^{13}C, DEPT 135, 2D NMR, and HRMS. The UV-vis. spectroscopy revealed the presence of intramolecular charge transfer phenomenon. All the four compounds fluoresce giving excitation emission fluorescence spectra with a red shift ranging from 64 to 151 nm. Interestingly, the nitro group in one of the products does not act as quencher; instead, it enhances the quantum yield to make it highest in this series. The products exhibit electrical conductivity which increases linearly with temperature. The scanning electron microscopic (SEM) studies reveal a distinct morphology with holes which facilitate flow of electrons as manifested by their electrical conductivity. The DFT investigation at the B3LYP/6-31+G(d) level of theory indicates an alternate donor acceptor stacking pattern in the products.

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P-40: Iron-Catalysed Regioselective Addition of C─H Bond in Indoles to Alkenes via Weak Chelation Assistance

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Earth abundant, less toxic and cheaper iron-catalyzed regioselective C−H bond alkylation of indoles with various alkenes is accomplished under mild conditions. This method allows the straight forward synthesis of C-2 alkylated indoles employing a well-defined simple iron catalyst, $Fe(PMe_3)_4$, providing a solution to the limitations associated with hydro(hetero)arylation of alkenes with excellent regioselectivity. A strikingly wide variety of alkenes can be used for this reaction, and the high-yielding anti-Markovnikov addition of indole C−H bonds to allyl derivatives was achieved for the first time using this catalyst system. A detailed mechanistic study (DFT) provides the evidence for the high selectivity of anti-markovnikov addition over markovnikov one.

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P-41: Ru-Catalyzed Benzannulation of Vinyl Sulfoxonium Ylide with Electron-Deficient Alkynes and Alkenes

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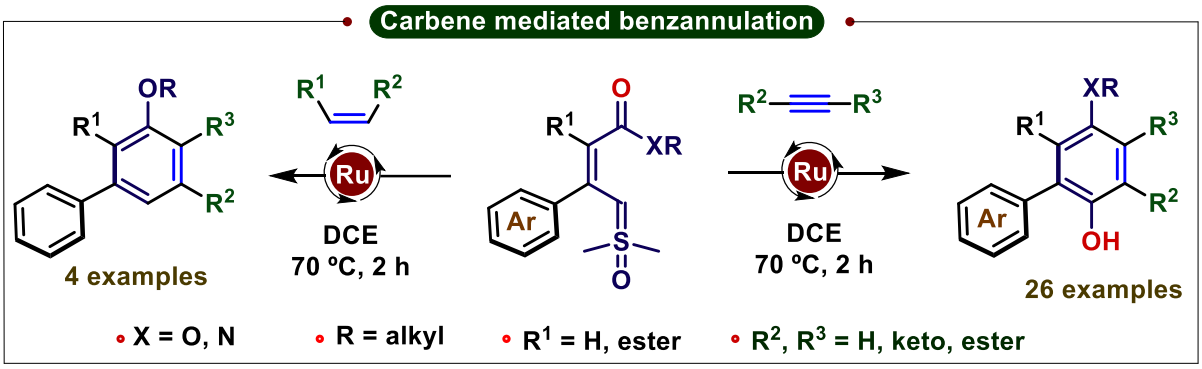

We report carbene-mediated benzannulation of vinyl sulfoxonium ylides with electron-deficient alkynes and alkenes to synthesize oxygenated arenes. This protocol features excellent regioselectivity, a broad substrate scope, and mild reaction conditions. Mechanistic studies revealed that the reaction proceeds through furan generation, cycloaddition, ring cleavage, and aromatization cascades. The synthesized arenes have been utilized in diverse product transformations and arene ring homologation.

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P-42: Hydrogen Peroxide-Mediated Rapid Room Temperature Metal Free C (sp2)-H Thiocyanation of Amino Pyrazoles, Amino Uracils, and Enamines.

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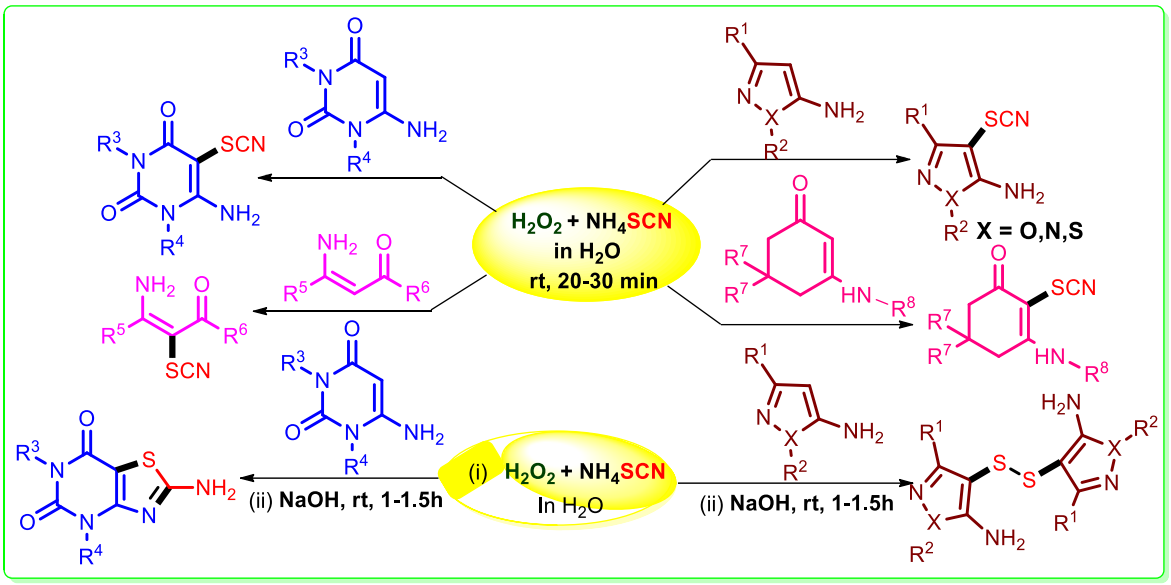

Fig 1 - Schematic representation of thiocyanation of aminopyrazole and aminouracil derivative and their functionalization.

A rapid metal and additive-free room temperature method for C(sp^2)-H thiocyanation of aminopyrazoles, aminoisoxazole, aminoisothiazole, amino uracils as well as aliphatic enamines has been developed in aqueous medium using hydrogen peroxide as benign oxidant and ammonium thiocyanate as thiocyanating agent. On the other hand, the reaction of hydrogen peroxide, ammonium thiocyanate followed by one-pot addition of NaOH provides corresponding disulfides in the case of amino azloles and pyrimidine fused 2-amino thiazoles were observed in case of aminouracils.

References:

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P-43: Solubilization of Curcumin and its Precursor (CurcumaLongin) Conventional and Deep Eutectic Solvents with and without Ionic Surfactants

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Curcumin shows several biological activities and acts as a natural antioxidant. It is a plant-based polyphenolic excipient that can be extracted from Curcuma Longa (CL, turmeric). Curcumin aqueous solubility is one of the major challenges in utilizing its complete potential in the bio-medical field [1]. Present studies show that curcumin solubility can be enhanced in water-based deep eutectic solvents (DESs). Water-based DESs (aquoline) are recently reported designer greener solvents which has water like properties with a wider window of temperature (for use) [2]. DES can be obtained by blending hydrogen bond donors (HBDs, e.g., urea, water, glycerol, malonic acid, etc.) with hydrogen bond acceptors (HBAs, e.g., choline chloride (ChCl)) [3]. The solubility of curcumin/CL has been determined, spectrophotometrically, in water, ethanol, and various aquolines (ChCl: nH2O, n = 2, 3, and 4). It has been found that λmax values (~425nm) are nearly the same for ethanol, water, and aquolines. Solubility shows an order: water< aquolines< ethanol. The effect of ionic surfactants (sodium dodecyl sulphate (SDS) and cetyl trimethyl ammonium bromide (CTAB)) has been investigated on the solubility behaviour of pristine material. It has been found that solubility augments in aquoline + surfactant and increases with an increase in [surfactant]. This behaviour has been interpreted in the light of the micellization (CMC values of SDS and CTAB are 4.69 mM and 0.87 mM, respectively) process as observed in an aqueous solution. The study allows us to conclude that aquoline-based micellar systems can be used as a potential vehicle for drug/gene delivery due to their physiological compatibility.

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P-44: A Metal-free Approach Towards Reductive Amination of Carbonyl Compounds

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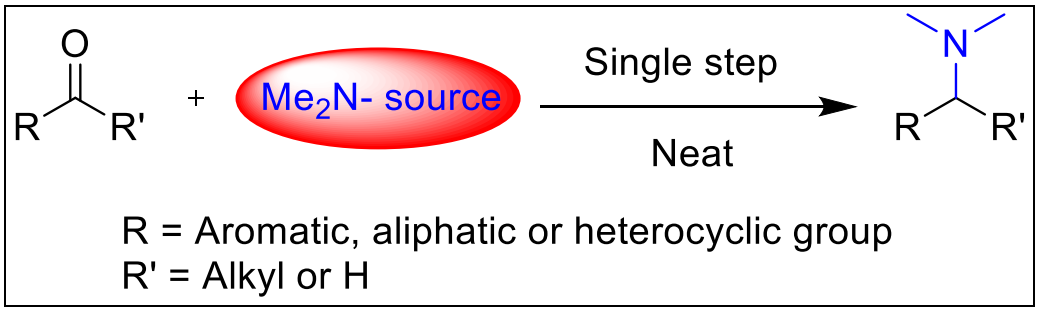

Tertiary amines are ubiquitous in nature and play a pivotal role in organocatalysis, pharmaceuticals, and fine chemicals.[1] Amongst various synthetic procedures known, the reductive amination of carbonyl compounds has been found to be a proficient method. Over the past few decades, various synthetic strategies for reductive amination have been developed. [2] Most of them suffer from the use of transition metals and/or harsh reaction conditions. Here, we present an efficient, operationally simple protocol for the chemoselective reductive amination of carbonyl compounds to furnish the tertiary amines (Scheme 1). The protocol encompasses broad substrate scope under the metal-free condition at room temperature and does not require any solvent.

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P-45: Functional Activities of UO_2(VI) Ion On Interaction with (O, N) and (O, N, S/Se) Based Acyclic and Cyclic Donor Bases

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Understanding the chemical behavior of uranyl (UO_2^{2+}) ion in various environments remains challenges because of the use of uranium compounds as nuclear fuel in global electricity generation. Indeed, the hexavalent oxidation state of uranium is the most stable form and appears exclusively in the form of (UO_2^{2+}) ion. Furthermore, uranium is often oxidized in (UO_2^{2+}) form in aquatic and aerobic environments and therefore studied extensively. [1] A Chemist's perspective on the role and nature of (UO_2^{2+}) ion underpins its chemistry involved from mining to conversion into highly enriched nuclear fuel, all the way to nuclear waste reprocessing and management, safe geological disposal, environmental impacts, and lastly, decommissioning of nuclear power plants.[2] These operations lead to serious environmental concerns at every stage. Conclusively, the present research work was an attempt to examine the unusual behavior of (UO_2^{2+}) ion in the presence of various acyclic and cyclic donor species. The formation of $[UO_2(NO_3)_3]^-$ has primarily been established computationally on various occasions, whereas the formation of this species remains hypothetical in the aqueous solutions of uranyl ion. e.g., the extraction of (UO_2^{2+}) ion before fabrication as and after reprocessing of nuclear-spent fuel is being extracted to organic/ ionic liquid media from conc. HNO_3 medium and prove to be highly problematic. In such cases, the speciation of (UO_2^{2+}) ion in solution state as $[UO_2(NO_3)_3]^-$ remains hypothetical in most of the high-level theoretical studies. Of course, in a few examples, the structure of $[UO_2(NO_3)_3]^-$ has been examined and with alkali or alkaline metal as counter cation where all the three nitrates bonded to (UO_2^{2+}) ion symmetrically. Undoubtedly, looking at the behavior of $[NO_3]^-$ ion may prove helpful in improving the extraction process using organic donor or ionic liquids applicable in nuclear technology.

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P-46: Salt-induced Inhibition and Disaggregation of Protein Amorphous Aggregates

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Protein amyloids and amorphous aggregates are implicated in various neurodegenerative disorders as well as in biotechnology and food industry.[1] Recent studies have revealed that solution parameters such as pH, ionic strength, temperature, and so forth play pivotal roles during protein amorphous aggregation mediated by an interplay of electrostatics and hydrophobic interactions. However, a detailed structural information on proteinaceous amorphous aggregates remains elusive. Additionally, it is important to devise suitable disaggregation strategies which will either arrest or abolish protein aggregation. Here, I will describe our recent study on salt-induced inhibition and disaggregation of protein amorphous aggregates.[2] Using a biophysical toolbox, we demonstrated that protein aggregation could be influenced by the solution ionic strength mediated by electrostatic screening. Additionally, our findings revealed salt-induced dissolution of preformed protein aggregates leading to a restoration of the protein native structure to a greater extent. This approach provides a potent strategy to design electrostatically-targeted inhibitors for protein aggregation.

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P-47: Unveiling the Three-component Phosphonylation on Alkynylaldehydes: Toolbox Towards Fluorescent Molecules

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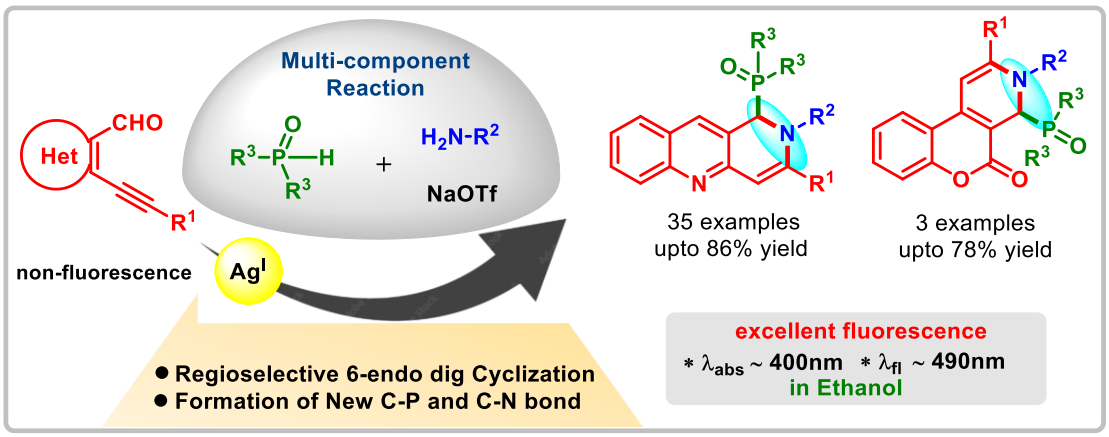

A regioselective tandem approach for annulated napthyridines/isoquinolines embedded with phosphine oxide group under mild reaction conditions in good to excellent yields has been achieved. The designed strategy involves the triflate-induced formation of new Csp^3-P and Csp^2-N bond formation in one-pot. This protocol was also well tolerated for the construction of densely functionalized organo-phosphorylated chromenes in good yields. Further, phosphino derived sulfamethazine and sulfamethoxazole drugs were also successfully synthesized in good yields. The mechanistic studies revealed the ionic pathway and the formation of regioselective *6-endo dig* cyclized products were confirmed through X-ray crystallographic studies. Interestingly, photophysical studies of selectivity selected compounds revealed their stimulating fluorescence properties.

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P-48: BODIPY immobilized MCM-41 based Solid Optical Sensors for Heavy Metal Ions Detection and Removal from Aqueous Medium

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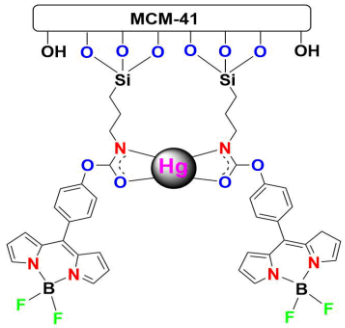

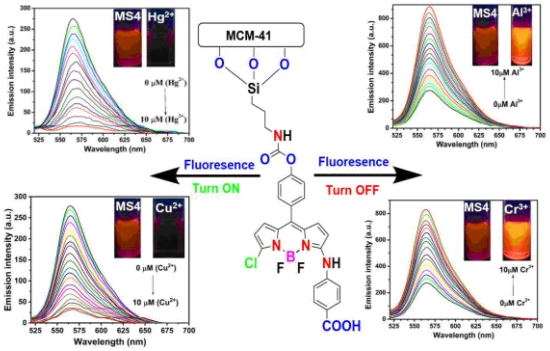

Heavy metal contamination has severely threatened the environment and human health. High levels of heavy metal ions, such as Mercury(Hg), Aluminium(Al), Lead(Pb), and Chromium(Cr), show an adverse effects on the ecological system and human health. All these metal ions are the most toxic non-biodegradable pollutants that exhibit acute toxicity to the human body, even in low concentrations.[1] Therefore, developing a rapid sensing method for selective determination and separation of these metal ions from an aqueous environment is a substantial task for researchers. In the present work, BODIPY functionalized MCM-41 based solid chemosensors BODIPY-propylsilyl@MCM-41 (MS1), and BODIPY-(COOH)-propylsilyl@MCM-41 (MS2) were synthesized and used for the efficient detection and removal of heavy metal ions such as Hg^{2+}, Cu^{2+}, Al^{3+} and Cr^{3+} in aqueous mediaum. The synthesized chemosensors MS1 and MS2 were well characterized using N_2 adsorption-desorption, powder X-ray diffraction, TEM, FT-IR, and thermal analysis. Chemosesnsor MS1 shows turn-off emission response slesctivly for Hg^{2+}, where as the emission intensity of MS2 is enhanced multifold in the presence of trivalent (Cr^{+3},Al^{+3}) metal ions and is completely quenched in the presence of divalent (Cu^{+2}, Hg^{+}) metal ions. The limit of detection was calculated to be a nanomolar range for Cr^{+3}, Al^{+3}, Cu^{+2} and Hg^{+} in pure aqueous media for both the chemosesnsors. Also, MS1 and MS2 were demonstrated the removal of respected metal ions from the pure water samples up to 98%.

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P-49: Palladium-Catalyzed N-Protecting Group Controlled Regiodivergent Cascade Cyclization/Alkoxylation of Allenamides

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Herein, we have developed a palladium-catalyzed domino Heck-cyclization/alkoxylation of allenamides to furnish regiodivergent indole and indoline derivatives. The palladium-catalyzed reaction provided indole and indoline at room temperature with good substrate scope. The N-protecting group on allenemides controls the outcome of the reaction. The mechanistic studies indicate the rearrangement of an indoline-derived intermediate to indoles to access free (NH) indoles with N-acetyl allenamides.

References:

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P-50: Domino reaction of tryptamines and diazo compounds to access hexahydropyrroloindoline derivative under Cu-catalysis

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Here in, we have developed a method for generating three consecutive stereogenic center in a single step. The cascade reaction of cyclopropanation/ring-opening/iminium cyclization of tryptamine derivatives with donor–acceptor diazo compounds furnished pyrroloindolines. The copper-catalysed reaction protocol provides pyrroloindolines at room temperature with broad substrate scope.

References:

1. Dharmendra Kumar,[a,b] Dhananjay Chaudhary,[a] Km Ishu,[a] Suman Yadav,[a] Naveen Kumar Maurya,[a,b] Ruchir Kant[c] and Malleswara Rao Kuram *Org. Biomol. Chem.*, **2022**, *20*, 8610.

P-51: Enhanced photoelectrochemical response of reduced graphene oxide covered inexpensive TiO_2-$BiFeO_3$ composite photoanodes

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We show enhanced photoelectrochemical response of reduced graphene oxide covered inexpensive TiO_2-$BiFeO_3$ composite photoanodes for photoelectrochemical water splitting reaction. The photoelectrochemical activity of TiO_2-$BiFeO_3$ composite electrodes increased by creating heterojunction of TiO_2-$BiFeO_3$ and rGO. Structural, optical and morphological analysis of pristine and composite samples was done by characterizing them using X-ray diffraction, UV–vis spectrometry and scanning electron microscopy. The photoelectrochemical water splitting reaction revealed that composite TiO_2-$BiFeO_3$ with 20 wt.% $BiFeO_3$ has higher photocurrent density. Further this composite electrode with rGO layer exhibits more than tenfold photocurrent density at onset and as well as higher potential. Graphene oxide layer acts as rich source of electrons caused better separation of the photogenerated electron hole pairs at heterojunction. Finally, this system shows high photocurrent density of 3.5 mA cm^{-2} at 0.95 V/Ag/AgCl with good stability under light conditions.

Keywords: TiO_2-$BiFeO_3$ composites, Photoelectrochemical response, Cost effective, TiO_2-$BiFeO_3$/rGO heterojunction, Hydrothermal

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P-52: Protecting-Group-Directed Stereodivergent Tsuji-Trost Cyclization: Total Synthesis of (+)-Petromyroxol

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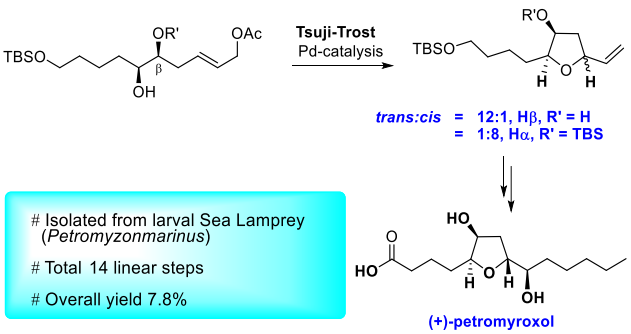

The Tsuji–Trost reaction over the last three decades has emerged as a convenient approach for construction of carbon–carbon and carbon–heteroatom bonds.[1] In 2012, Gandon and co-workers[2] disclosed the counteranion-directed catalysis (CDC) for the synthesis of 2,3,5-trisubstituted-THFs via Tsuji–Trost reaction. (+)-Petromyroxol was first isolated by Li and co- workers in 2014, as a non-racemic 64:36 mixture of (+)/(–) enantiomers from >100000 L of water conditioned with larval Sea Lamprey (*Petromyzon marinus*)[3] A stereodivergent protecting-group-directed Tsuji-Trost cyclization with efficient synthesis of both 2,5-cis- and 2,5-trans-disubstituted-THF scaffolds have been realized. Presence of β-O-silyl group in allyl acetate results in cis-2,5-disubstituted-3-oxygenated THF in a good up to 8:1 dr. Alternatively, when the free OH at the β-position is available for acetate co-ordination, it gives trans-2,5-disubstituted-3-hydroxy THF scaffold almost as single diastereomer (up to 12:1 dr). The THF scaffolds synthesized were carried forward in the total synthesis of (+)-petromyroxol.[4]

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P- 53: Modulation of Supramolecular Chirality by Stepwise Axial Coordination in a Nano Size Zn(II)porphyrin Trimer

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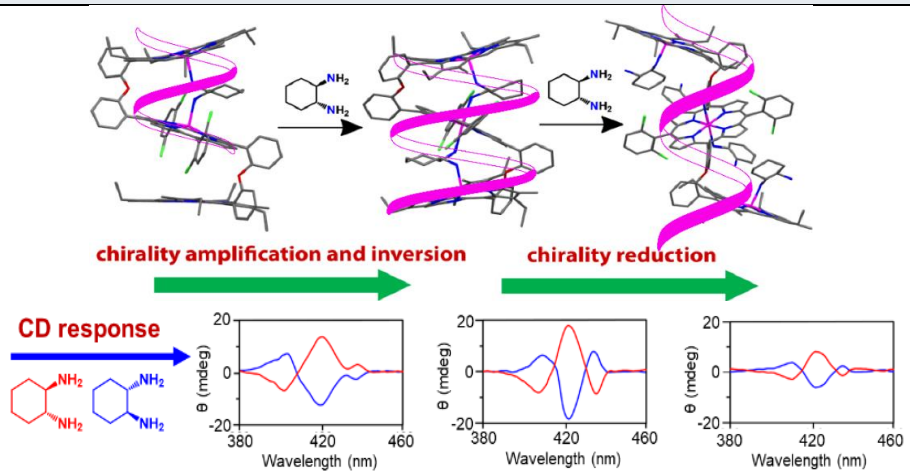

Supramolecular chirogenesis is one of the most important interdisciplinary fields to be looked into, because of its occurrences in many natural (DNA double helix, heme proteins, secondary α-helix structure of proteins, etc.) and artificial systems. Exciton Coupled Circular Dichroism (ECCD) is a nonempirical spectroscopic method that is based on detecting the through-space exciton interaction between helically oriented independently conjugated chromophores. Step-wise induction, amplification and inversion, and reduction of molecular chirality have been realized in a single molecular framework through successive coordination of chiral diamines with an achiral trizinc(II)porphyrin trimer host due to change in the interporphyrin interactions and helicity. The origin of chirality transfer from guest to host is clearly rationalize by experimental and computational studies.

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P-54: Quantum Chemical Investigation of Post Combustion CO_2 Capture Using N-Heterocyclic Systems

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As we struggle through the alarming levels of CO_2 emission worldwide, carbon capture and sequestration (CCS)[1] offer an area of intensive research. Among various materials available for carbon capture, this work focusses on quantum chemical investigation of several under-explored N-heterocyclic systems, such as the isomers of dihydrooxazole family. This includes the anions generated from oxazoline, oxadiazoline and oxatriazoline as potential azolate based CO_2 capture systems. In another study, we have used quantum chemical methods to determine possible pathways for the reactions between CO_2 and various positional isomers of methylpiperidines (N-methyl, 2-methyl, 3-methyl, 4-methyl). As methylpiperidines are an already known CO_2 capture material, the preference for carbamate *vs*. bicarbonate pathway[2] is evaluated and compared depending on reaction conditions. The possibility of multiple products (due to their various plausible conformations, *cis-trans*/*ax-eq*) resulting from these pathways are also explored. Quantum chemical methods are efficient in predicting atomic interactions, reaction mechanisms, physicochemical properties and thermodynamic data.

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P-55: Insight into the High Proton Conductivity of One-/Two-Dimensional Cadmium Phosphites

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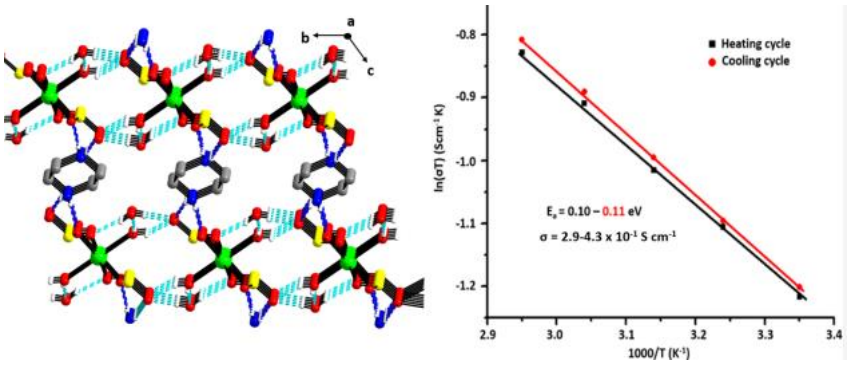

Figure 1. H-bonded network in **2** as well as Arrhenius plot for both heating and cooling cycle.

The study describes the synthesis and structural attributes of two new cadmium phosphites, [Cd{OP(O)(OH)(H)}$_2$(4,4′-bipy)] (**1**) and [H_2pip][Cd(HPO_3)$_2$(H_2O)]·H_2O (**2**). The structure of **1** adopts a two-dimensional motif featuring alternate [Cd-μ2-O]$_2$ and [Cd-O-P-O]$_2$-cyclic rings, while the inorganic chains are held together by 4,4′-bipyridine. The presence of strong hydrogen bonding interactions between the appended H2PO3 groups (O---O = 2.55 Å) provides a facile proton conduction pathway and results in a proton conductivity of 3.2×10^{-3} S cm^{-1} at 75 °C under 77% relative humidity (RH). Compound **2** comprises an anionic framework formed by vertex-shared [Cd−O−P−O]$_2$-cyclic rings, while the [H_2pip] cations between the adjacent chains assist a well-directed O-H---O hydrogen-bonded network between coordinated water, lattice water, and phosphite groups. The bulk proton conductivity value under conditions as in **1** reaches 4.3×10^{-1} S cm^{-1}. For both **1** and **2**, the proton conductivity remains practically unchanged under ambient temperatures (25−35 °C), suggesting their potential in low-temperature fuel cells.

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P-56: Chalcogen Bond-mediated Cellular Uptake of Fluorescent Compounds

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Efficient cellular delivery of bioactive molecules plays an important role in the discovery and development of novel drugs. Targeting intracellular proteins in cytosol and other cellular components by small molecules is a challenging task. As such, these molecules must cross the lipid bilayer plasma membrane, which acts as a barrier for its direct delivery. Although small molecules such as oxygen, carbon dioxide and nitric oxide can cross the plasma membrane by simple diffusion, large molecules such as protein, peptides, nucleic acids require membrane transporters and receptors for their efficient uptake.

Recently, it was reported that introduction of halogen atoms enhances the cellular uptake of small fluorescent molecules and specifically the iodine atom substitution shows remarkably higher uptake compared to that of other halogen substituted compounds[1,2]. As halogen bond plays an important role in cellular uptake, similarly chalcogen bond may play a key role in efficient cellular uptake of small molecules. We found that introduction of chalcogen atom increases the cellular uptake of small fluorescent molecules specifically it is higher for selenium atom containing molecules. We also found similar type of increase in cellular uptake in different types of fluorescent probes. Detailed investigation suggests that these compounds transport through an energy independent carrier mediated pathway. This provides a novel strategy for efficient delivery of small molecules in living cells.

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P-57: Schiff Base Ligand Based Complexes as Electro Catalysts for Proton Reduction

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Solar energy harnessing is a promising way to meet the increasing global energy needs.[1-7] An important approach in this context is artificial photosynthesis (AP) wherein water is split into hydrogen and oxygen using electrocatalysts incorporating different chromophores.[8-9] For the reductive side of AP (H_2 generation), a highly active catalyst, stable in the presence of water and designed using earth abundant materials is preferable. Identifying a robust, active, and efficient electrocatalyst is hence, a crucial first step in this direction. Though Pt is active for proton reduction, the widespread application of Pt is limited due to its rare nature. Keeping this in mind, efforts have focused on using abundant elements such as Fe, Co, Ni, Mo and different combinations of ligands for designing the proton reduction catalysts. For the ligand platforms in developing the catalysts with inexpensive components, Schiff base ligands have received special attention in the past few years. Based on the above-mentioned facts, tetradentate Schiff base ligands N, N'- Bis (salicyldiene)ethylenediamine(**L^1**),2,2'-((1E-1'E)-(ethane1,2diylbis(azanylyidene))bis(ethane-1-yl-1-ylidene))diphenol(**L^2**) and 3-(2-(E)-(hydroxynaphthyl)methyl)imido)propylamine) (**L^3**) were reacted with $MCl_2.6H_2O$ (M = Co, Ni). The synthesized Schiff base complexes [Co^{II}(**L^1/L^2/L^3**)] **1-3** and [Ni^{II}(**L^1/L^2/L^3**)] **4-6** were characterized by FTIR, NMR and UV-Vis spectroscopic techniques, mass spectrometry, elemental, and thermal analysis.

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P-58: Heterogenization of non-precious homogeneous catalysts within MOF pores for borrowing hydrogen catalysis

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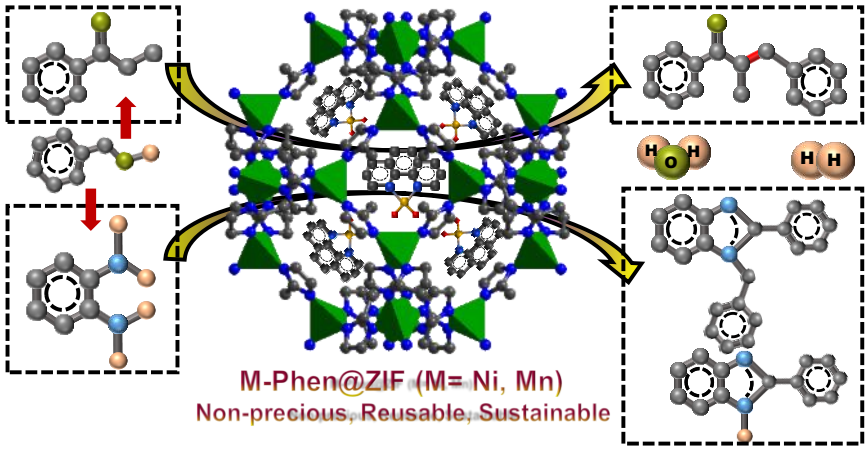

Into the cavities of metal organic framework ZIF-8, homogeneous Ni-phenanthroline and Mn-phenanthroline complexes were successfully immobilized. Here, the as synthesized heterogeneous catalysts designated as M-phen@ZIF-8 where M= Ni & Mn, are demonstrated as first MOF based catalysts for the selective synthesis of mono – or 1,2 disubstituted benzimidazoles & functionalized branched ketones where alcohols being used as renewable coupling partners, respectively. Superior stability of catalysts under harsh basic conditions well examined by SEM, TEM, BET, PXRD, TGA and EDX elemental mappings. The borrowing hydrogen strategy was validated through mechanistic studies and deuterium labelling experiments. The released hydrogen gas was also measured by water displacement method or quantified by GC. Defects, additional lewis acid sites, pore amplification in the M-phen@ZIF-8 during the reaction, all contributed to higher activity and selectivity.

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P-59: Development of Green Multicomponent Approach to Synthesize Biologically Active 2,3-Dihydrofurans and 2,3-Dihydrofuro[3,2-c] Coumarins

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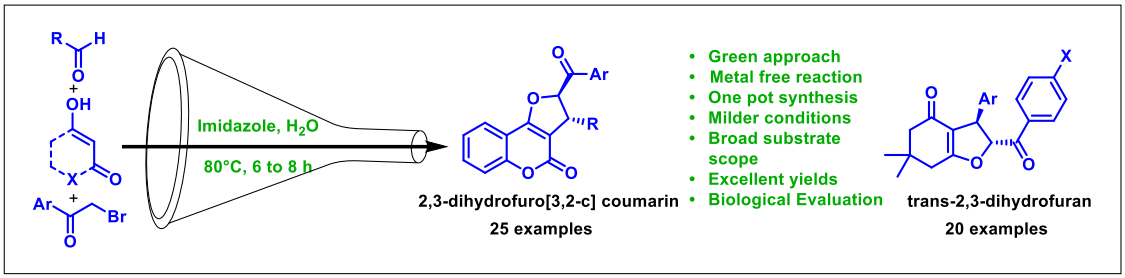

Development of green multi component reactions as an efficient synthetic methodology for the construction of biologically active molecules have received great attention in last couple of decades. In addition, organic scaffolds such as 2,3-Dihydrofurans and 2,3-dihydrofuro[3,2-*c*] coumarins displayed an extremely wide range of biological activities, however, they were yet to be succumb in greener way. Following the nature's footsteps, herein we reported the first time, an eco-friendly, inexpensive, and efficient one-pot green multicomponent approach to synthesize functionalized *trans*-2,3-dihydrofuro[3,2-*c*]coumarins (DHFC) and their derivatives using imidazole and water as a catalyst and solvent, respectively, under mild conditions.[1] Applications of the developed catalytic process in water medium revealed the outstanding activity, productivity, and broad functional group tolerance, affording a series of newly designed DHFC and derivatives in excellent yields (72-98%). Moreover, the human serum albumin (HSA) binding ability of the synthesized DHFC derivatives have been covered through the detailed *in silico* and *in vitro* based structure-activity analysis.[1] Furthermore, developed strategy was also applied for the synthesis of bioactive heterocycle i.e., dimedone fused 2,3-dihydrofuran derivatives using imidazole and water as a green catalyst and solvent, respectively, under mild conditions in excellent yields (70-99%). The synthesized dimedone based 2,3-dihydrofuran derivatives have been found to inhibit SaTR *in vitro* at low to medium micromolar (μM) concentrations.[2]

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P-60: Fe-catalyzed Sequential Oxidative Cleavage and Nucleophilic Addition of Peroxyoxindole Towards the Spiro[indoline-3,4'-pyran]-2-ones, 2-(2-oxoindolin-3-ylidene) Malononitriles and Spiro [dibenzo[c,h]xanthene-7,3'-indolin]-2'-ones.

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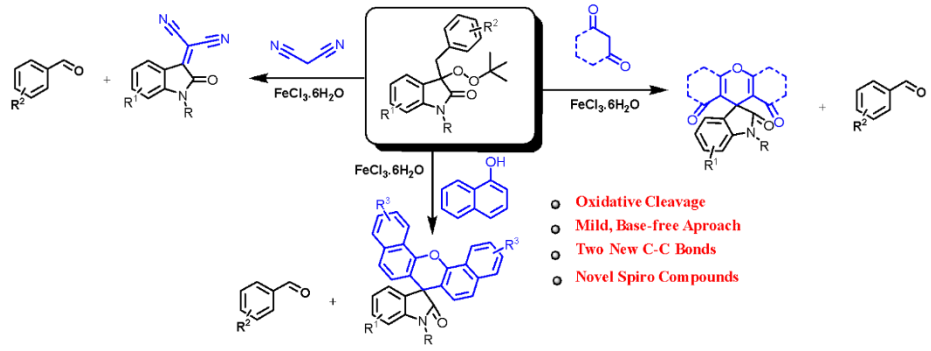

Organic peroxides are prevalent intermediates in organic synthesis.[1] These peroxides can be readily cleaved in the presence of a catalyst, light, or heat to generate new reactive species due to weak O−O bond, which can be exploited in many oxidative transformations and rearrangement reactions for the synthesis of heterocyclic compounds.[2] Herein, we developed a new approach for the direct synthesis of a series of biologically important pyran and xanthene-containing spiro oxindole derivatives via oxidative cleavage of peroxyoxindoles. The rearrangement of peroxyoxindole in the presence of $FeCl_3$ generates the isatin intermediate, which undergoes sequential reactions with cyclic-1,3-diketone such as Knoevenagel condensation, Michael addition, and dehydration. The present method is a simple, mild and base-free method to synthesize variety of spirooxindoles by using the most abundant Fe-catalyst. A plausible mechanistic pathway for this transformation has been reported with experimental evidence and control experiments, and this approach is also applicable for the synthesis of 2-(2-oxoindolin-3-ylidene) malononitriles as well as for the synthesis of spiro [dibenzo[c,h]xanthene-7,3'-indolin]-2'-ones.

References:

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3. Gokul S. Londhe, and Boopathy Gnanaprakasam; (**Unpublished Work**)

P-61: Ligand-Enabled Pd (II)-catalyzed [3+2] Annulation via C(sp3)-H and C(sp2)-H Bond Activation

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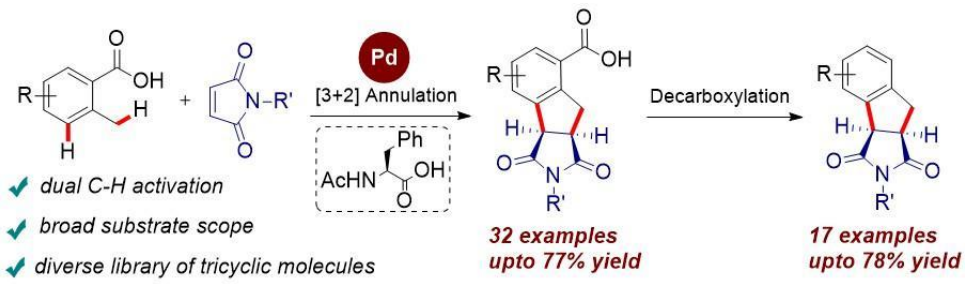

The transition metal-catalyzed annulation reaction *via* C−H bond activation is an interesting method to synthesize structurally complex organic moieties effortlessly. In the last few decades, six-membered cyclic rings generated through [4+2] and [2+2+2] annulation reactions through C−H bond activation were widely explored. Similarly, seven, five and four-membered cyclic rings can be synthesized through [3+4], [3+2], and [2+2] cyclization reactions, respectively. The annulation through dual C−H bond activation reaction is a highly interesting and demanding method in contrast to mono C−H bond activation because it can overcome the difficulty of the existing method in the construction of complex organic frameworks. Recently, palladium-catalyzed [3+2] annulation *via* double C−H bond activation has emerged as a powerful and straightforward method to construct a five-membered cyclic ring.[1] In this conference, I will present a palladium-catalyzed [3+2] annulation of substituted benzoic acids with maleimides leading to tricyclic heterocyclic molecules having a free carboxylic group. The protocol has been developed in a high atom- and step-economical manner without incorporating any exogenous directing. The annulation reaction proceeds *via* dual C−H bond activation such as C(sp^3)−H at the benzylic position and C(sp^2)−H bond at the meta position of substituted aromatics. An external ligand (MPAA) is crucial for the success of this protocol. Further, the decarboxylation of the free carboxylic acid group of observed products was carried out and a plausible reaction mechanism has been proposed for the [3+2] annulation reaction.[2]

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P-62: New Directions in Diene Functionalization: Oxidative Cleavage and Hydroalkoxylation

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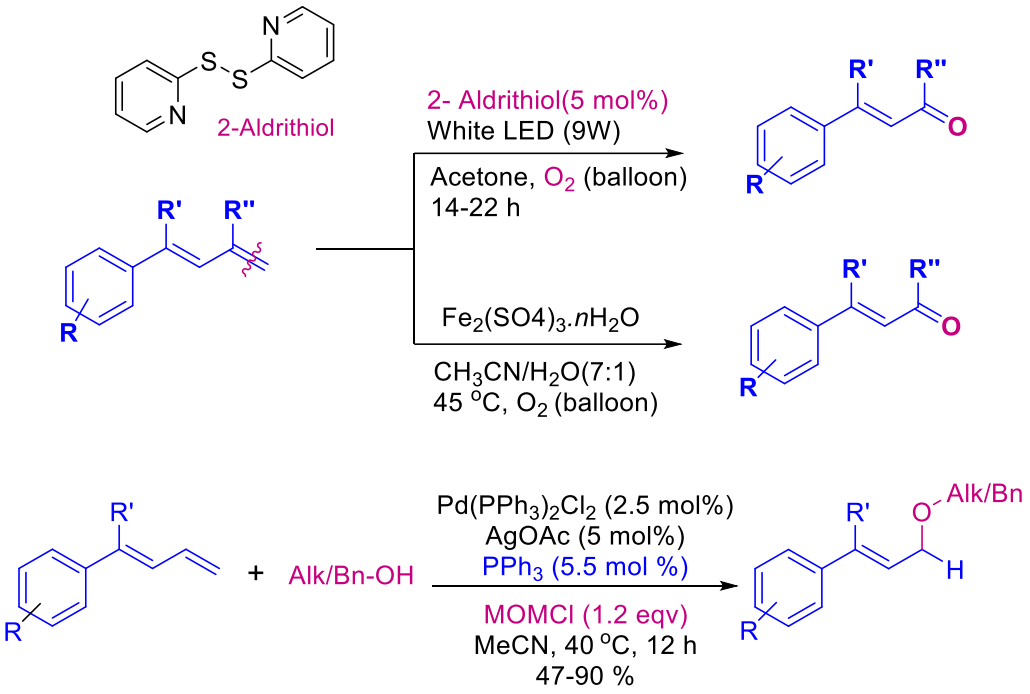

An interesting oxidative cleavage of 1-arylbutadiene proceeded with the use of Fe(III) sulfate/O_2 conditions.[1] Later, a metal-free oxidative cleavage of dienes under a simple, efficient, and environmentally benign disulfide-catalyzed conditions in presence of light was developed.[2] To extend further, we recently explored the regioselective hydroalkoxylation of 1-aryl-butadienes in presence of the Pd-catalyst and additive chloromethyl methyl ether (MOMCl).[3] All these works will be presented.

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P-63: Boron Based Dual emissive Single Fluorescent Probe for Differentiating Autophagy and Apoptotic Cells/Tissue

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Autophagy and apoptosis are crucial intracellular processes for maintaining cellular homeostasis and cell survival.[1] Autophagy is a ubiquitous degradation process during which damaged cellular organelles and misfolded or aggregated proteins are selectively degraded. On the other hand, apoptosis, known as the programmed cell death pathway, removes the aged or damaged cells. The hallmark of apoptosis is the disassembly of dying cells into small membrane-bound vesicles termed apoptotic bodies (ApoBDs). Recent studies on the autophagic and apoptotic processes have demonstrated that these two processes have complicated crosstalk in cell death.[1,2] In many conditions, autophagy is considered as a cell survival mechanism; however, emerging evidence suggests that it may function as programmed cell death when apoptosis is prohibited. It has also been reported in the literature that many cytotoxins can trigger both autophagy and apoptosis under specific conditions. The imbalances in these two processes' can result in several neurodegenerative diseases such as Parkinson's disease (PD), Alzheimer's disease, Huntington's disease, cancer, etc. Thus, it is vital to understand how the interplay between these two processes controls the fate of a cell. To date, several fluorescent probes based on protein and small molecules have been developed to image autophagy and apoptosis. However, a small molecule-based single fluorescent probe that can image both processes is yet to be reported. Thus, developing fluorescent probes that can image and differentiate autophagy and apoptosis processes is exciting, but it is a challenging task. Considering all these facts, we designed and developed two boryl anilines, **1** and **2,** composed of dimesityboryl acceptors and the 10-amino(/dimethylamino)anthryl group as donors. The cytotoxicity and imaging studies on these molecules indicated that probe **1** was more cell-permeable than **2**. Compound **1** can also differentiate late and early apoptotic cells. We have successfully developed a single probe for simultaneously and differentially imaging apoptotic and autophagic cells.[4] These results will be discussed in detail in this poster.

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P-64: Graphitic Carbon Nitride as Responsive Photocatalyst for Expeditious C-H activation /Oxidative Dearomatization in Organic Synthesis

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In the arena of solar energy conversion, environmental remediation, and recently in organic synthesis graphitic carbon nitride (g- C_3N_4) is a fascinating conjugated polymer that has drawn wide interdisciplinary interest as a metal-free and visible- light- responsive photocatalyst.[1] Researchers are attracted to it by its appealing electronic band structure, its high physicochemical stability, and its "earth-abundant" nature. To improve the photochemical stability and electrical band structure of g-C_3N_4, and to decrease charge recombination rates, and to improve light- harvesting performance some modifications are required.

Here we have used oxidized g-C_3N_4 (CNO) for the generation of singlet oxygen. As one of the most reactive oxygen species (ROS), singlet oxygen ($^1O_2$) has many applications, including selective organic synthesis. By incorporating carbonyl groups into g-C_3N_4, we have significantly enhanced triplet-exciton yield by promoting spin-orbit coupling and reducing the matrix's singlet–triplet energy gap, thus facilitating the generation of $^1O_2$ through energy transfer and suppressing ROS simultaneously.

Oxidized Graphitic Nitride application is explored for “Regioselective Ring-Opening Nucleophilic Addition of Aziridines[2] again developed another mild and effective method for asymmetric synthesis of C2- quaternary Indoline-3 ones directly from 2- Arylindoles via oxidative dearomatization.[3]

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P-65: Synthesis of 2-Quinolinone Derived -Quinone Methide via Ring Expansion of Isatins using 1,2-Phospha-Brook Rearrangement

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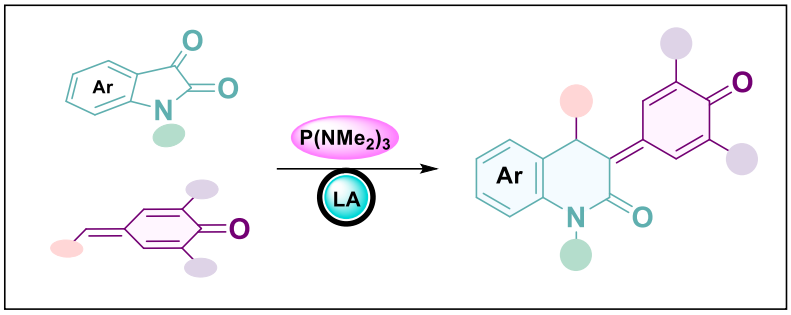

An efficient and regioselective one-carbon homologation approach for installing 2-quinolinone cores packed with para-quinone methides has been developed. Further, post-synthetic transformations affording functionalized 3,4-dihydroquinolinones by constructing of C-P, C-S, and C-C bonds have been elegantly demonstrated.

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P-66: Evaluating the *in vitro* potential of novel benzimidazole derivatives as *Helicobacter pylori* IMPDH inhibitors

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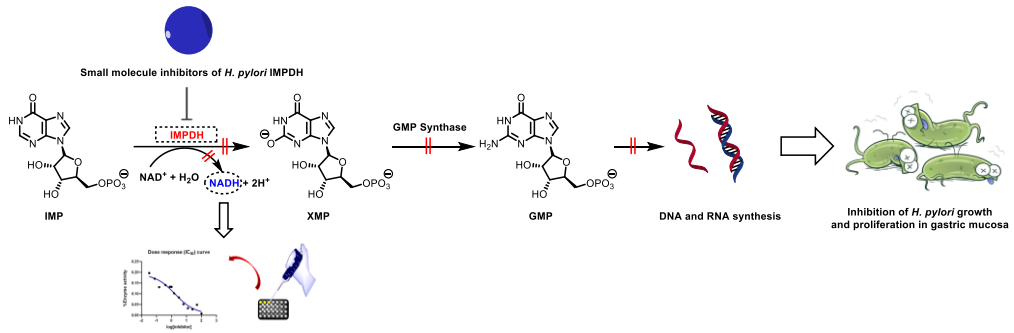

Helicobacter pylori (*H. pylori*) infection, leading to gastric inflammation, peptic ulcers and eventually gastric cancer[1] affects almost 50% of the total world population and over 80% of the Indian population[2,3]. The anti-bacterial resistance shown by these bacteria has resulted in an increasing demand for a novel therapeutic strategy. One of the recent drug targets identified to combat *H. pylori* is the metabolic enzyme inosine-5'-monophosphate dehydrogenase (*Hp*IMPDH) involved in the first step of the *de novo* purine biosynthesis pathway[2]. Owing to the promising therapeutic potential of benzimidazoles against *H. pylori*[4], and taking inspiration from the hit molecule C91[2], the present study identifies a novel class of benzimidazole derivatives which would act as potential small-molecule inhibitors of *Hp*IMPDH. Benzimidazole at its second position was substituted with a methyl pyrazole, and aryl derivatives of the linker part of this scaffold were synthesized, characterized and tested *in vitro* using fluorescence-based assay, along with *in* silico studies. The design, synthesis and *in vitro* biological evaluation of these 2-(2-(1-methyl-1H-pyrazol-3-yl)-1H-benzo[d]imidazol-1-yl)-N-arylacetamide derivatives would help us in determining their inhibitory potential against *Hp*IMPDH, which would further improve the drug development process to treat the infection.

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P-67: Transition from innocent to non-innocent character by changing the *meso*- substitution on corrole

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Cobalt-corroles are a great model to investigate the coordination-induced spin crossover, due to their rigid planar coordination framework. A spin transition from S=1 to S=0 results from the coordination of one or two axial ligands to the metal core.[1]. Depending on the number of ligand coordination (n = 4, 5, or 6), it is known that complexes of cobalt (III) can exist in two distinct spin states. Co^{3+} frequently exhibits a high spin (paramagnetic, S = 1) state in square planar complexes (n = 4). Low spin cobalt (III) is most often diamagnetic (S = 0).[2]. Here, we demonstrate the existence of a stable molecular spin switch at normal temperature. We designed and synthesized two cobalt corrole molecules to understand the coordination induced effect on the spin states of cobalt. Azo derivatives of phenyl and pyridine have been thoughtfully incorporated into the design, enabling us to modify the coordination number upon exposure to light or by switching the *meso*- position from EWG to EDG, in addition to invoking non-innocent character.

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P-68: Germyliumylidene catalyzed hydrosilylation of aldehydes and ketones

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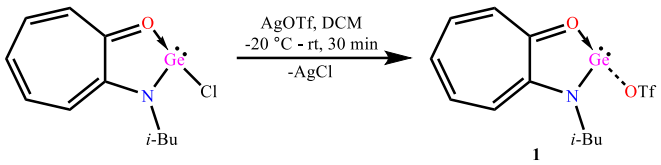

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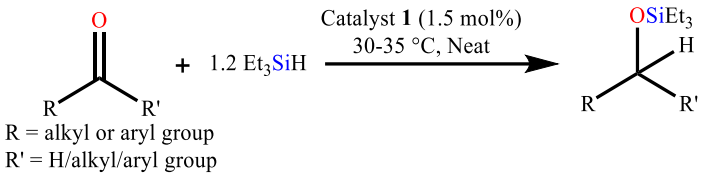
Scheme 1: Synthesis of germylene cation **1**.



Scheme 2: Hydrosilylation of aldehydes and ketones catalyzed by germylene cation **1**.

The use of main-group compounds as catalysts for organic transformations has advanced significantly. Germylenes, a class of low-valent main-group compounds, have been used as catalysts for the hydroboration and cyanosilylation of carbonyl compounds.[1] Hydrosilylation of CO_2 using germylene→borane adduct and germylene cation are also reported recently.[2,3] However, the hydrosilylation of carbonyl compounds using a germylene catalyst is hardly known. In this regard, this poster reports the aminotroponate (AT) ligand stabilized germylene cation [(*i*-Bu)ATGeOTf] (**1**) (Scheme 1) as a valuable catalyst for the hydrosilylation of various aldehydes and ketones. Using 1.5 mol% of compound **1**, benzaldehyde was hydrosilylated in 4.25 h with 99% conversion (TOF = 15.5 h^{-1}) (Scheme 2). The substrate scope, effectiveness of various other germylene cations, and detailed mechanistic insights will be presented in the poster.

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P-69: Prochlorperazine targeting mutant *KRAS* and its response in non-small cell lung carcinoma

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KRAS mutations has been associated with drug resistance/sensitivity and poor patient outcome in various cancers. *KRAS*-oncogenic mutations are dominant in lung carcinoma and is considered as leading cancer with the highest mortality. Therefore, identification of new biomarkers to treat NSCLC patients targeting the *KRAS* mutant is needed. Moreover, the development of effective radiosensitizing agents will be necessary for further improvement in the radiation therapy for NSCLC. In pursuance of the search for a novel radiosensitizer, high-throughput screening of FDA-approved drugs was performed at active site of K-Ras. Prochlorperazine (PCZ), an antipsychotic drug, showed good binding affinity with KRAS-mutant proteins. Towards this effort, evaluation of the radiosensitization profile of Prochlorperazine showed a positive response in inhibiting of Ras/Raf/MEK/ERK signalling with PCZ + radiation treatment in NSCLC and suggested decreased cell viability in vitro and regression of *KRAS* G12S tumours. Gene enrichment analysis obtained from RPPA data shows downregulated proteins were mainly annotated to negative regulation of apoptotic process, positive regulation of transcription and significantly enriched in ErbB, PI3K-Akt, and FoxO signalling pathways.

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P-70: Detection of Assorted Analytes by Coumarin-Based Chemosensors

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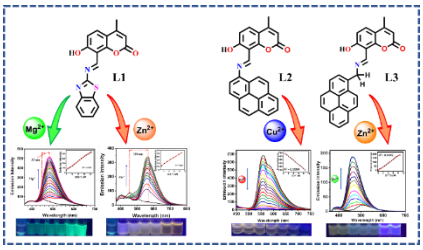

Development of selective yet sensitive chemosensors for the detection of various analytes is of immense significance due to their role in various biological, medicinal and industrial processes. Coumarin and its derivatives continues to be exploited in the field of chemosensing as they offer strong and stable emission, high quantum yield, impressive biocompatibility, good structural flexibility as well as versatile chemical functionalization. Our research laboratory has been working on developing chelate-based chemosensors where chelation-induced-emission "Turn-On" as well as "Turn-Off" phenomena have been effectively utilized for the detection of assorted analytes (cations, anions, gases, drugs, etc.).[1] Taking inspiration from the earlier work, a series of coumarin-based chemosensors (**L1-L3**) have been designed for the detection of different metal ions. A coumarin-benzothiazole based fluorescent chemosensor **L1** was utilized for the dual-channel "*Turn-On*" detection of Mg^{2+} (at 483 nm) and Zn^{2+} (at 560 nm) ions at two different wavelengths with large Stokes shifts.[2] On the other hand, two pyrene-linked coumarin-based chemosensors **L2** and **L3** exhibited selective detection of Cu^{2+} and Zn^{2+} ions. The chemosensors **L2** and **L3** differed by a methylene spacer that significantly changed their detection profiles by an emission "*Turn-Off*" response of **L2** towards the Cu^{2+} ion and a "*Turn-On*" behaviour of **L3** with the Zn^{2+} ion.[3,4]

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P-71: Greener and Efficient Transamidation Protocol for Weakly Nucleophilic Aromatic Amines with N-Acyl-2-Piperidinones

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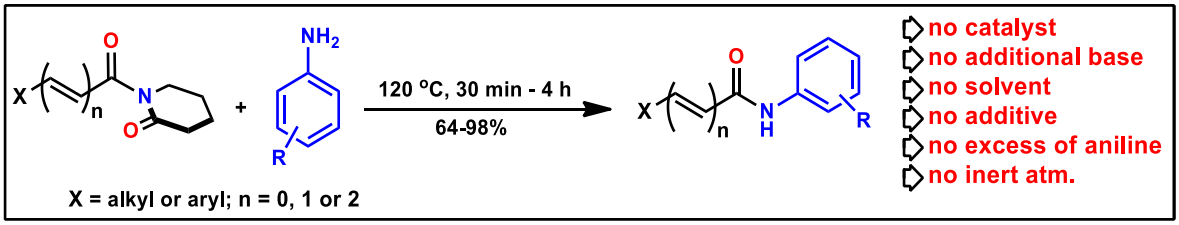

Amides are essential components of the biological system and medicines. It becomes more crucial than ever to create innovative approaches for amide bond formation, preferably under mild and metal-free environments. Transamidation (amide reacts with an amine to generate a new amide) emerged as a promising alternative for amide bond formation. However, amidic resonance and thermoneutral properties make transamidation difficult[1]. In this context, the amide bond twist associated with *N*-acyl-2-piperidones is exploited to overcome the aforementioned limitations (**Scheme 1**). Here, transamidation of *N*-acyl-2-piperidones is demonstrated to occur with non-nucleophilic amines, such as anilines[2] in absence of catalyst, base, additive or solvent. Off-note the developed protocol is chemoselective and operationally simple yet effective at ambient condition. A mixture of *N*-acyl-2-piperidones and anilines was stirred at 120 °C under neat condition furnishes the transamidation product in moderate to excellent yields (64-98%). Electronically diverse anilines were screened as fruitful substrates. Markedly, amines bearing protic hydroxy and carboxylic acid groups were compatible under the reaction condition. To showcase the synthetic usefulness synthesis of bioactive natural products, Avenanthranamide-A, and piperamides was demonstrated. By-product, 2-piperidinones was isolated in 48% for re-synthesis of *N*-acyl-2-piperidinones. Our results suggest that the devised approach potentially be used for the environmentally safe, protection-deprotection-free synthesis of peptides and amide-based medicines.

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P-72: Nano-encapsulation of melatonin into polydiacetylene-phospholipid assembly for sustained-release and enhanced bone formation in zebrafish

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Melatonin, an indoleamine hormone, that is secreted primarily by the pineal gland present in the brain. It regulates the sleep-wake cycle and promotes osteogenesis to prevent bone deterioration.[1] The low bioavailability of melatonin limits its effective antiosteoporosis activity. In the present study, the polymer-supported liposome is used to encapsulate the melatonin in order to enhance its bone formation activity. More specifically, the melatonin drug has enwrapped into a polymer/lipid hybrid nanovesicle (Lip-mel) by the self-assembly of 10,12-pentacosadiynoic acid (PCDA) and 1,2-dimyristoyl-sn-glycero-3-phosphocholine (DMPC) through thin-film hydration method. The liposome-encapsulated melatonin was characterised well by UV – Vis absorption spectroscopy, fluorescence microscopy, energy-dispersive X-ray analysis (EDX), and dynamic light scattering (DLS) measurements. The conjugated yne-ene chain of polymeric backbone of polydiacetylene (PDA) facilitates the formation of stable nanoaggregate[2] from which only 50% of the encapsulated melatonin was leached out even after 72 h under physiological conditions. The Lip-mel shows alkaline phosphatase activity (ALP) and calcium deposition in mouse mesenchymal stem cells more efficient than non-encapsulated melatonin. Furthermore, the Lip-mel elevated the expression of key transcription factors (Runx2, type1 col mRNAs) and secretion of extracellular matrix proteins that are related to osteoblast differentiation. Interestingly, the bone formation in zebrafish model was also enhanced after exposure of Lip-mel compared to melatonin. Thus, the nano formulation of melatonin could be developed as efficient antiosteoporosis drug with better pharmacokinetic properties than that of free form of melatonin.

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P-73: C-H Bond Chlorination by Ni(II)-Biguanide Complexes

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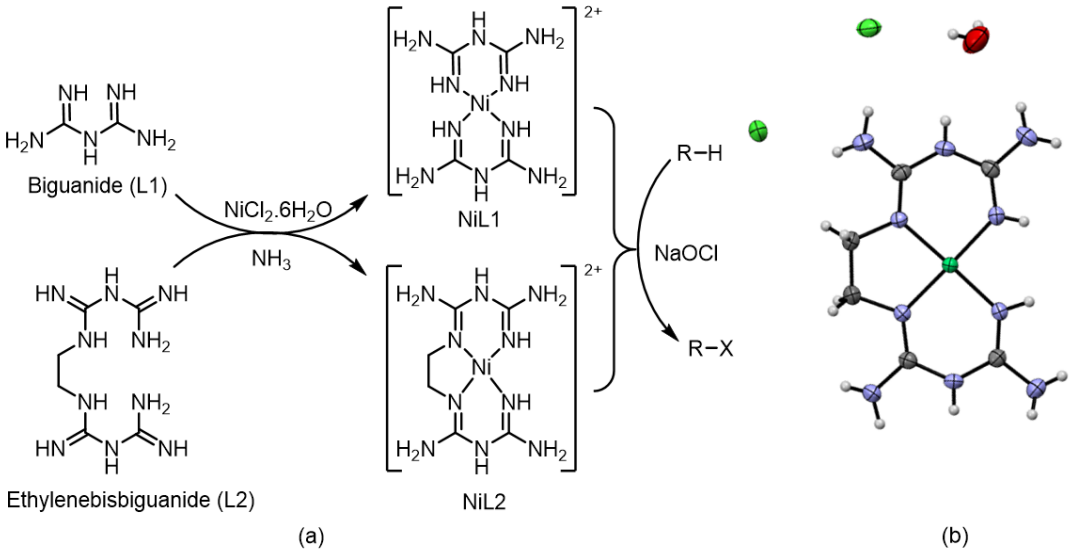

Nickel (II)-biguanide complexes (ML1, ML2, M = Ni^{II}) were synthesized and characterized by various analytical techniques such as single crystal XRD (S-XRD), cyclic voltammetry (CV), ultraviolet-visible (UV-Vis) and high-resolution mass spectroscopy (HR-MS) etc. Ni complexes successfully carried the C-H chlorination of a series of substrates using sodium hypochlorite (NaOCl) as an oxidant and a source of chlorine in water using acetic acid at room temperature (RT). The bond dissociation energy of the $C(sp^3)$–H bond of the substrates varies from 99.3 kcal mol^{-1} (cyclohexane) to 87 kcal mol^{-1} (ethyl benzene). Exclusively chlorinated products (TON: 931 for Toluene) were obtained without any hydroxylated products, thus mimicking the activity of the halogenase enzyme.

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P-74: Insights into calcium-induced aggregation of milk proteins using spectroscopic tools

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The uncontrolled and spontaneous self-assembly of soluble monomeric intrinsically disordered proteins (IDPs) leading to the formation of ordered fibrillar amyloids and/or disordered amorphous aggregates are implicated in various neurodegenerative diseases and systemic amyloidosis. One such IDP namely, casein (CN) is a major constituent of milk which is known to be associated with Corpora Amylacea comprising of casein amyloids that is linked with bovine mammary cancer. Nevertheless, caseins are also used as traditional food ingredients in food processing industries. Among various caseins, β-casein (β-CN) acts as a natural emulsifier and foam stabilizer, and such properties are highly altered during food processing that raises concerns about food quality. Studies have demonstrated that β-CN undergoes self-association in the presence of divalent calcium ions, however, the molecular mechanism remains elusive. We have investigated the structural underpinnings of bovine β-CN aggregation as a function of protein concentration, temperature and varying ionic strength in the presence of calcium chloride utilizing several spectroscopic and microscopic techniques. Our findings revealed that calcium ion is a prerequisite for β-CN aggregation mediated by an interplay of electrostatics and hydrophobic interactions that can be modulated by other milk proteins and varying ionic strength.

P-75: Carbon Quantum Dots embedded Screen-Printing Electrodes electrochemical Aptasensor development for Chlorpyrifos detection

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Organophosphorus based pesticides are commonly used to protect plants from pests but higher exposure could also cause serious health issues on consumer's human health[1]. Among the presence of many organophosphate pesticides, Chlorpyrifos is one of the commonly used organophosphates in the agricultural products by the farmers but high-volume usage in fruits and vegetables is a serious concern about food safety. Also, pesticide contamination leads to several acute and chronic diseases such as Alzheimer's disease, damage of central nervous system and reproductive system etc. Conventional techniques are available such as Gas Chromatography (GC), High performance liquid chromatography (HPLC), Mass Spectrometry (MS) etc. for detection of pesticides,[1] but these are expensive, time consuming and used sophisticated instruments for testing of food samples. Hence, simple, in-expensive, rapid and sensitive method is required to resolve the detection issues. Aptamer based biosensors is one of the selective and sensitive approach to detect the analytes due to large surface to volume ratio, excellent conductivity, good optical and electrochemical properties. Aptamers are single stranded nucleotides having specific and strong binding affinity with target molecules through Vander walls interactions or strong electrostatic interactions[2]. Designing of electrochemical aptasensor require three major steps such as immobilization, signal amplification and assay approaches[3]. In this work, microwave synthesized carbon quantum dots (CQDs) have been drop-casted onto Screen-printed electrodes for fabrication of electrochemical biosensors. CQDs based nanomaterial shows tremendous potential and provide good electro-optical properties, improve bioconjugation and enhance catalytic properties which lead to enhance the biosensing characteristics of the aptasensor such as reproducibility, detection range and selectivity of the aptasensor. Fabricated Aptamer/CQDs/SPE platform used for the detection of chlorpyrifos using electrochemical cyclic voltammetry and chronoamperometric techniques. This aptasensor for chlorpyrifos works in the range of concentration from 0 pM to 500 nM with a detection limit of 0.834 pM and sensitivity of 21.39 µA pM^{-1} cm^{-2} (R^2 = 0.973). Moreover, fabricated aptasensor has shown 5 months stability when stored at 4˚C. Such CQDs based electrochemical aptasensor can be further utilized for the other pesticides detection.

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P-76: Cytotoxic Photoactive Ruthenium (II) Polypyridyl Oxalate Complexes: Synthesis, Characterization, Biological Interaction, and their Anticancer Activity against HepG2 Cells

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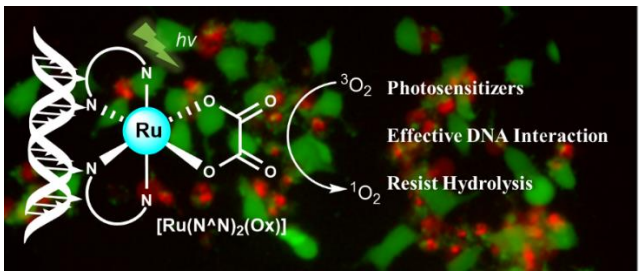

Ruthenium (II) complexes offer multiple drug design opportunities owing to their structural diversity, physiologically accessible variable oxidation states, tunable electronic structure and kinetic lability, rich amenable physicochemical and photophysical properties.[1,2] Ru(II)-polypyridyl complexes though thermodynamically stable, however, they undergoes photoactivation to generate reactive oxygen species (ROS) and ligand dissociation involving low-lying ^{3}MLCT, ^{3}MC or IL excited states which could be exploited in designing photodynamic and photoactivated chemotherapeutic (PDT/PACT) agents respectively.[3,4]

Herein, we present a series of photoactive ternary octahedral Ru (II)-polypyridyl complexes: [Ru(NN)$_2$(Ox)] constructed from two *N*,*N*-donor bidentate ligands (phen, dpq, dppz) as photosensitizer cum DNA binder and an *O*,*O*-donor oxalate ligand. The complexes were thoroughly characterized and their physicochemical and photophysical properties were extensively studied. These octahedral Ru (II) complexes show strong binding affinity with CT-DNA and BSA as confirmed by UV-vis, fluorescence, and CD-spectral titrations. The complexes effectively generate $^1O_2$ upon photoactivation in visible light. We observed potent antiproliferative and anti-migratory effects on liver hepatocellular carcinoma (HepG2) cells. Enhanced photocytotoxicity was observed upon low energy photoirradiation, suggesting their potent PDT/PACT efficacy.

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P-77: Stereoselective Synthesis of Isoxazolidine via Alkyne–Oximium Cyclization

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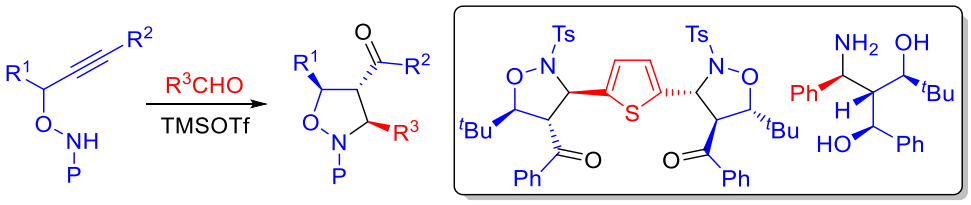

A TMSOTf-mediated alkyne–oximium cyclization on *O*-propargyl hydroxylamines give highly diastereoselective access to isoxazolidines.[1] Various alkene-based approaches for the synthesis of isoxazolidine *via* 1,3-dipolar cycloaddition reaction are well documented in the literature.[2] Surprisingly, synthesis of isoxazolidine from alkyne has received much lesser attention.[3] This method provides new approach to synthesize isoxazolidines bearing three contiguous stereocenters. The strategy could be applied in the synthesis of enantiomerically enriched isoxazolidines. Moreover, the synthetic potential of methodology is demonstrated by synthesizing the corresponding 1,3-aminodiols with precise control over all stereocenters formed.

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P-78: Iodine Catalysed Tandem Stereoselective Acetalation-Glycosylation of Reducing Sugars Using Acetals/Ketals: Application in the Synthesis of EIDD Molecules

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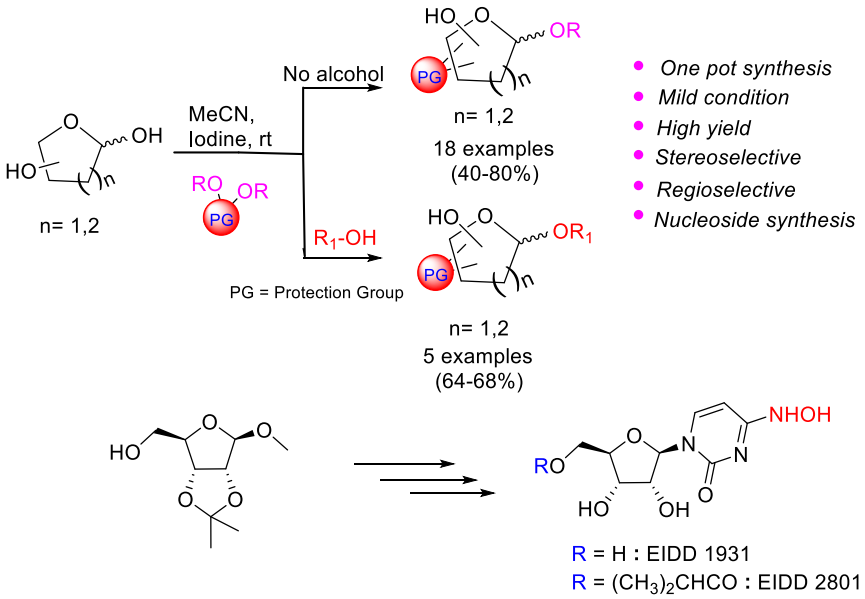

A convenient and efficient one pot method has been developed for molecular iodine catalysed tandem synthesis of acetonide protected *O*-glycosides from reducing sugars using acetals/ketals. Various free sugars reacted smoothly with both acetals and ketals to form orthogonally protected *O*-glycosides using insitu generated alkoxy group in good yields under mild reaction conditions. The methodology works well in presence of external alcohol where in external alcohol present in excess amount subdues intramolecular attack. Acetonide protected methyl riboside thus formed was converted into ribose donor locked up in furanose form and utilized further for synthesizing EIDD 1931 & 2801 molecules the latter being the only orally drug currently in use for treating COVID-19 thus showcasing the applicability off such building blocks.

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P-79: Derivatives of NNO based pincer type ligands as an Inorganic Antibiotics

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Antibiotic resistance-induced infectious diseases are the foremost cause of death worldwide.[1,2] The increasing morbidity and mortality resulting from the resistance of bacteria to antibiotics, accompanied by high medical costs, has become a severe ultimatum to global public health.[3,4] Therefore, it is an immediate need to develop novel antibacterial agents. In this perspective, the work illustrates the synthesis and characterization of a new series of pincer-type NNO donor atom-based ligands and their copper and zinc complexes in high yield (85-87 %). All ligands were characterized by the ^{1}H, $^{13}C\{^{1}H\}$ NMR, and Mass spectroscopy and structure of the ligands and complexes were further confirmed by single crystal X-ray studies. The synthesized compounds were screened against five bacterial strains, *A. baumannii*, *E. coli*, *S. aureus*, *P. aeruginosa*, and *K. pneumoniae*. The ligands and their copper/zinc complexes showed potent activity against *Staphylococcus aureus* (gram-positive bacteria) with MIC in the range 2-16 µg/mL and 16-64 µg/mL, respectively, with low hemolytic and cytotoxic activities. SEM and AFM imaging studies were performed to understand the mechanism of cell death, and the results revealed that cell wall disruption is the main reason for bacterial cell death. The results were further supported by the live/dead fluorescence experiments of the most promising compound, H_2L^{11}, on the cell membrane of *S. aureus*. Time-kill kinetics of H_2L^{11} at the different concentrations on *S. aureus* revealed its tendency to effectively hindered bacterial growth even at 0.25x MIC. It also showed good antibacterial activity against vancomycin-resistant *Enterococcus (VRE) and* vancomycin-sensitive *Enterococcus* (VSE) with MIC in the range of 2-8 µg/mL. The lead compound displayed high activity against clinical isolates of MRSA (methicillin-resistant *S. aureus*) and VRSA (vancomycin-resistant *S. aureus*) with MIC values in the range of 2-4 µg/mL. Taken together, the study shed light on the class of potent antibacterial and antibiofilm agents for combating *S. aureus* infections.

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P-80: Design and Synthesis of a Library of Short Peptide Sequences and In-silico Screening Against pf-DHFR for Antimalarial Chemotherapy

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One million people die from malaria each year, a potentially fatal illness that affects 500 million people globally. The etiological agents of malaria in humans are Plasmodium species *P. falciparum* and *P. vivax*[1]. Since *Plasmodium falciparum* Dihydrofolate Reductase (pf-DHFR) has been identified as a key target for the development of antimalarial drugs, much effort is being put into generating inhibitors of this enzyme. However, drug-resistant strains with mutant DHFR genes have emerged, reducing the effectiveness of the molecule on the parasite[2].

We hypothesised that inhibitors would be extremely selective given the considerable structural differences between human and plasmodium DHFR enzymes. In order to achieve this, we chose to screen potential inhibitors and then analyse the hits *in vitro*. We created a library of peptides using ChemDraw and computationally tested them for interactions with pf-DHFR. The binding energies of the hits and the methotrexate and pyrimethamine controls were compared. At first, we screened for tripeptides with increased binding energies compared to controls. However, during the screening and interaction analysis of hits, we discovered an empty cavity located deep within the enzyme's active site that might be filled with an additional amino acid. We reasoned that tetrapeptide sequence would bind to the enzyme most effectively. Thus, we focused our attention to tetrapeptides in order to fill cavity in the active site and enhance the number of interactions between enzyme and ligand. Solid phase peptide synthesis (SPPS) was used to synthesise and characterise the best post-screen tetrapeptide hits using mass spectrometry.

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P-81: Expedient Access to Polyaromatic Biaryls by Unconventional Ag-Catalyzed Cycloisomerization of Alkynylthiophenes and Au-Catalyzed Double C−H Activation

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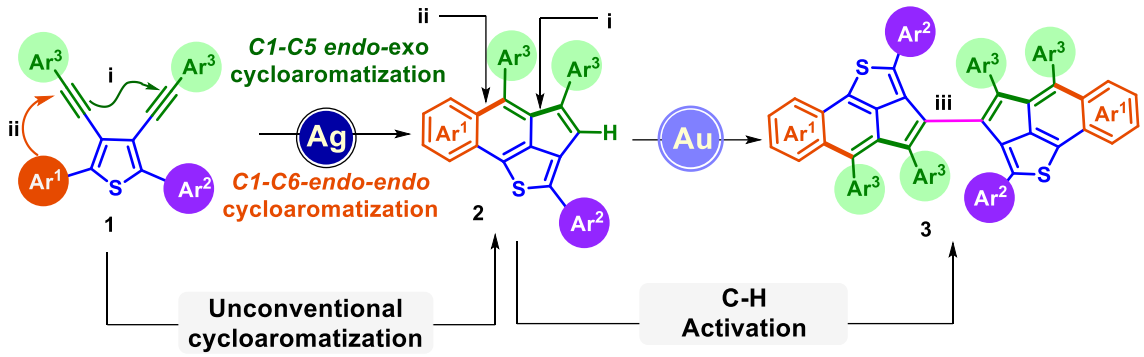

An unconventional approach for the regioselective synthesis of polyaromatic biaryls via site-selective Ag-catalyzed two-fold electrophilic cycloisomerization followed by Au-catalyzed double C−H activation is described. Previous examples have principally been 6-*endo*-dig/6-*endo*-dig, 6-*endo*-dig/5-*endo*-dig, 5-*exo*-dig/6-*exo*-dig cyclization for the synthesis of fused polyaromatics/thienoacenes; however, little is known about 5-*endo*-dig/6-*endo*-dig cascade cyclizations. The developed process allows the synthesis of highly decorated biaryls with excellent regioselectivity. As revealed by DFT computations, the reaction represents a rare example of a 5-*endo*-dig cyclization preceding a 6-*endo*-dig cyclization. The formation of the 6-membered ring is predicted to be the fruit of an uncommon SE_{Ar} on a vinyl carbocation.

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P-82: Kinetic Resolution of Electron Deficient Bromohydrins via Cu (II) Catalysed C-C Bond Cleavage

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The catalytic asymmetric halo functionalization of unactivated alkenes is a powerful synthetic tool for constructing chiral halogenated organic compounds, which are of great synthetic utility. Despite the versatility of these reactions, only a few enantioselective reactions[1] have been reported. Enantioselective halo functionalization with "inert" nucleophiles lacking coordination to the catalyst is less explored.[2,3] Herein, we report the first kinetic resolution (KR) of α, β - unsaturated ketone-derived from bromohydrins (up to S = 250) via the cleavage of C-C bonds, which is enabled by Cu(II)-Ph-Box catalysis in the presence of N-Bromo succinimide. The one-pot synthesis and KR of bromohydrins have also been achieved with excellent enantioselectivities (up to 99% ee). The extended synthetic utility of this process has been demonstrated by exploring a new strategy to convert the recovered enantiomer into optically active epoxides.

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P-83: Organo-catalyzed synthesis of α, β-unsaturated carbohydrate enals (Perlin's aldehyde)

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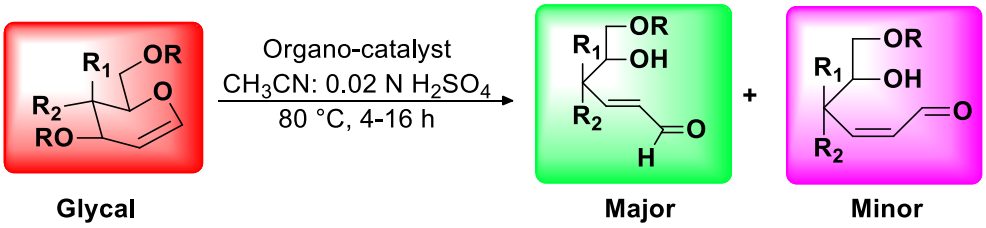

Glycal **Major** **Minor**

α, β-unsaturated carbohydrate enals (Perlin's aldehyde)[1] is a very important precursor for the synthesis of various natural products and their derivatives.[2] It also used in medicinal chemistry for the synthesis of drugs and drug like molecules viz. anti-fungal, anti-bacterial etc. There are two available methods for the synthesis of α, β-unsaturated carbohydrate enals (Perlin's aldehyde) from acetyl, benzyl and alkyl protected glycals. First one is by using $HgSO_4$ and H_2SO_4 and second one is by using mixed Lewis's acid ($HfCl_4$ and ZnI_2).[1,3-4] Recently $InCl_3$ mediated synthesis of Perlin aldehydes was reported by N.G Ramesh et. al.[5] But due to the toxic nature of Mercury (Hg^{2+}) and high cost of Hafnium and Indium (Hf and In), our objective was to explore the synthesis of α, β-unsaturated carbohydrate enals (Perlin's aldehyde) from acetyl and benzyl protected glycal by using various organo-catalysts. The details of this finding will be reported in this poster.

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P-84: Microemulsion route-based synthesis of lanthanum oxides-based nanomaterials and to study their magnetic and photoelectrochemical properties

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Ruddlesden-Popper (RP) compounds are layered complex oxides having K_2NiF_4-type structure with alternating rock-salt-like and perovskites layers. Lanthanum Nickel oxides (La_2NiO_4) and their doped counterparts are of significant interest because of their interesting electronic, magnetic and catalytic properties.[1,2] Traditionally solid-state methods have been extensively used to prepare bulk La_2NiO_4 oxides which preclude control over size and morphology.[3,4] Nanoscale materials are of interest for fundamental as well as applied research because many material properties are governed by the crystallite size and morphology. In this work we tailored different forms of La_2NiO_4 and other related nanostructures through low-temperature reverse micellar route[5] Also, magnetic and photoelectrochemical properties of the different morphological forms of La_2NiO_4 have been studied[,6] in detail which will be presented.

Keywords: Ruddlesden-Popper type structure, Reverse-micelles, Nanostructures, Magnetic properties

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P-85: Manganese Catalyst for α-Alkylation of Nitriles with Alcohols

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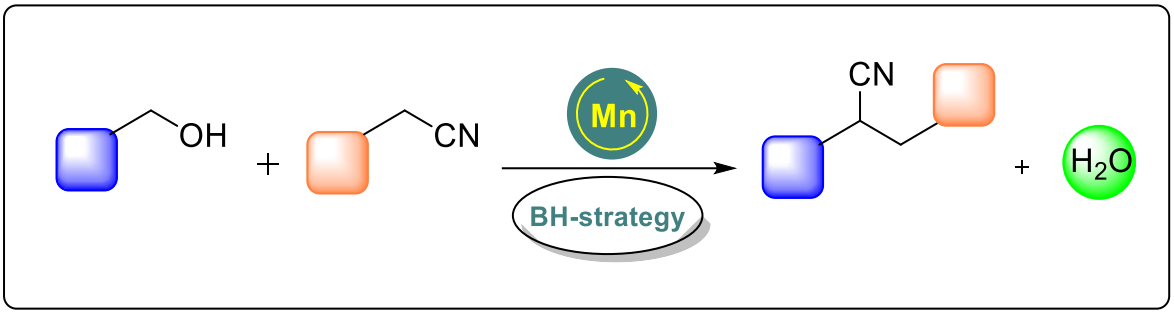

Scheme 1. Mn(I)-catalyzed α-alkylation of nitriles.

Alkylated nitriles are essential building blocks in various biologically active drug molecules and pharmaceuticals.[1] Conventionally, alkylated nitriles were synthesized from organohalides, leading to copious waste generation and making product separation difficult. Amongst the several methods employed for synthesizing alkylated nitriles, the borrowing hydrogen (BH) strategy with the alcohol and nitrile in the presence of an Mn(I) catalyst has shown promising activity.[2] Herein, we present a simple and easy-to-use Mn(I) catalytic system for the alkylation of various nitriles with alcohols (Scheme 1). The catalytic reaction proceeds under benign conditions and results in the formation of α-alkylated products in good to excellent yields.[3] Notably, water is the by-product generated during the catalytic process. This protocol represents a greener footstep for generating various alkylated nitriles under mild conditions.

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P-86: Exploiting the Versatility of 7-Azaindole for Mechanistic Study of Chan-Lam Type Coupling

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The detailed structural and electronic information on reaction intermediates of a new copper(II)-DBU catalytic system for the N-arylation of 7-Azaindole has been studied through multiple spectroscopic techniques, along with single-crystal X-ray analysis. A plausible mechanism using the dimeric copper(II) complex as a catalyst for the coupling reactions has been proposed.[1,2] The role of DBU as a base and also as a ligand has been established. UV-vis spectroscopic studies has helped to demonstrate the transmetalation step involving monomeric aryl-copper(II) species generated from the dimeric unit oxidized by another equivalent of copper(II) to yield an aryl-copper(III) intermediate for facile N-arylation.[3] The regeneration of the copper(II)-catalyst by aerial oxidation of colorless copper(I) species is confirmed by mass and absorption spectroscopy. Detailed DFT and TD-DFT studies has been carried out to propose the reaction intermediates and their corresponding electronic transitions. Moreover, the involvement of Cu(II)/Cu(III)/Cu(I) species in the Chan-Lam type of coupling has been confirmed via HRMS of copper(I)-7-azaindole intermediate.

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P-87: Organophosphorus Catalyzed Stereoselective Borylative Ring-Opening of Vinylcyclopropanes: A Route of δ-Valerolactones

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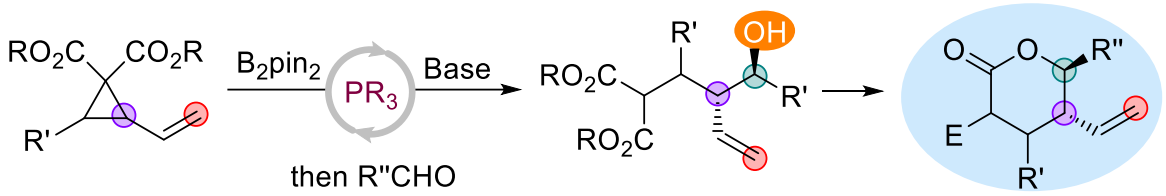

♦ Transition Metal-Free ♦ Diastereoselective ♦ Versatile Products

δ-Valerolactones (DVL) are important bio-feedstock chemicals used as synthons in material sciences and agrochemical industries.[1] DVLs are prominent in several biologically important molecules and commercially used drugs.[2] So far, accessing lactones with stereodefined substituents has often been laborious.[2-3] Herein, we demonstrate an organophosphorus-catalyzed borylative ring-opening of donor acceptor vinylcyclopropanes affording allyl boronates through an umpolung process. A facile coupling of allyl boronates with aldehydes affords homo-allylic alcohols, which undergo lactonization under basic conditions to provide highly functionalized δ-valerolactones. Further, the synthetic utility of obtained allyl boronates and homoallylic alcohol has been demonstrated. A plausible mechanism for borylative ring-opening reaction has been proposed based on the control experiments.

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P-88: Electrochemically synthesized highly stable double zwitterionic Naphthalenediimide from ultra-electron deficient molecule

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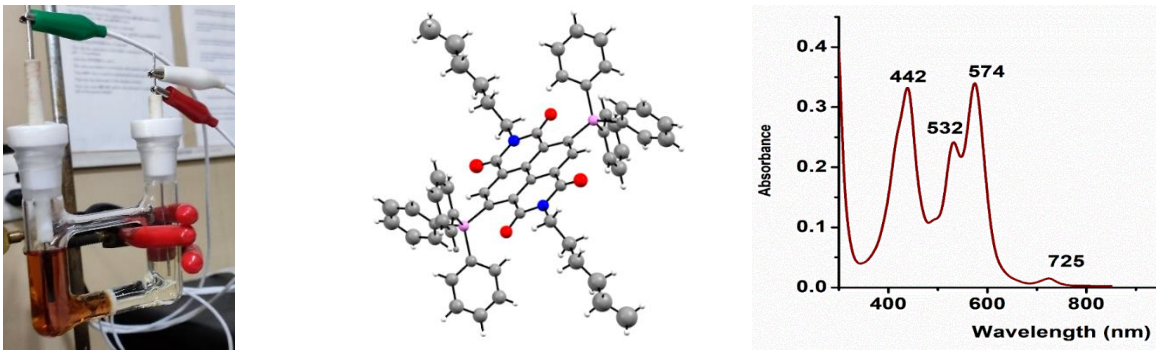

Figure: a) ($C_6(PPh_3)_2$-NDI) Crystals grown in Electro-crystallization setup in MeCN b) X- ray crystal structure of ($C_6(PPh_3)_2$-NDI) ORTEP representation c) UV-vis-NIR spectra of ($C_6(PPh_3)_2$-NDI) in DCM

Here, we synthesized doubly- Zwitterionic, Di- reduced Naphthalenediimide (NDI) through electrochemical method from ultra- electron deficient $(C_6(PPh_3)_2\text{-NDI})^{2+}$ $2BF_4^-$ (E_{LUMO} value is -4.90eV) NDI molecule which is difficult through classical method. This is validated by single crystal X-ray crystallography data and spectroscopic method. Its crystal shows brown and blue colour according to its reflecting angle of polarised light. In this method we were avoiding all kind of hazardous reducing agent and it is easy to synthesis also repeatable.

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P-89: Deep LUMO based Terrylene Diimide with NIR emission

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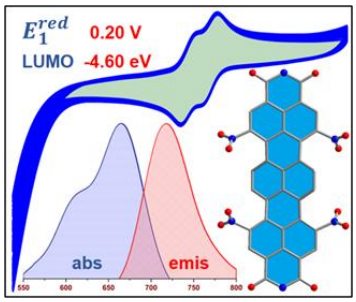

Molecules having emission in Near-infrared (NIR) are gaining high attention due to their applications in Organic Light Emitting Diodes (OLEDs), in organic solar cells (OSCs), and suitable for photobiomodulation (PBM).[1] However, obtaining stable electron deficient NIR emitting molecules with deep-LUMO (≤-4.5 eV) levels are challenging. This can be due to the p-extension strategy utilized for this purpose make them electron rich. Generally, nitro aromatics (having high Electron Affinity) are known to stabilize LUMO levels efficiently, but due their non-emissive nature, are less explored.[2] Shorter Rylene Diimides (RDIs) with electron-withdrawing substituents are shown to attain deep-LUMOs, albeit with no emission.[3] However, nitration of electron rich longer aromatic molecules such as terrylene diimide (TDI) can be an effective platform owing to their absorption and emission spectra in longer wavelength region. Additionally, their less crowded multiple core positions makes them more suitable for above mentioned purpose. In this work, we have synthesized the deep-LUMO based TDI derivatives with emission in the NIR region, using nitration as a strategy. These nitro derivatives demonstrates deep-LUMO levels values ranging from -4.06 eV to -4.60 eV (vs SCE) with excellent redox stability. Interestingly, a LUMO value of **-4.60 eV** observed for Tetra-nitrated TDI (**T_{abcd}**), the lowest observed LUMO for any longer RDIs.

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P-90: Photoinduced apoptosis by Mitochondria targeting Pyrene-mercaptobenzimidazole conjugate due to mitochondrial cardiolipin disruption

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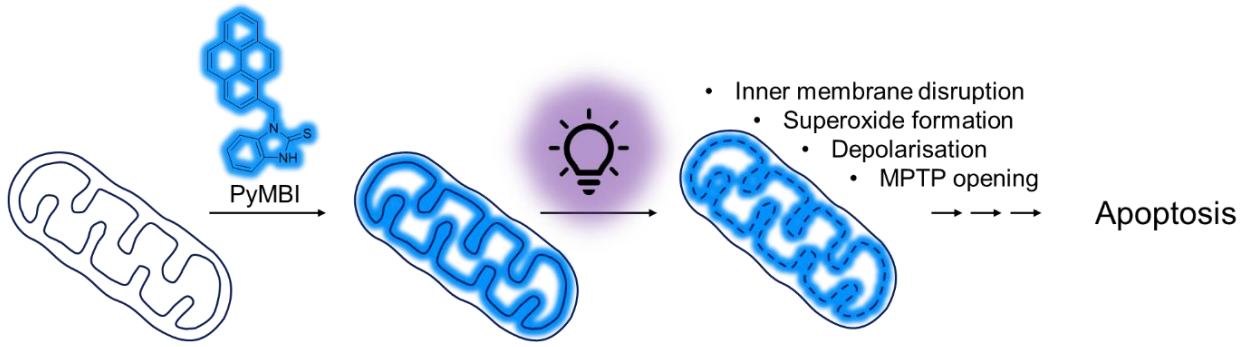

Mitochondria is the powerhouse of cells. It generates ATP, the energy currency of cells. For the first time in 1988, a mitochondrial protein (Bcl-2) was identified as the regulator of apoptosis, a programmed cell death. Mitochondria regulate apoptosis, and thus it is the target of several molecules which specifically induce apoptosis. We designed mitochondria targeting molecule, PyMBI, based on the chemical structures of mitochondrial complex I inhibitors. These inhibitors have heterocyclic moieties attached to the hydrophobic group. To get a light-activated response, we chose Pyrene as a hydrophobic group and attached it to the mercaptobenzimidazole, which quenches Pyrene fluorescence. The photochemical studies suggested a photoinduced electron transfer from mercaptobenzimidazole to pyrene, forming a charge-separated state within femtoseconds. This quickly recombines to create a triplet state on pyrene.

Upon irradiation, PyMBI disrupts mitochondrial cardiolipin and generates superoxide radicals in mitochondria. This triggers apoptotic cell death, which is reversed by decylubiquinone pre-treatment.

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P-91: Controlling the fluorescence intermittency of water-soluble BSA-conjugated Quantum Dots with Super resolution of Lysosome

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The high fluorescence intermittency with short OFF time creates intrinsic limitation for the applications of semiconductor quantum dots in super resolution microscopy, despite their other great advantages over the organic dyes. Here, we show that, bovine serum albumin (BSA) in biocompatible phosphate buffer saline (PBS) media, not only tuned the intermittency of water soluble CdTe QDs, but also helped in specifically staining the lysosomes via endocytotic pathway uptake. Finally, lysosomes were super-resolved to get the image with their size down to ~ 60 nm. The blinking statistics changed from truncated power law to inverse power law from water soluble QDs to the BSA-PBS media. This suggests that the rich electron centre in this system reduces the trap states, tuned the ON-OFF time and finally increases the photons per cycle substantially, leading to the enormous improvement in localization precision.

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P-92: Iron-catalysed alkylation of 2-methyl and 4-methyl azaarenes with alcohols *via* C-H bond activation

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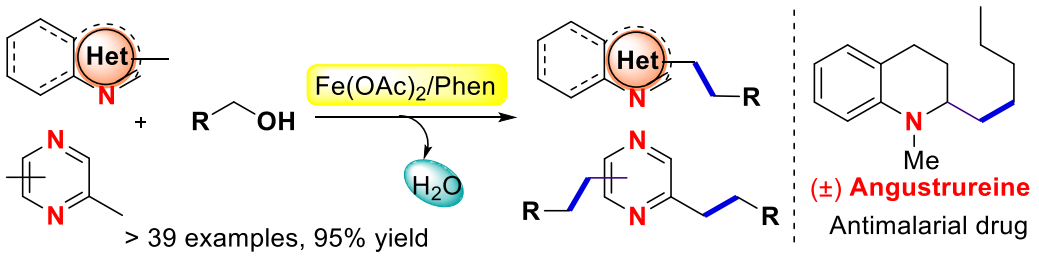

- Non- precious metal-catalyst
- (iso) quinaldine, lepidine, pyrazine and pyridine derivatives
- Mechanistic studies
- scope witharyl, heteroaryl and aliphatic alcohols
- Gram scale reaction
- Multi- functionalization/drug synthesis

N-Heteroaromatics and their derivatives are ubiquitous in various important pharmaceuticals and bioactive compounds and significantly used as lifesaving drugs. Therefore, metal catalysed functionalization of C(sp^3)-H bonds in such azaarenes enables access to valuable *N*-hetero aromatics.[1] In general, the selective functionalization of C(sp^3)-H bonds is associated with high energy barriers. Thus, often metal-catalysed alkylation of such C-H bonds was performed involving directing group assistance in combination with activated olefins or related derivatives.[2] Hence, developing an atom-economic alkylation process for C(sp^3)-H bonds in *N*-heteroaromatics following sustainable technology is a challenging goal.[3] Herein, the first Fe-catalysed alkylation of 2-methyl and 4-methyl-azaarenes with a series of alkyl and hetero-aryl alcohols is reported (>39 examples and up to 95% yield). Multi-functionalisation of pyrazines and synthesis of anti-malarial drug (±) Angustureine significantly broaden the scope of our methodology. The preliminary mechanistic investigation, deuterium labeling and kinetic experiments including trapping of the enamine intermediate were also studied.

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P-93: Drug design, Green Synthesis, Hirshfeld Analysis and anticancer activity of dihydropyriminidone analogs

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DHPM hold a significant value in medicinal chemistry due to its broad spectrum of biological activities antiviral, antitumor and antibacterial etc. In this study, Citrus macroptera juice was used for the first time to synthesize dihydropyrimidine (DHPM) derivatives via the Biginelli reaction, which showed better yield, shorter reaction time, and no organic solvent was required. The synthesized compounds were then crystallised, characterized, and their molecular geometries were established by the single-crystal x-ray
diffraction method. The weak intermolecular interactions in the molecular packing of the synthesized compounds are then investigated and demonstrated. The analysis of self-assembly of synthesized compounds in crystal packing revealed that they expand their supramolecular network mainly by N-H···N, N-H···O, C-H···N, C-H···O, C-H···π, lone pair··π and π··π interactions. Further, the anticancer activity of DHPMs were evaluated in vitro using A549 lung adenocarcinoma cells which significantly inhibited proliferation at 200 μM. The molecular docking study was also carried out to investigate the non-covalent interactions and binding mode of DHPMs in the active site of human kinesin Eg5 protein.

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P-94: Thermodynamic Studies of interaction between basic ligands and DNA

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DNA condensation is a phenomenon in which long DNA fragments experience compaction and aggregate into ordered, highly condensed states. DNA condensation is achieved by positively charged proteins and positively charged amino acids. In DNA condensation DNA, a large structure is wrapped around protein and amino acid so that DNA compaction takes place. It has a role in gene therapy.

In this study we used a lysine and arginine-rich protein. A histone is a special group of proteins found in nuclei of eukaryotic cells responsible for DNA folding and chromatin formation. These proteins prevent DNA from becoming tangled and protect it from DNA damage. Because this protein is positively charged and DNA has a negatively charged phosphate group there occurs electrostatically interaction between protein and DNA

Objective of this study to determine the nature of interaction involved in binding of basic protein with nucleic acid through thermodynamics studies. One of the goals of my research is to investigate the biological and kinetic aspect of DNA condensation.

Importance of study, to determine the interaction of the basic protein with DNA at simulated physiological conditions (pH 7.4) was studied using different spectroscopic approaches. I have observed that there is a presence of electrostatic interaction between protein and DNA because my protein is positively charged and DNA has a phosphate group that is negatively charged.

I have done UV- Vis spectrometer, Fluorescence, Agarose gel electrophoresis these three method used for determine interaction present between basic protein and DNA all method show that there is presence of electrotactic interaction present between basic protein and DNA.On increasing the salt concentration there is a decrease in electrostatic interaction between DNA and protein because of the interference of salt between protein and DNA.

Keywords: Protein, DNA, Interaction between protein and DNA, UV-Vis spectroscopy, Fluorescence, Agarose gel electrophoresis, Salt concentration

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P-95: UV-Light Promoted Oxidative Cleavage of 2,5-Diarylphenanthreno-[*c*]-thiophenes to 9,10-Diaroylphenanthrenes

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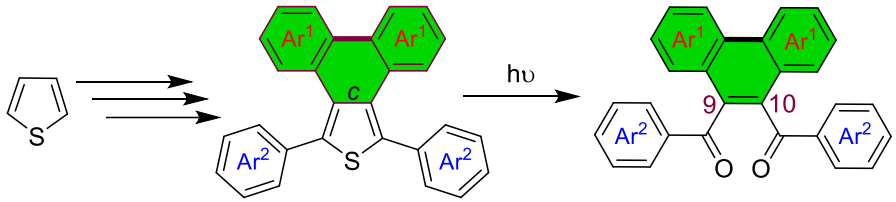

Catalyst-free Light-mediated Broad substrate scope Good to excellent yield

The building block of phenanthrene establishes a group of natural products that are popular for biological activities.[1] The synthetically important 9,10-diaroylphenanthrenes were previously formed via an oxidative cleavage of benzo[*c*]heterocycles employing an oxidant.[2] The most prevalent catalyst-free oxidation strategy for preparing 9,10-diaroylphenanthrene derivatives has not been reported till date. We have developed an unprecedented photocatalyst-free method (Scheme 1) that uses UV light to transform phenanthro-[*c*]-thiophene scaffolds to 9,10-diaroylphenanthrene derivatives under aerobic conditions; the required phenanthro-[*c*]-thiophene precursors were obtained by a metal-free oxidative C–C coupling of 3,4-diarylthiophenes. The developed new method is clean, highly efficient, and affords phenanthrene derivatives in good to excellent yields. In view of the rich chemistry possible with 9,10-diaroylphenanthrene derivatives for the synthesis of annulated arenes and functional hetero-annulated congeners, the former are valuable products.[3,4] In this poster, the oxidative synthesis of 9,10-diaroylphenanthrenes from the commercially available thiophene using UV light will be presented.[5]

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P-96: Circular Polarised Light Directed study in Chirality Regulation of Amino Acid Capped Nickel Nanoparticles

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Induced chirality, chirality transfer, and synthesis of inorganic chiral nanomaterials have attracted increasing recognition due to their multifaceted optical properties[1]. Here we report the one-pot synthesis of L/D-cysteine (L/D-Cys) modified chiral nickel nanoparticles (L/D-Cys@NiNPs). A red shift in the CD signal of the L/D-Cys@NiNPs soluble in an acidic solution, from pure L/D-Cys, signifies the induced chirality[2] by chiral ligands on nickel nanoparticles. Further, the variation in the chirality of L/D-Cys@NiNPs is observed upon irradiation of circularly polarised light. The Absorption of left (L)/right(R) circular polarised light (CPL) communicates the change in the chirality of (L/D-Cys@NiNPs). A change in the extent of chirality (*g*-factor) by left (L)/right(R) circular polarised light is due to the light-matter interaction-induced change in morphology of (L/D-Cys@NiNPs). The chiral L/D-Cys@NiNPs can be utilized as catalysts in asymmetric synthesis and spintronic devices.

keywords: Circular dichroism, Circularly polarised light, Anisotropic dissymmetry factor, Optical chirality

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P-97: Metal-Organic Framework Encaged Monomeric Cobalt (III)-Hydroperoxides Enable Chemoselective Methane Oxidation to Methanol

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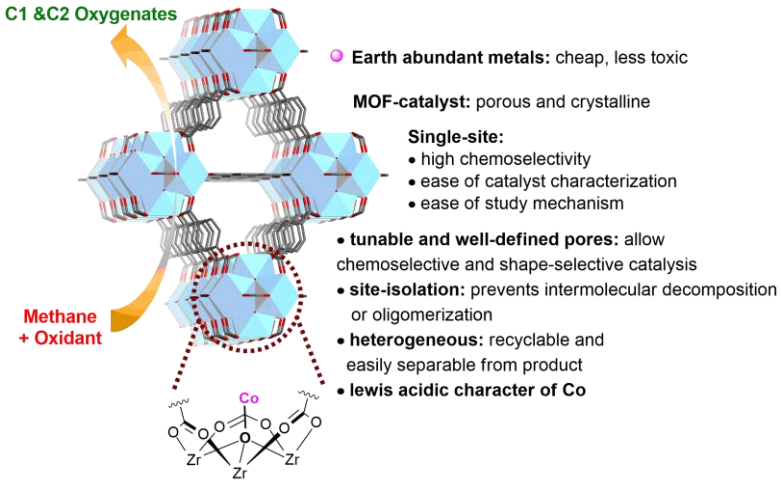

Figure 1. Earth abundant metals anchored onto the SBUs of UiO-66 MOF

We have synthesized a UiO-66 MOF supported cobalt catalyst with the highest ever reported methanol yield, to the best of our knowledge using a non-noble metal, along with more than 90% selectivity and a decent conversion in water along with an oxidant. Mercury test further ruled out the possibility of any activity of leached metal nanoparticles. MOF also showed recyclability and stability with a slight decrease in methanol yield in each run with minimal leaching of post synthetically attached metal or zirconium.

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P-98: Phytochemical profiling and GC-MS analysis of Nigella sativa (black cumin) seeds.

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Nigella sativa (black seed) is an annual flowering plant from Ranunculaceae family, native to southwest Asia. The use of its seeds and oil is common for treatment of many diseases, including rheumatoid arthritis, asthma, inflammatory diseases, diabetes and digestive diseases. *N. sativa* has many biological effects such as anti-inflammatory, anti-hyperlipidemic, anti-microbial, anti-cancer, anti-oxidant, anti-diabetic, anti-hypertensive, and wound healing activities. The GC-MS analysis revealed the presence of seventeen bioactive compounds which include p-cymene, acetophenone, thymoquinone, 1,8,11-Heptadecatriene, Octadecenoic acid, Glycidyl palmitate. Compounds were purified by silica gel column chromatography and preparative thin layer chromatography.

Keywords: *Nigella sativa*; Black seed; GC-MS analysis; Chromatography 0.Z.

P-99: *tert*-Butyl nitrite mediated azo coupling reactions of imidazole derivatives and sulphur containing amino compounds

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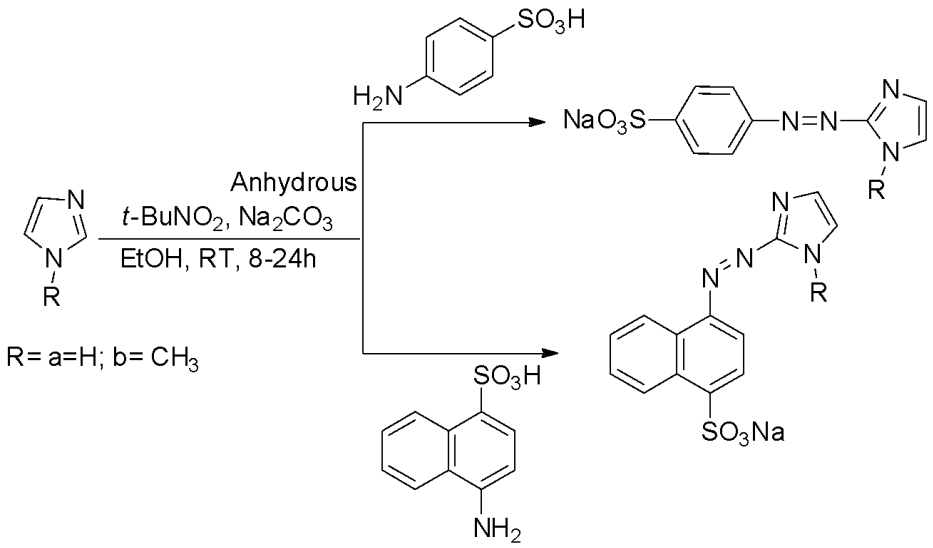

The heterocyclic azo compounds have received special attention owing to their applications in cosmetics, therapeutics, dyes and pigments and in biomedical investigations.[1] A wide range of syntheses and applications of different heterocyclic azo compounds have been reported, but very few reports are accessible, wherein imidazoles are used as coupling agents in diazotisation reactions. In view of this, four new, dark yellow to red azoimidazoles were synthesized *via* non-aqueous diazotization reaction using *tert*-butyl nitrite at room temperature**.** The structures of the synthesized compounds were confirmed by HRMS, IR, ^{1}H and ^{13}C and 2D NMR spectral techniques. The solvatochromic behaviour of the synthesized compounds was investigated in DMSO, DMF, methanol and water using UV-vis spectrophotometer. The use of the synthesized compound as a dye on the silk fabric was also investigated. The colour strength and overall fastness properties were investigated using Gray Scale method. It is found that the compounds exhibit moderate to good fastness property with reference to washing, perspiration, ironing and rubbing.

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P-100: Redox Induced Diverse Functionalization of Bis (aldiimine) Ligands on Electron Rich Ru-Platform

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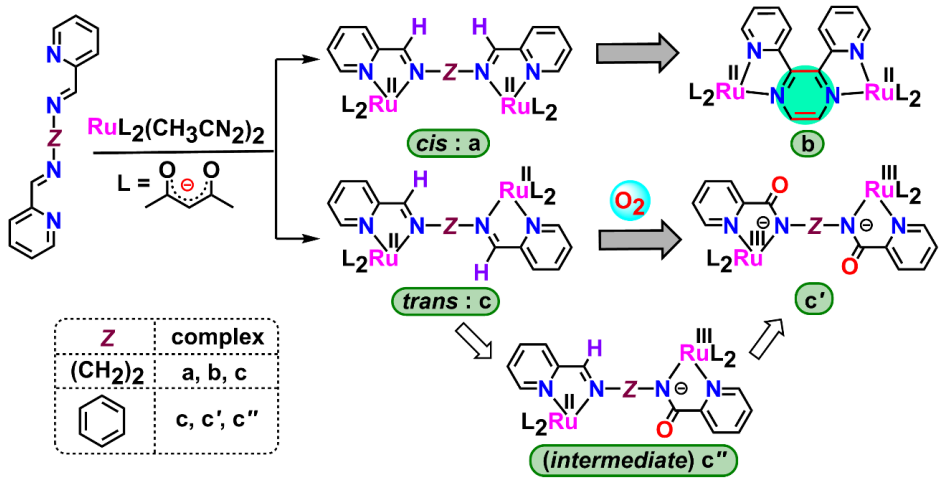

Electron shuttling on the metal-ligand interface facilitated variegated functionalization[1] of redox non-innocent bis(aldiimine) derivatives in presence of electron rich ruthenium {Ru(acac)$_2$}. The modes of functionalization principally varied based on the nature (aliphatic versus aromatic) of the linker (Z). In this context, acyclic BPE (N,N′-bis(2-pyridylmethylene)ethylenediamine) (Z= $(CH_2)_2$) derived *cis*-diruthenium complex (a) underwent redox mediated transformation into cyclic DPP (2,3-bis(2-pyridyl)pyrazine) *via* intramolecular C-C coupling, [2] whereas, PBP (*p*-phenylene-bis(picoline)aldimine) (Z = Ph) derived *trans*-diruthenium complex experienced stepwise activation of molecular oxygen to generate (bis(pyridine carboxamide)benzene) derived isovalent ($Ru^{III}Ru^{III}$, S=1) complex via the formation of ((*E*)-*N*-(4-((pyridin-2-ylmethylene)amino)phenyl)picolinamide) derived mixed valent ($Ru^{II}Ru^{III}$, S=1/2) intermediate under aerobic condition.[3] The detailed mechanistic outline for the generation of all the functionalized products was authenticated by experimental (UV-vis. kinetics, hydrogen evoluation) and theoretical (transition state) investigations.

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P-101: Sulfonyl Promoted Michaelis-Arbuzov Type Reaction: An Approach to S/Se-P bonds.

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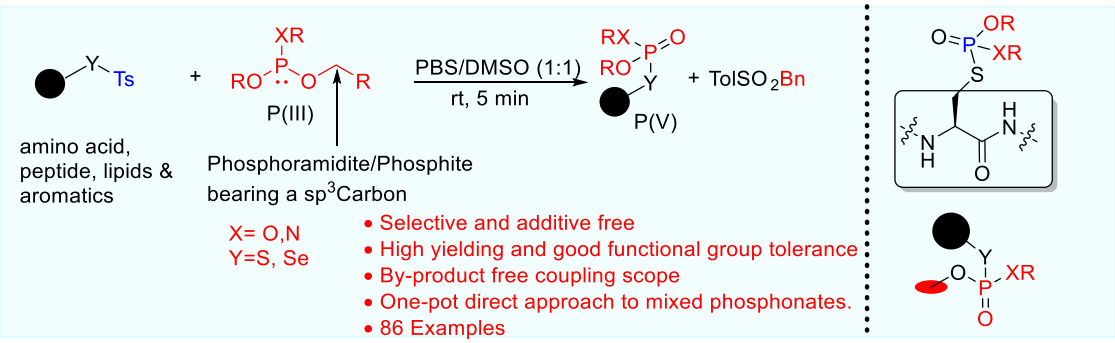

By chemical conversion of thiols to thiosulfonates, phosphoramidite/phosphite bearing sp^3 hybridized carbon serve as ideal coupling materials to forge new connections at room temperature. In this work, functional group induced, additive free, novel, S-P bond forming approach is presented. This protocol exhibits good functional group tolerance with wide applications that includes phosphorylation of cysteine derivatives, development of one pot approach to mixed unsymmetrical thiophosphonates and extension of the concept to different Se-P bonds. Meticulously, our reaction also generated S-P bond against cyclic 1,2-dithiane-1-dioxide in a by-product free manner. These Michaelis-Arbuzov type reactions are easy to conduct, works efficiently in reduced reaction time and are applicable to gram-scale preparation as well.

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P-102: Furan Appended Benzothiazole Based Schiff Bases For a Highly Selective Visual and Fluorimetric Detection of Cu^{+2} ion with Density Functional Theory Studies and its Application For Real-life Samples.

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A recent research problem is the design of an efficient and compact analytical method to find a trace amount of hazardous metal ions in environmental samples. A new Schiff base receptor **(R1)** was synthesized by an equimolar reaction between conjugated furfural and 2-hydrazinobenzothiazole in an ethanol solution. Subsequently, **R1** was deployed for the ratiometric detection of Cu^{2+} ions in the THF medium. **R1** receptor show both chromogenic and fluorogenic responses in the presence of copper ions. The absorption study of the chromogenic receptor of Cu^{2+} displayed a discernible color change from yellow to copper brown color with a red shift ($\Delta\lambda \approx 60$ nm) and also reveals the astonished quenched emission spectrum at (λ_{em} = 529 nm) with high selectivity and sensitivity in a linear concentration range 0 -120 μL of Cu^{2+}. The remarkable water tolerance of the **R1** is up to 90% and is an excellent probe for testing biological and real-time samples. **R1** is stable between pH 2 to 10 and R1-Cu^{2+} complex is stable in acidic pH. The Job's plot, which showed a 2:1 ratio of **R1** and Cu^{2+} ions was used to determine the stoichiometric ratio, and the LOD was found to be 1.3 x 10^{-8}M by the photoluminescence spectroscopic techniques. Based on these findings, the probable applicability of **R1** for identifying Cu^{2+} in environmental samples and vegetable extract is confirmed; the recovery rates were around 97 and 98% respectively. When a R1-$Cu2^{+}$solution was coated on paper strip it shows a colour change and therefore used as the solid support sensor. The **R1** and complex formation was confirmed by (FT-IR) Fourier Transform Infrared Spectroscopy, (^{1}H-NMR) Nuclear Magnetic Resonance spectroscopy, (HRMS) High-Resolution Mass Spectroscopy, (UV-vis) Ultraviolet-visible spectroscopy, (FL) Fluorescence spectroscopy, B-H plot, Job's plot, and (DFT) Density Functional Theory calculations.

Keywords: Furan, Benzothiazole, Schiffs base, Fluorogenic Sensor, Cu^{2+} detection, DFT

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P-103: Synthesis and mechanistic studies of Isatin-pyrazole hydrazones as bacterial MetAP Inhibitors

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To explore the antimicrobial potential of novel *N*-heterocyclic containing scaffolds, we designed and synthesized Isatin-pyrazole hydrazone conjugates (**PS1-14**) and screened them as bacterial methionine aminopeptidases *(MetAPs)* inhibitors. The results indicated **PS9** emerged as a potent and selective inhibitor of prokaryotic *MetAPs* i.e. *Mt*MetAP1c, *Ef*MetAP1a, and *Sp*MetAP1a with ***K***i values of 0.31, 0.69.3 and 0.37 µM respectively compared to *Hs*MetAP1b with ***K***i (631.7 µM). All the conjugates were also screened for their antibacterial activity, and the results identified compounds **PS3, PS6, PS9**, and **PS11** as growth inhibitors which were further validated by Minimum bactericidal concentration (MBC), disk diffusion assay, growth curve, and time-kill curve assays. Moreover, the best inhibitor **PS9** did not show any cytotoxic effect on human red blood cells (*h*RBCs), Human Embryonic Kidney cells (HEK293), and *Galleria mellonella* larvae *in vivo*. **PS9** further inhibited growth of multidrug-resistant environmental bacterial isolates with low MIC values than the standard drugs. Overall, the study led to identification of a potent antimicrobial compound **PS9,** with high and selective affinity towards bacterial MetAPs, no significant toxicity in mammalian cells and effective growth inhibitors of sensitive as well as MDR resistant bacterial strains.

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P-104: Evolution of IBX based oxidation: Transformation of alcohols into corresponding aldehydes and Ketones

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Transformation of alcohols into their corresponding carbonyl compounds is a very common practice in organic synthesis.[i] A different class of oxidant has been developed for the same purpose. Hypervalent iodine reagents are very popular for controlled oxidation of alcohols into aldehyde or ketone.[ii] IBX was first synthesised in late 19th century (1893) by Hartmann and Meyer. It was a two-step methodology which involves transformation of 2-iodobenzoic acid into 2-iodosobenzoic acid (IBA) followed by treatment IBA with alkaline $KMnO_4$.[iii] This periodinane (IBX) was unexploited due to its insolubility in common organic solvent. A century later in 1983 Dess and Martin developed its acetyl derivative which was able to oxidize alcohols into aldehyde or ketone in dichloromethane under mild reaction condition.[iv] Earlier we have developed an IBX-TfOH based system which has shortened the oxidation time of alcohols under mild reaction condition. This methodology involves very easier purification and isolation of oxidised product.[v] In continuation we have developed a camphor sulfonic acid assisted, IBX based oxidation methodology. The methodology involved *in-situ* generation of IBX based oxidant and it was confirmed by HRMS. Mild reaction condition, broad substrate scope, easier isolation makes this methodology very useful in organic synthesis.[vi]

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P-105: Vanadium-based Mixed Metal Oxides for effective removal of Toxic Pollutants

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Wastewater is a major environmental issue that is becoming more prevalent in many industries. This issue has been identified as a major bottleneck in the textile industry. The textile industry uses a lot of synthetic dyes and dumps a lot of colored dyes into the water(Holkar et al., 2016). Toxic pollutants in water make it murky and increase its toxicity, both of which are undesirable. In this context, various nanomaterials have been explored to remove or degrade the pollutants present in wastewater. Vanadium is the most abundant element having many catalytic applications in the fields of lithium-ion storage batteries, electrochemical properties, photochemical catalysis, and in ceramic industries. Vanadium-based mixed metal oxides show their property as an adsorbent in the effective removal of dye from wastewater. In this work, these nanomaterials have been synthesized via the hydrothermal technique, and they were characterized by several analytical techniques. These synthesized nanomaterials exhibited successful adsorption of methylene blue (MB) dye. The kinetic studies were analyzed in detail to know the mechanistic aspects. This study displays the use of vanadium-based nano adsorbent in a simple, cost-effective, and easy method for the efficient removal of pollutant dye (Muthukumaran et al., 2016).

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P-106: Aromatic C-H Activation by Bioinspired Cu(II)- complexes

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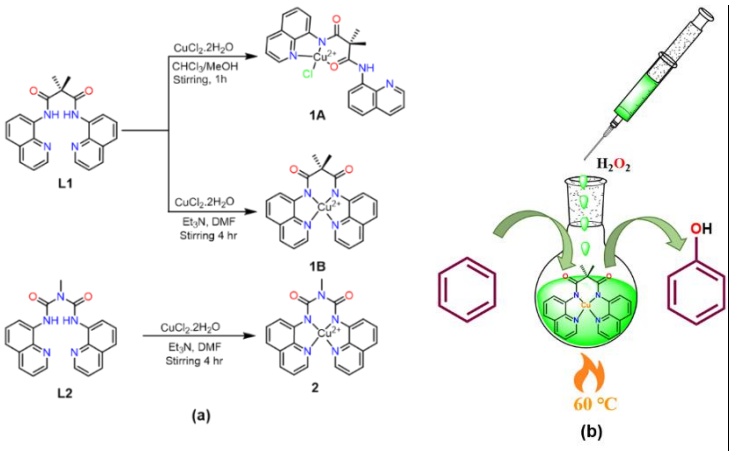

- ✓ Green Oxidant
- ✓ Low catalyst loading (0.01mol%)
- ✓ Phenol Selectivity > 90 %
- ✓ Acid & Base free
- ✓ TOF 2.5/min
- ✓ TON>800

Cu (II) complexes consisting of tetradentate-amidoquinoline ligands (L1 and L2) were synthesized (Scheme 1a) and characterized by various analytical methods (Single crystal XRD, UV-Vis, HR-MS, EPR and CV). All these complexes effectively catalysed the single-step hydroxylation of aromatic C-H bonds using hydrogen peroxide as an oxidant without using an external base and afforded greater than 90% selectivity for phenol with a TON of 810 for benzene. The kinetic isotope effect (KIE) values (1.1-1.3) supported the involvement of metal-bound oxygen species.[1] Formation of Cu(II)-OOH species was also proved by UV-Vis, HR-MS and EPR spectroscopy.[2] The negative value (-0.167) obtained from the Hammett plot of substituted arenes helped in the interpreting the electrophilic aromatic substitution pathway.[3] Based on our experimental findings and density functional theory (DFT) calculations, a plausible mechanism for aromatic C-H hydroxylation was proposed.[4]

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P-107: Effect of Dehydrating Agent on the Kinetics of Ligand/G-quadruplex DNA Interaction

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G-quadruplex (G4) structures in nucleic acids takes part in various molecular processes in cells such as replication, gene-pausing, expression of crucial cancer-related genes and DNA damage repair. Several targeting G4-drugs usually bind to the G4 DNA structures, some of them can also facilitate the G4-folding of unfolded G-rich sequences and stabilize in absence of ions.[1] The kinetics of ligand binding to G-quadruplex DNA (GqDNA) structures has a paramount importance for comprehending (possible) ligand-induced anticancer activity involving GqDNA within cells.[2-3] Although only few earlier studies dealt with deciphering the kinetics of ligands/GqDNA interactions in dilute solution,[4-5] such studies in cell-like crowded milieu are limited. However, cellular environment is crowded with variety of small- and macro-molecules that occupy ~30 - 40% of cell-volume.[6] In this investigation we elucidate the effect of dehydrating agent on the kinetic steps of association and dissociation of a rhodamine dye containing a fluorescent xanthene core; specifically, Rhodamine 6G (RhG), with parallel-GqDNA structure using fluorescence correlation spectroscopy (FCS), followed by other methods. For this study we used ethanol as dehydrating agent, the steady-state fluorescence results show that the binding constant of the ligand to the GqDNA decreases in presence of 20% ethanol as compared to buffer solution. These results have further important implications in the context of ligand/GqDNA interactions within the crowded cellular environment.

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P-108: Phytochemical study of Petroleum Ether Extract of Seeds of *Psoralea Corylifolia* by GC-MS

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Psoralea corylifolia belongs to the family Leguminosae and subfamily papilionacea, commonly known as babchi, is a popular herb, which has since long been used in traditional Ayurvedic and Chinese medicine for its magical effects to cure various skin diseases. This plant is also pharmacologically studied for its chemoprotective, antioxidant, antimicrobial, and anti-inflammatory properties. Roots, stems, leaves, and seeds treat obstinate skin problems, such as leukoderma, skin rashes, infections, and others in the ayurvedic system of medicine. Its oil has a powerful effect on the skin Streptococci. In addition, it helps fight vitiligo, a disorder in which patches of skin lose their pigmentation. Herbalists also prescribe seeds of this plant in inflammatory diseases, mucomembranous disorders, dermatitis, and edematous skin conditions. It treats itching red papules, boils, itching skin eruptions, extensive eczema with the thickened dermis, ringworm, rough and discoloured dermatosis, and dermatosis with fissures. It purifies blood therefore also used to address scabies. The air-dried Seeds of Psoralea corylifolia (4kg) were coarsely powdered and then extracted with petroleum ether for 12*3 hours on a water bath. The petroleum ether extract was filtered, removal of the solvent under reduced pressure gave viscous oily extract. The GC-MS analysis revealed the presence of twenty-three bioactive compounds which include 4- [3,7-dimethyl-3-vinyl-1,6-octadienyl] phenol, Isopsoralen, Ficusin, trans, trans-9,12-Octadecadienoic acid, propyl ester, and dichloroacetic acid tridec-2-ynyl ester.

Keywords: -Psoralea corylifolia, babchi, GC-MS analysis, antimicrobial activity.

P-109: Stereoselective Synthesis of Densely Functionalized Indenes via Regioselective Cascade Iodoalkylation of Alkyne

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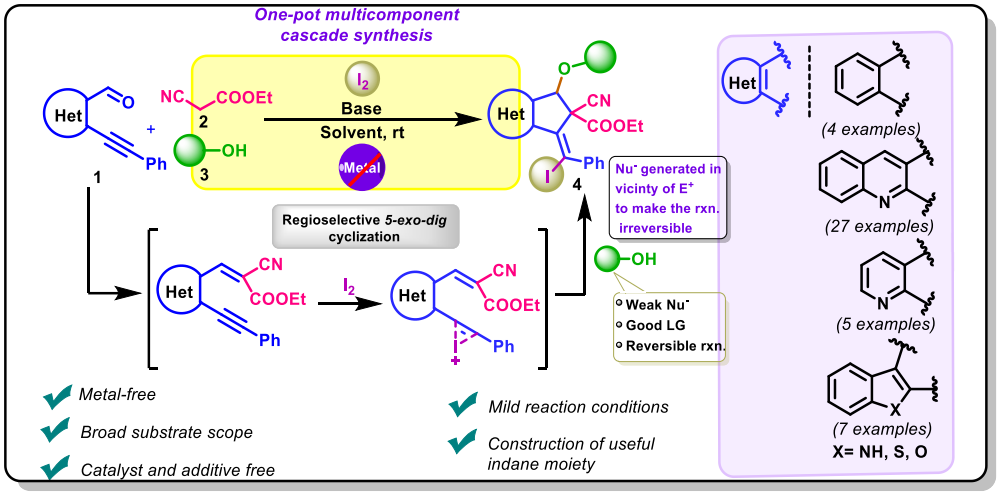

Herein, one pot two-step approach for the stereo-selective construction of privileged indene skeleton has been achieved under the metal and additive-free conditions via base promoted regioselective cascade iodoalkylation of alkyne. Michael addition of methanol to the carbon-carbon double bond initiated the consecutive formation of C–O, C–C, and C–I bond in a single operation. The synthesised product contains exocyclic double bond along with numerous groups like -CN, -COOEt,-I and -OMe which can be easily transformed to afford biologically active pharmacophores.

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P-110: Chiral iron(II)-catalysts within valinol-grafted metal-organic frameworks for enantioselective reduction of ketones

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Chiral amino alcohols, prepared by reducing chiral amino acids, are an important class of organic compounds containing both an alcohol and an amine functional group. Although optically active amino alcohols are primarily used to synthesize chiral oxazolines,[1-2] their application in asymmetric metal catalysis as chiral ligands is limited due to lack of steric substituents leading to the formation of multinuclear catalytic species. We have developed amino alcohol functionalized metal-organic frameworks (MOFs) that could be used as solid chiral ligands to prepare robust single-site earth-abundant metal catalysts via site-isolation for asymmetric organic transformations. The L-valinol-functionalized MOF (L-valol-UiO) was synthesized by post-synthetic treatment of L-valinol and aldehyde-functionalized Zr-UiO-68 MOF. The metalation of L-vol-UiO with $FeCl_2$ in THF afforded the corresponding Fe-functionalized MOF (L-vol-UiO-FeCl). At a 0.5 mol% Fe-loading, L-vol-UiO-Fe was an active heterogeneous catalyst in hydrosilylation of ketones at room temperature to afford the corresponding silyl ethers with high yields and excellent enantiomeric excesses up to 99%. The MOF-catalysts could be recycled and reused multiple times, and the leaching of iron into the supernatant was very low. The oxidation state and the coordination environment of the iron-centre within L-vol-UiO-Fe were established by XANES and EXAFS studies. The detailed mechanistic investigation of the catalytic hydrosilylation reactions by kinetic, spectroscopic, and computational studies will also be discussed.

Keywords: asymmetric catalysis, chiral amino alcohols, metal-organic frameworks, enantioselectivity

References:

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P-111: Brookhart's Acid-Catalyzed Switchable Regioselective *N*-Alkylation of Arylamines/Heterocyclic Amines with Cyclopropylcarbinols by Temperature Regulation

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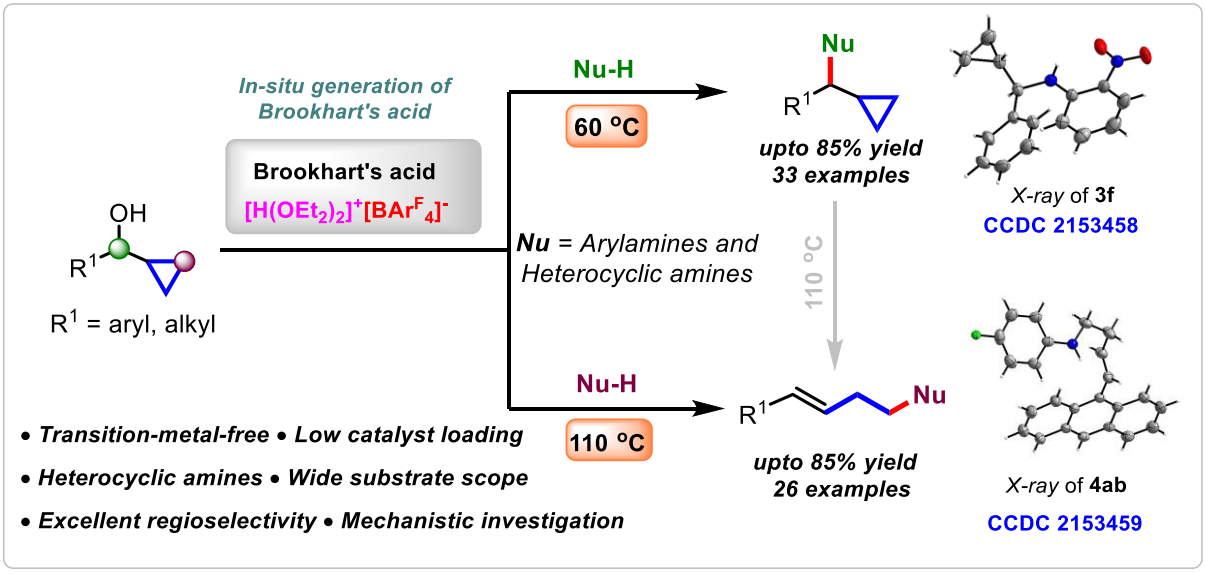

An unprecedented, Brookhart's acid catalyzed temperature switchable regioselective divergent approach for *N*-alkylation of arylamines and heterocyclic amines by utilising cyclopropylcarbinols is presented herein. The reaction offers *N*-alkylated cyclopropyl derivatives and homoallyl amines by employing 2.5 mol% catalyst loading at different temperatures in excellent regioselectivity and yields. This method has shown to be relevant with a wide range of cyclopropylcarbinols, including aliphatic ones. Several control experiments and spectroscopic studies have been performed to gain insight into the reaction mechanism. Further, the synthetic utility of the protocol has also been described.

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P-112: Mononuclear/Binuclear [$V^{IV}O$]/[$V^{V}O_2$] Complexes Derived from 1,3-Diaminoguanidine and Their Catalytic Application for the Oxidation of Benzoin via Oxygen Atom Transfer

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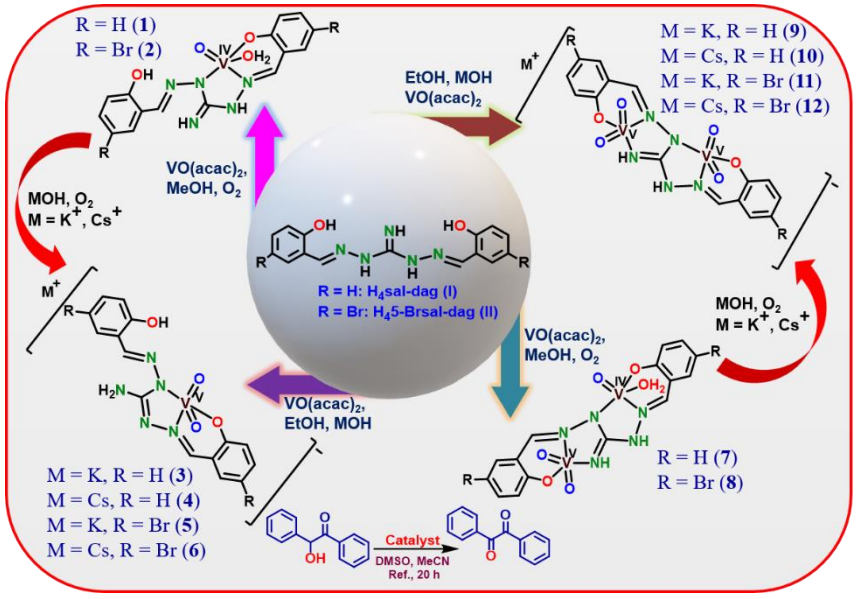

Twelve different vanadium complexes with 1,3-diaminoguanidine based ligands [**I** and **II**] have been prepared by reacting them with suitable vanadium precursors in the molar ratios of 1:1 and 1:2 in the presence/absence of O_2 and/or K^+/Cs^+ salt. These complexes are effective catalyst for the oxidation of benzoin to benzil via oxygen atom transfer (OAT) between DMSO and benzoin. Independent of catalysts used, a stable oxidovanadium(IV) intermediate is the proposed active species involved in the catalytic cycle.

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P-113: Photo-Induced Decarboxylative Radical Cascade for Synthesis of Quaternary-CF_3 Containing Oxindoles and Indoline-Alkaloids

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Oxindole and its related alkaloids are common skeletons found in various natural products, and exhibit diverse biological activities.[1] Additionally, the presence of an electronegative fluorine atom modifies the physicochemical properties of a molecule,[2] hence 3-trifluoromethylated (-CF_3) oxindole derivatives have become very attractive scaffolds for drug discovery.[3] This metal and additive-free, photo-induced decarboxylative radical alkylation-cyclization of CF_3-acrylamides with alkyl redox-active esters enabled corresponding quaternary CF_3-oxindole derivatives in good yields. The present approach has been extended for concise synthesis of CF_3-attached bio-active indoline alkaloid analogues. Further, the reaction is likely to proceed through initial photoexcitation of redox-active ester followed by SET process with acrylamide.

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P-114: Bolaamphiphilic Surfactants Derived From L-Lysine and L-Glutamic Acid

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The noun "bola" relates to the shape of a South American missile weapon.[1] The simplest form of "bola" consists of two balls which are attached to both ends of a cord. The term "bolaform electrolyte" (short form: "bolyte" or "bolion") was introduced by Fuoss and Edelson in 1951 for a chain of hydrophobic groups connecting two hydrophilic end groups. For less water-soluble analogues, the name "bolaform amphiphiles" (short form: "bolaamphiphiles") is preferred.[2] Bolaamphiphiles are an extensive family of molecules with interesting chemical structures, which give self-assembled supramolecular architectures with a wide spectrum of applications. The biological and biochemical applications of amino acids and synthetic peptides have evolved over the years, offering an effective means to satisfy the technological demand of modern biomaterials. Design of peptide-based bolaamphiphiles offers a simple and facile means to organize peptide and amino acid motifs with the aid of nonbiological hydrophobic Centres, realizing a protein-mimetic configuration at the molecular level. Inspired by these thoughts, we have synthesised a new class of amino acid based bolaamphiphilic surfactants derived from L-Lysine and L-Glutamic acid residues and have studied their aggregation properties. The results of our studies in this direction are presented in the poster.

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P-115: Substituent-controlled selective synthesis of 1,2-diketones and internal alkynes from terminal alkynes and arylboronic acids *via* α-stilbene radicals obtained from heteroleptic Cu(I) complexes under visible light

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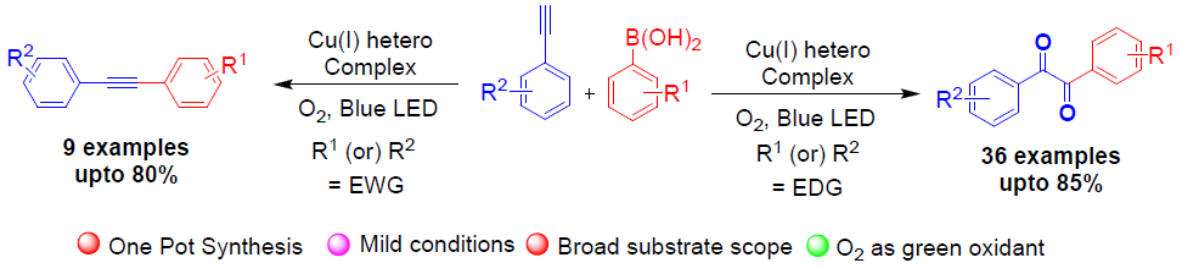

Diaryl 1,2-diketones scaffolds are important structural motifs which are present in various natural products[1]. Therefore, a variety of synthetic strategies have been developed for their synthesis. Herein, we report a substituent-controlled synthesis of 1,2-diketones and internal alkynes from terminal alkynes and arylboronic acids *via* α-stilbene radicals obtained from heteroleptic Cu(I) complexes under visible-light irradiation. The *in situ* generated α-stilbene radical Cu (II)-complex was achieved by photoinduced C_{sp}–C_{sp}[2] coupling of copper(I) acetylides[2] and aryl radicals catalysed by heteroleptic Cu(I) complexes. This photochemical approach offered high atom economy with a low *E*-factor and functional group tolerance under mild reaction conditions. Mechanistic insights clearly show that the reaction proceeded *via* copper(I) acetylides and the phenyl radical intermediate pathway.

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P-116: Diastereoselective Decarboxylative Alkylation of Coumarins via Dual Synergistic Role of Cerium in Ligand-to-Metal Charge Transfer and Lewis Acid Catalysis

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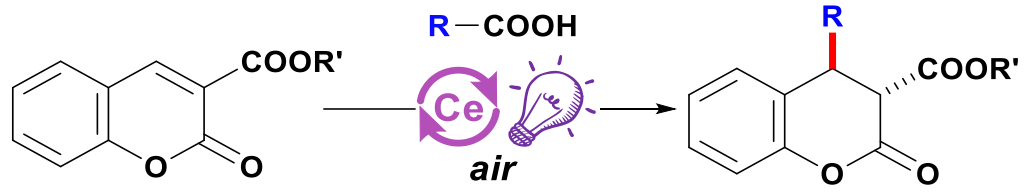

- *Operationally simple and mild reaction conditions*
- *Feedstock carboxylic acids*
- *Inexpensive catalyst system*
- *Highly diastereoselective*

We herein report the synergistic dual role of cerium for the photoinduced ligand-to-metal charge transfer (LMCT) process leading to generation of the alkyl radical followed by its subsequent Lewis acid catalysis for the construction of stereodefined C–C bonds. This operationally simple, and efficient photocatalytic method for the diastereoselective direct C-4 alkylation of coumarin derivatives. This paradigm utilizes inexpensive and earth abundant cerium catalysts, for accessing alkyl radical from feedstock carboxylic acid. This methodology is based on bimodular role of cerium i.e., for visible-light-triggered ligand to metal charge transfer (LMCT)-process for the generation of the alkyl radical from feedstock carboxylic acid and simultaneously as an active Lewis's acid for diastereoselective alkylation of coumarins. Detailed mechanistic studies using UV-Vis spectroscopy in combination with *in-situ* FTIR spectroscopy supports the reaction to undergo photoinduced LMCT/homolysis event through the CO_2 extrusion. Furthermore, this mild and atom economical methodology allows the late-stage modification of pharmaceuticals.

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P-117: Regiocontrol via electronics: Ru/Cu co-catalyzed site-selective alkylation of isoquinolones by C-C bond activation of cyclopropanols

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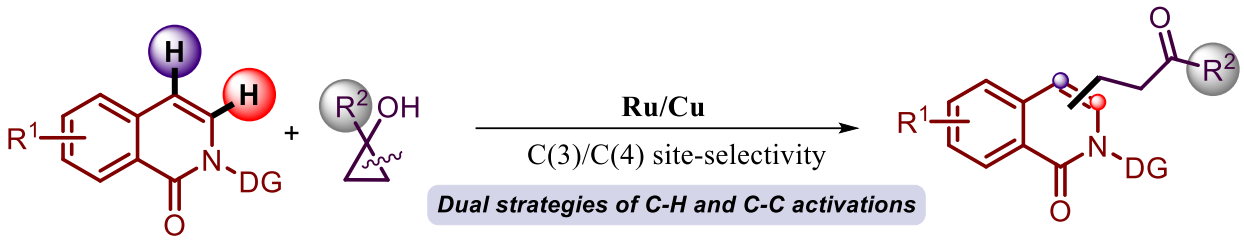

Isoquinolines and their analogues are a dominant class of heterocyclic motifs found in various pharmaceuticals and natural products.[1] Therefore, methods pertaining to their site-selective functionalization are vital, and create an optimum tool-box for their diversified syntheses.[2] Our present work focuses upon the site-selective alkylation of isoquinolones by employing cyclopropanols as alkylation congeners.[3] The Ru/Cu co-catalyzed strategy avails the dual approach of C-H and C-C bond activations, thereby generating a wide spectrum of regioisomeric products. The ratio of regioisomers follows directly from the electronic nature of the coupling partners in deciding the site-selectivity (C3 *vs* C4). Extensive mechanistic investigations and control experiments suggest a dual catalytic pathway operating in a single-pot. Synthetic transformations and late-stage functionalization of the product further enhance the utility of the methodology.

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P-118: Giant electron transport properties of functionalized superparamagnetic nanoparticle

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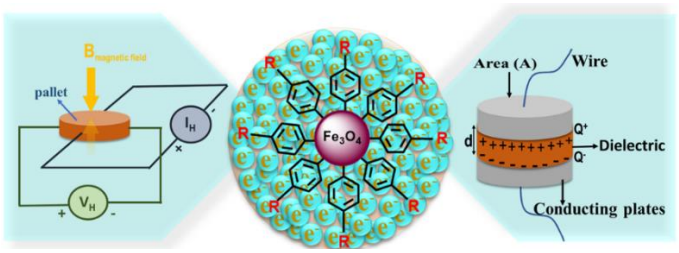

Superparamagnetic Fe_3O_4 nanoparticles (NPs) play gigantic roles in material science due to their high surface-to-volume ratio, optical and electrical properties which found enormous applications in catalysis, photothermal cancer treatment, nanofluids, and data storage. However, high surface energy caused fast agglomeration and limited the utilization of Fe_3O_4 nanoparticles.[1] Hence, there is a pressing need for proper surface functionalization to achieve the desired material properties. In this regard, small molecules can be used to functionalize the nanoparticles, which can lead to several exciting phenomena at the nanoscale. In the present study, organic molecules with different functional groups (-SO_3H, -OH, -COOH) were attached to the surface of Fe_3O_4 NPs through a radical mechanism forming covalent bonds onto the surface of Fe_3O_4 NPs. X-ray diffraction analysis confirmed the formation of well-crystalline single-phase NPs after surface functionalization.[2] Room temperature dielectric measurement reveals the strong dispersion behavior at low frequencies due to the presence of oxygen vacancy and space charge polarization in the system. Electrical impedance spectroscopy (EIS) was used to evaluate the contribution of grain and grain boundaries. The semiconducting nature of modified Fe_3O_4 NPs was ensured by four-probe Hall measurements. These results open very promising avenues to design surface-functionalized superparamagnetic Fe_3O_4 NPs for electronic applications.[3 4]

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P-119: Theoretical and Experimental Investigation of Influence of Solvents and Electrode Roughness on Potential of Zero Charge

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Equations based on the mean-field theory for the potential of zero charge and electronic dipolar capacitance for metal surface with steps is analysed and compared with experimental data. These electrochemical properties studied for different dipolar solvents, viz. acetonitrile (MeCN), propionitrile (EtCN), butyronitrile (PrCN) and valeronitrile(BuCN). The experiments were performed at the platinum electrode in 0.1 M $TBAPF_6$ as the supporting electrolyte. The change in the homologous series of different dipolar solvents led to the change in physical properties, i.e., size and dipole moment of solvents, which influence the electronic-dipolar capacitance and PZC of the metal. Determination of the potential of zero charge is crucial because it reveals details about the electrode/electrolyte interface's structure. Finally, our theory explains the experimental observation of PZC and electronic-dipolar capacitance for the stepped platinum electrodes.

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P-120: Anchoring of Phosphine on Metal-oxide Nanostructure for Heterogeneous Catalysis.

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Triphenylphosphine (Ph_3P) is commonly used as a basic chemical reagent for Appel, Mitsunobu, Staudinger, and Wittig reactions for industrial scale preparation of alkyl halide, ester, secondary amine, and alkene, respectively. Notably, triphenylphosphine oxide (Ph_3PO) is the dead-end side-product formed in all these chemical reactions. (Ph_3PO) is produced in several thousand tons per year as chemical waste. However, a huge consumption of phosphorus per year leads to an exponential drop of the global storage and urgently requires a regeneration scheme. By now purification of Ph_3PO from organic products and subsequent recycling of it to Ph_3P are two major challenges. Available Ph_3PO purification techniques are chromatography, distillation, co-crystallization, and metal-complexation. However, all these techniques have some pros and cons while organic products have different reactive functional groups. In this context, immobilization of organophosphine on the heterogeneous nanostructure surface[1] enables us to recover the organic product via straightforward techniques, mechanical/gravitational force (centrifugation). Details of this will be presented in the poster.

References:

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P-121: Crystal facet-engineered $NaNbO_3/Ag_2S$ stable inks for visible light photoelectrochemical water splitting

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Tuning the light-harvesting range for absorption in the visible region and suppressing the quick recombination of photogenerated charge carriers are the primary focus for photoelectrochemical water splitting. Herein, we explain the importance of the facet-selective approach for enhanced photoelectrochemical water splitting based on the surface energies of facets of $NaNbO_3$. The core@shell heterostructures wherein faceted $NaNbO_3$ as core material and Ag_2S as shell material have been synthesized using a surface functionalization approach owing to their absorption in the visible region. When two different facets are exposed in two different morphologies of $NaNbO_3$, the mechanism of inter-facet charge transfer varies and hence, different photoelectrochemical efficiency. In the present work, an enhancement in the photoelectrochemical efficiency of the cubic $NaNbO_3$ has been observed as compared to the truncated cube morphology owing to its higher surface catalytic activity, low electron-hole combination, and higher charge injection at its exposed facet.

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P-122: Surface Modulated Free-standing Copper Electrodes for Nitrate to Ammonia Synthesis

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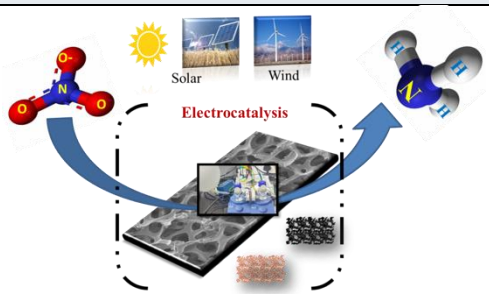

To fulfil the global ammonia demand (H_2 storage and fertilizer), alternative ways of NH_3 generation is on high demand. To overcome the issues related the Haber-Bosch's process (high-level consumption of energy and CO_2 generation), the electrochemical reduction process is one of the most promising pathway. However, the future of this low-cost process is compromised by the low yield rate and poor selectivity, due to the inert N≡N bond and ultralow solubility of N_2. In that sense, nitrate (NO_3^-) to ammonia synthesis by electrochemical reduction of nitrate (NO_3RR) can address the environmental as well as energy issues efficiently. In the NO_3RR process, the hydrogen evolution reaction (HER) is the limiting reaction which decreases the faradaic efficiency of the process. Hence, the catalyst with modulated surface is on high demand to be developed which can deliver higher Faradaic efficiency. The lower H^+ adsorption energy over copper (Cu) surface limits its activity towards HER, and NO_3^- could adsorb over Cu surface with a donation electron from the highest occupied molecular orbital of NO_3^- into the empty levels of the Cu atom assisted by backdonation from the fully occupied Cu 3*d* orbital into the NO_3^- lowest unoccupied molecular orbital. Such an interaction implies a charge transfer between NO_3^- and Cu which gives better selectivity towards the NO_3RR. Here we developed a high-performance free-standing, surface modulated Cu catalyst (copper-cobalt alloy) that delivers a high NO_3RR Faradaic efficiency which is ~98% and high ammonia yield (~10,000 $\mu g\ h^{-1}cm^{-2}$) at -0.91V vs. RHE. The observed high NO_3RR catalytic activity enables nitrate conversion into ammonia, from a low concentration usually industrial wastewater (1000-2000 ppm), maintaining the higher Faradaic efficiency enables the lower consumption of energy.

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P-123: Efficient Synthesis of Triazole Bridged Indole-based Glycohybrids

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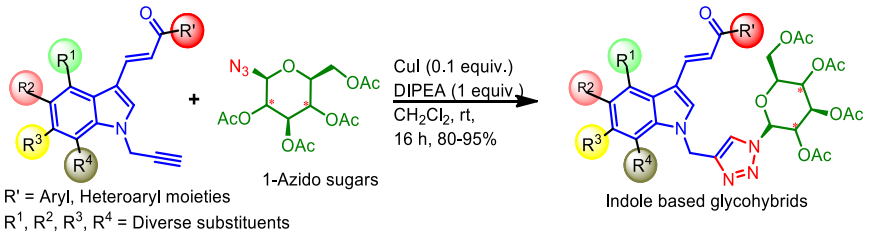

Indole nucleus consists of fused benzene and pyrrole ring is known as privileged structure motif. The presence of basic nitrogen atom in pyrrole ring of indole proclaims various biological activities like antimicrobial, anti-HIV, anti-inflammatory**,** anticonvulsant, antioxidant**,** antifungal, anticancer, antiviral, anti-tubercular, anti-diabetic, anti-malarial, antihistaminic, plant growth regulator, antihypertensive, enzyme inhibition, anti-leishmanial**,** anti-hepatitis, tubulin polymerization inhibitor, and analgesic, etc.[1,2,3] Indole nucleus is present in different kind of plants, marine organism and used as efficient chemical precursors for generating biologically active structures.[4,5] Therefore many researchers explored efficient synthesis of indole derivative for biological applications.[6] Our group is working on the efficient synthesis of glycohybrids in order to improve the selectivity, efficacy, stability and solubility of bioactive molecules.[7,8] The detailed synthetic approach will be present therein.

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P-124: Power of Protons on Porphyrin Macrocycle

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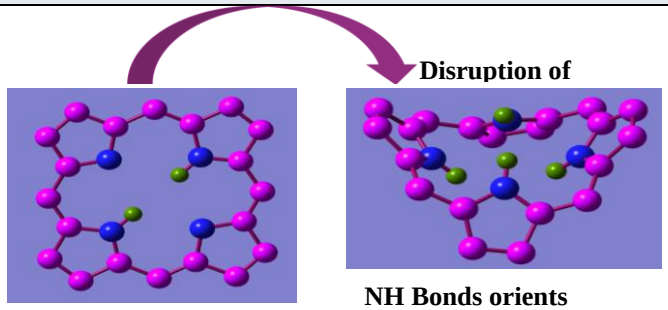

The redox properties of porphyrins can be modulated by protonation of the macrocyclic core. Free base porphyrins exhibit characteristic spectral and conformational features upon protonation and deprotonation in solution.[1] Herein, we report all possible deprotonated and protonated species of 2,3,5,10,12,13,15,20-octaphenylporphyrin (OPP) ring systems *viz*. planar and nonplanar macrocycles using spectral changes, electrochemical and DFT studies. Protonation leads to the crowding inner hydrogen atoms attached to the pyrrole nitrogen atoms of the porphyrin core which induces macrocyclic ring distortion.[2] This non-planarity in macrocyclic ring is experimentally observed in a single step. The macrocycles display incrementally increasing nonplanarity with protonation which follows the order, OPP < $OPPBr_4$ < $OPPBr_3NO_2$. The progress of the protonation was monitored by UV-Vis spectroscopy, which was also used to calculate logβ for proton addition to the core nitrogen atoms of the macrocycle. Planar porphyrins such as OPP shows a greater red shift in the electronic spectral features and downfield of NH protons as compared to nonplanar porphyrins $OPPBr_4$, $OPPBr_3NO_2$ on protonation. This can be attributed to the planar porphyrin ring in OPP, which experienced greater distortion during the course of protonation as compared to already distorted macrocycle in case of $OPPBr_4$ and $OPPBr_3NO_2$. DFT results clearly indicate that protonation and deprotonation results in tilting of pyrrole ring from the mean porphyrin plane which is verified by the spectral as well as electrochemical results.

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P-125: Reactivity Switch for Selective Nucleoside Formation from 2-Acetoxy Methyl Glycals: Synthesis of C-2 Methylene and C-2-Functionalized Nucleoside Mimetics

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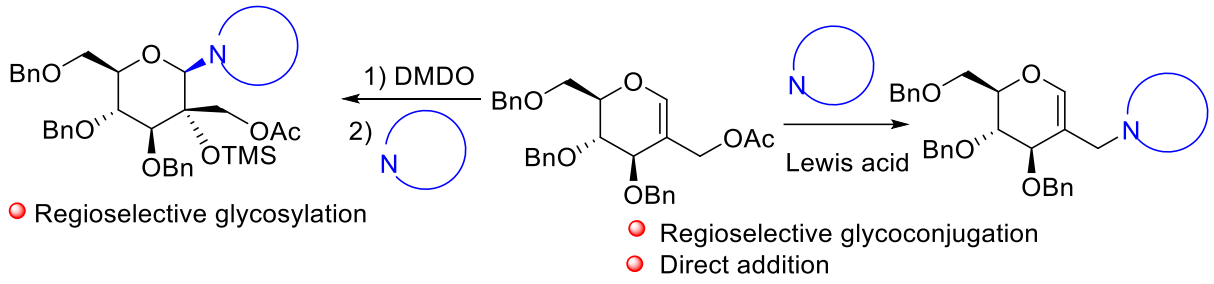

Nucleosides and their derivatives are profoundly important molecules in medicinal chemistry.[1]But the natural nucleosides have the drawback of instability against both acidic and enzymatic hydrolysis, and severe side effects to the host. Several approaches were made to overcome the instability, one of which is the replacement of the sugar ring of nucleosides with carbocyclic and thiofuran rings.[2] In another approach, the ring size of sugar moiety has been modified.[3] Herein we reported the synthesis of Novel C-2 methyl-linked glycal nucleoside mimetics by regioselective glycoconjugation of C-2 acetoxymethyl glycals with nucleobases in the presence of Lewis acids. Such glycal derivatives can also be utilized for the regio and stereoselective synthesis of C-2 functionalized nucleosides by adopting epoxidation followed by Lewis acid-catalyzed glycosylation with epoxy ring opening sequence.[4]

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P-126: Synthesis of Benzofuran and Indole Scaffolds *via* One-Pot Domino Sonogashira Coupling/Cyclization using Abnormal NHC based Pd-PEPPSI Complexes

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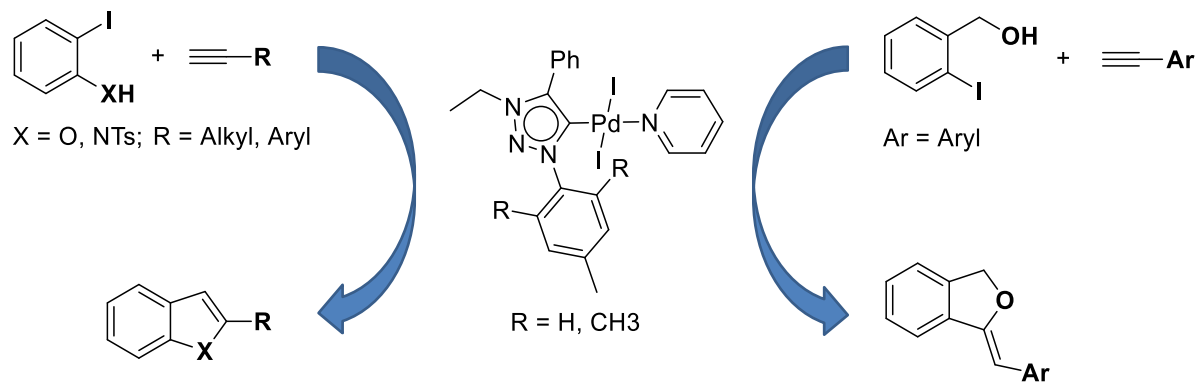

Benzofuran and indole scaffolds are common framework of several biologically and pharmaceutical active molecules. Due to comprehensive presence of these heterocycles, researchers are much interested to develop an efficient synthetic procedure for these molecules.[1] 1,2,3-Triazole based N-heterocyclic carbenes are extensively used as a fascinating ligand in metal catalysed organic transformations. Strong σ-donor and weak π-acceptor nature of tzNHCs provides highly attracted ligands in place of traditional phosphine ligands.[2] tzNHCs supported Pd-PEPPSI (Pyridine Enhanced Precatalyst Preparation stabilization and Initiation) complexes are one of the most important classes of metal complexes for C-C bond forming reaction.[3] In this work, we disclose the preparation and characterization of 1,2,3-triazolylidenes based palladium PEPPSI complexes in good yields. These catalysts were used for one-pot tandem synthesis of benzofuran and indole scaffolds via sonogashira coupling followed by cyclization in moderate to good yields with wide substrate scope.

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P-127: Enhance antioxidant and cytotoxic activity of ferrocenyl-substituted curcumin via stabilization of promoter c-MYC silencer element

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We are reporting a successful attachment of ferrocenyl moiety at the active methylene carbon atom of β-diketone of curcumin via Knoevenagel condensation reaction, to utilize the optimum selectivity toward biological targets. The formation of ferrocenyl curcumin (i.e., Fc-cur) has been confirmed by ^{1}H NMR,^{13}C NMR, and FT-IR spectra analysis. Further, circular dichroism (CD) spectroscopy, thermal denaturation, absorption, and fluorescence spectroscopy have been used to understand the association of ligand (i.e., Fc-cur) with G-quadruplex. Based on this analysis, the binding mechanism of the ligand i.e., Fc-cur to the parallel and hybrid topology present in different G-quadruplex has been proposed. Further, the binding and modes of the interaction of Fc-cur with Pu27 c-MYC silencer element and H-telo G-quadruplexes have unravelled selective and stronger binding via intercalation with parallel topology of c-MYC G-quadruplex rather than the hybrid topology of H-telo quadruplex. The manifestation of better antioxidant activity of Fc-cur has been demonstrated by showing a stronger radical scavenging capability than pristine curcumin. The cytotoxicity analysis of the proposed ligand i.e., Fc-cur against Vero and HeLa cells have clearly reflected the nontoxicity toward Vero cells and quite effective against the HeLa cells which reduces the cancer cells more effectively than the already reported for curcumin.

P-128: Ultrasensitive fluorogenic detection of Hydrargyrum in Industrial Effluent and Utilization of Conjugated Thiophene Carboxaldehyde in Forensic Fingerprint Imaging with DFT Calculation

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The development of constructive precursors and products has led to indulging the synthesized compounds P1, P2 and P3 for multiple application. A newly synthesized Benzimidazole linked thiophene conjugated receptor P3 were utilized for the detection of hydrargyrum (Hg^{2+}) in industrial effluent through fluorogenic technique. P3 shown a very high sensitivity to Hg^{2+} ion through quenching effect. An outstanding LOD of about 2.12 X 10^{-11} M in a linear range between 0 to 110µL was obtained. The effect of heavy metal ion followed by electron transfer was the cause for quenching. Further the detection of Hg^{2+} was confirmed by UV selective and sensitive studies. The stoichiometric ratio of 1:1 for P3-Hg^{2+} was obtained through Job's plot; the binding mechanism was further confirmed through NMR titration, HRMS and Infra-Red Spectroscopic technique. The investigated experimental values were in correlation with the theoretically obtained DFT and TD-DFT calculations using B3LYP/6-31+G** basis set.

In addition to metal ion detection in real time samples, the comparative studies were carried out for all compounds. The optical band gap was obtained through Tauc's plot; which reveals a decrease in band gap from P1 to P3, the decline in band gap was attributed due to an extended conjugation of the products. All three compounds shown a positive solvatochromic effect with increase in solvent polarity and have wide range of pH stability. P1 and P2 exhibited an Aggregation Induced Emission Enhancement (AIEE) in solvent:water ratio up to 80% and 50% respectively, whereas P3 exhibited Aggregation caused Quenching (ACQ) effect. The Aggregation effect was then confirmed with SEM image. The thermal and electrochemical properties were also investigated for the synthesized compounds. Alongside, the crystalline structure P2 was confirmed by single crystal XRD having monoclinic crystal system with P21/c space group. Due to an enhanced solid-state emission and AIEE property of P2 than P1, P3; it was employed for Latent finger print imaging in forensic studies. A porous and non-porous surfaces like glass plate, plastic and steel were used for observing the finger print images.

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P-129: Chloroform-COware Chemistry: An Emerging Tool for Palladium-Catalyzed Aminocarbonylation

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Synthesis of carbonylated compounds remains an intriguing area of research for synthetic and medicinal chemists as carbonyl group forms an integral part of several drug molecules and materials. Handling toxic CO gas has several limitations. Thus, using safe and effective techniques for in or ex-situ generation of carbon monoxide from non-toxic and cheap precursors is highly desirable. Among several precursors that have been explored for the generation of CO gas, chloroform can prove to be a promising CO surrogate due to its cost-effectiveness and ready availability.[1] However, the one-pot chloroform-based carbonylation reaction requires strong basic conditions for hydrolysis of chloroform that may affect functional group tolerability of substrates and scale-up reactions.[2] These limitations can be overcome by a two-chamber reactor (COware) that can be utilized for ex-situ CO generation through hydrolysis of chloroform in one chamber and facilitating safe carbonylation reactions in another chamber under mild conditions.[3] The versatility of this "Chloroform-COware" technique is explored through palladium-catalyzed aminocarbonylation of medicinally-relevant heterocyclic cores.

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P-130: An investigation of 4-aminoquinoline-quinazoline (AQ-QN) molecular hybrids as potent antimalarial agents

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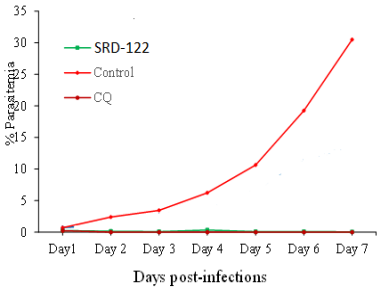

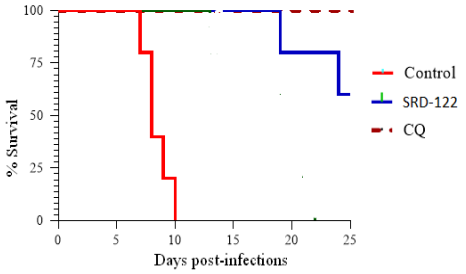

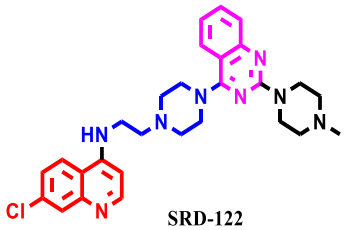

According to the latest **world malaria report**, there were 241 million cases of malaria in 2020 compared to 227 million cases in 2019. The estimated deaths stood at 6,27000 in 2020. [1]For a long time, aminoquinolines are known as a potent antimalarial drug but it was found that P. falciparum has developed resistance against these compounds.[1]Mechanistic studies show that Chloroquine (CQ) prevents the hemozoin (polymeric form of dimeric heme) formation by accumulating in the food vacuole (FV) of parasite. This leads to the accumulation of toxic un-polymerised heme in the FV, which results in parasite death. On the contrary, Mutated pfCRT is one of the main causes of CQ resistance in falciparum. It efflux CQ from FV and prevent the accumulation of CQ inside FV[2].Moreover, studies shows that Gefitinib (tyrosine kinase inhibitor), a quinazoline based anticancer drug can reverse the CQ resistance in the parasite[3]. Our group reported the **AQ-Pyrimidine hybrids** as excellent antimalarial agent[4] and based on QSAR study; incorporation of hydrophobic moiety on the fourth position of pyrimidine can upgrade antimalarial activity[5]. Here, we report the Design and synthesis of AQ-QN hybrids with potent antimalarial activity against both sensitive and resistance strains of plasmodium in nano molar range.

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P-131: Electrocatalytic Hydrogen Evolution Reaction by μ-Oxo Iron Complex bearing thiazolinium moiety as proton relay

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We present an oxo bridged pyridine dicarboxamide based Iron dimeric complex, FeL bearing a free thiazolinium moiety acting as proton relay for electrocatalytic hydrogen evolution reaction. Electrochemical investigation combining cyclic voltammogram and spectro electrochemistry measurements reveals that neutral FeL complex undergoes metal-based reduction followed by two sequential ligand-based reduction.[1] This complex displays two distinct mechanism depending on the strength(pKa) of exogenous acid and applied potential. Synergistical combination of DFT and experimental data provides a proton coupled electron transfer as initial step in the presence of strong acid but sequential electron and proton transfer in case of weak proton source in DMF.[2] This work draw attention to a unique example for hydrogen evolution reaction electrocatalyst involving a bridged oxygen and redox active proton responsive thiazolinium moiety acting as proton relay.

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P-132: Oxygen-bridged $CuMoO_4$ catalyst for C_{sp2}-*Se* cross-coupling

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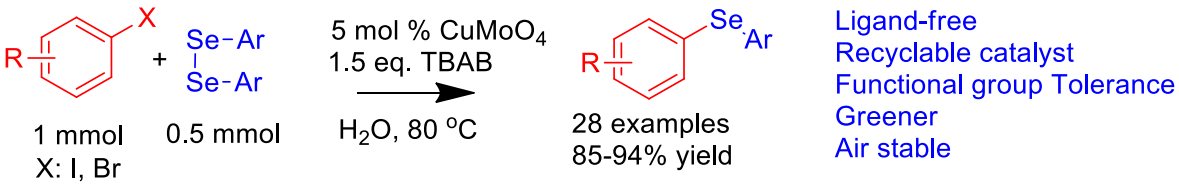

Scheme 1: C_{sp2}-Se coupling using oxygen-bridged $CuMoO_4$ bimetallic catalyst

Organoselenium compounds plays an important role in organic synthesis as synthetic reagents or intermediates. The selenoether molecules act as an anti-cancer, anti-oxidant agents and a promising donor molecules for conductive materials. The versatility of organo selenium compounds shows asymmetric catalysis and fluorescent properties.[1] These compounds are also appreciated in the field of biological and medicinal chemistry with their anti-oxidant, anti-tumor, anti-microbial, anti-viral and anti-cancer properties.[2] The previous developed methodologies need longer reaction period, harsh conditions, stoichiometric or greater amount of metallic reagents and have the moderate yield of products and mostly, these reactions were carried in homogeneous medium with *N*-derivative ligands and a coreductants.[4] Herein, we have synthesized a novel oxygen-bridged $CuMoO_4$ bimetallic catalyst for the C_{sp2}-*Se* coupling of diaryl diselenides with (hetero)aryl halides which is recyclable and shows high efficiency in product formation in water solvent(Scheme 1).[5-8]

Keywords: *Cross*-coupling, heterogeneous catalyst, water**,** synthetic methods

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P-133: When Organic Lewis Acid Turn out to be a Photooxidant to Build a New Avenue for Azolation of Unactivated Arenes

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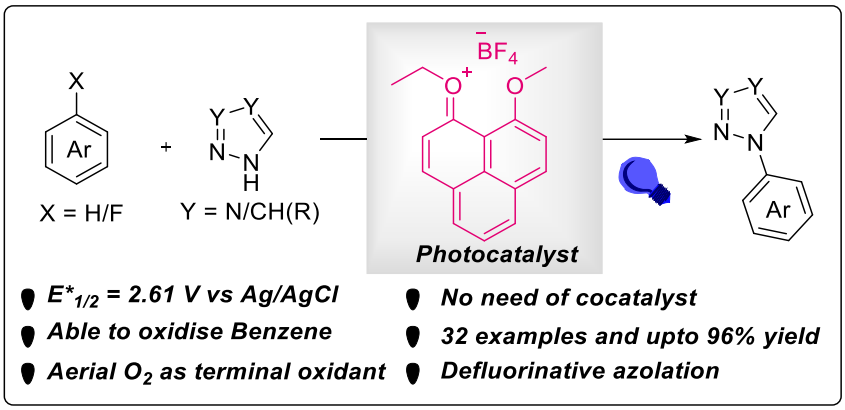

This article reveals the direct azolation of C-H bond in readily available and most unactivated arene system (like Benzene) via Photoredoxcatalysis that offers a straightforward simplification, albeit in most cases existing photocatalytic systems are unable to achieve such kind of activation. Because of the restriction to the energy of a single photon of visible light, it is hard to find a photocatalyst that can directly reach an excited state potential $E^*_{1/2} > 2.5$ V via single photon consumption. In this work, for the first time, we have successfully unlocked the excited state property of a Phenalenyl based organic Lewis acid to achieve an $E^*_{1/2} = 2.61$ V which is sufficient to oxidise benzene and other unactivated aromatic congeners. Being a Lewis acid at the ground state, this newly developed photocatalyst is able to overcome the necessity of Lewis acid cocatalyst needed to prevent catalyst deactivation in the reported multiple photon excitation protocols. Additionally, this method is compatible with many electron-donating, electron-withdrawing and heteroaromatic systems along with scaling up the reaction. A detailed mechanistic study including UV-visible spectroscopy, Fluorescence analysis, EPR studies, Cyclic Voltammetry experiments along with computational calculations revealed the possible pathways by tuning the solvent medium (DCE and HFIP). Furthermore, this protocol also exhibits the facile defluorinative C-N cross-coupling between fluoroarenes and azoles.

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P-134: Molecular Crowders Modulate Ligand Binding Affinity to G-Quadruplex DNA by Decelerating Ligand Association

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The study of kinetics of ligand binding to G-quadruplex DNA (GqDNA) structures is of paramount importance for comprehending (possible) ligand-induced anticancer activity involving GqDNA within cells[1-2]. However, cellular environment is crowded with variety of small- and macro-molecules that occupy ~30 - 40% of cell-volume[3]. While only few earlier studies dealt with deciphering the kinetics of ligands/GqDNA interactions in dilute solution[4-5], such studies in cell-like crowded milieu are absent. Here we investigate the effect of small and macro molecular crowders, glucose, sucrose and ficoll 70, on the kinetic steps of association and dissociation of a benzophenoxazine-ligand (Cresyl Violet: CV) with human telometic (hybrid) GqDNA structure using fluorescence correlation spectroscopy (FCS), aided by other methods. We find that the binding constants of the ligand to GqDNA in the absence and presence of crowders change appreciably with nearly five-fold decrease in the presence of ficoll 70, compared to that in pure buffer solution. FCS measurements unfold that this decrease of binding constants is mainly modulated by the viscosity-induced deceleration of the association of ligand to GqDNA in the crowded solution; however, the rate-determining dissociation rates remain nearly unchanged in the presence of crowders. These results have important implications in the context of ligand/GqDNA interactions within cellular environment which indicate that even if the binding affinity of ligand to GqDNA may be influenced by cellular crowders, they cannot influence the unbinding rates of ligand from a stable ligand/GqDNA complex formed by strong π-π stacking interactions.[6]

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P-135: A comprehensive Biophysical analysis of the effect of ss DNA binding on the fluorescence intensity of metal nanoclusters.

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In this study we integrated the biophysical basis of formation of a simple, low cost and highly fluorescent ss DNA based metal nanoclusters. In general, the reduction of metal salt solution in the presence of capping ligand leads to the formation of nanoparticle of diameter distributed in the range of 10-100 nm. But such type of particles do not show fluorescent property. The reason behind this phenomenon is highly metallic nature of such particles having no band gap[1]. In contrast MNCs are smaller in size (<2nm) and contain fewer number of atoms. As their size approaches the fermi wavelength of electron, MNCs display molecular like, size dependent optical property due to their discrete energy level, which allow radiative electronic transition. Because of their better photostability, biocompatibility and nontoxicity they show wide potential application in bioimaging and biosensing[2]. But the synthesis and stabilization of these small clusters is very challenging. Since they are growing spontaneously in the absence of stabilizer. Resulting into the formation of large and more stable nanoparticles with the loss of luminescence property. Therefore, it is highly desired to protect the environment of these nanoclusters. Metal nanoclusters stabilized with ss DNA scaffolds provides excellent photostability and electronic property[3]. Single Stranded DNA bounded metal ion prevent aggregation in solution and provide more favourable micro environment for the reduction of metal ion[1].

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P-136: Synthesis of 3-alkenyl-oxindole derivatives using Pd-catalyzed multicomponent reaction

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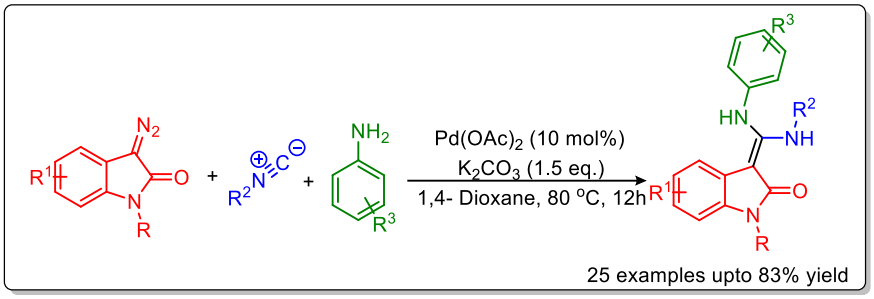

Oxindoles or its derivatives are important class of heterocycles because of their ubiquitous presence in various pharmacologically active molecules in which 3-alkenyl-oxindoles scaffolds are extremely crucial from biological perspectives due to their presence in various drug moieties. Therefore, 3 alkenyl oxindole derivatives have gained lots of attention during past many years. Although various methods have been reported to synthesize 3-alkenyl-oxindoles. However, they have few limitations like limited substrate scope, selectivity ratio for E/Z isomers and complicated starting materials. Due to wide range of biological activities possessed by 3-alkenyl-oxindole derivatives, a divergent synthesis is extremely required which is very important nowadays in medicinal chemistry. In this perspective, multicomponent reactions (MCR) perhaps most convenient and practical approach for the construction of biologically valuable frame works. Herein, we reported a novel diverse synthesis of *E*-selective 3-alkenyl-oxindole derivatives via Pd-catalyzed multicomponent reaction of N-substituted diazoisatin, isocyanide and aniline. To get deep insight into the reaction mechanism, we have also performed DFT study which suggested that this reaction undergoes isocyanide insertion/carbene coupling pathway to get E-selective 3 alkenyl oxindole derivatives.

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P-137: Sustainable synthesis of diverse molecular scaffolds via photoredox catalysis and electro-organic Synthesis

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Benzofused heterocycles play an important role in drug and natural products industries. For example, flavonoid, flavanols, degulin, naringenin, cromakalim etc. contains benzochromane moiety while methoxsalen, amiodorane, blasaminones etc. contains a benzofuran core. Thus sustainable synthesis of these derivatives has a huge demand and a highly desirable process for many industries. Herein we aim to develop a new methodology for the synthesis of benzo-fused heterocycles via photoredox catalyzed cascade reaction.

Fluorination and trifluoromethylation of drugs and bioactive molecules have a huge importance in pharmaceutical chemistry due to the increased efficacy of these molecules. Hence, we next attempted direct C-H functionalization of arylamines as these are ubiquitous molecules widely present in many natural products and drugs. In general, C-H functionalization requires a directing group and a transition metal catalyst to activate the C-H bonds, which reduces the atom economy and the synthetic viability of the method. In order to overcome these issues, we focused on direct & remote C-H functionalization of acetanilides and aryl ureas using electro-synthesis.

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P-138: Design and Development of small molecule activators to treat neurodegenerative diseases

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The stability and functional features of the proteome are achieved by protein homeostasis (proteostasis), which consists of an extensive network of components such as translational machinery, molecular chaperones, and cochaperones, the ubiquitin-proteasome system (UPS), and the autophagy machinery[1]. Recent studies have shown that the inefficient activity of protein degradation machinery such as UPS, autophagy-lysosome, and exocytosis has led to the accumulation of unwanted protein aggregates within neurons and causes various neurodegenerative proteinopathy. These studies have also established that aging decreases the activity of UPS and is the most risk factor in neurodegenerative disorders such as Alzheimer's disease (AD), Parkinson's disease (PD), dementia, Huntington's disease, and many others[2].

Furthermore, it is increasingly evident from recent reports that restoring the protein degradation activity of UPS leads to the clearance of unwanted protein aggregates in neurons. While neurodegenerative diseases affect millions of patients worldwide, there are insufficient available therapeutics to halt or slow down the progression of these diseases thus, UPS becomes a potential therapeutic target for curing neurodegenerative and other proteotoxic disorders[3,4]. In our venture we have designed and synthesized phenothiazine, imidazolines based small molecules. Molecular docking and molecular dynamic simulation studies on these protein-small molecule complexes show favorable binding on human constitutive 20S proteasome. In vitro protein activity assays also confirm the modulation of activity of the proteasome. The intriguing findings from these studies will be presented in the poster.

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P-139: Synthesis of Stable Perylenediimide-based Neutral Radicals with Switchable States

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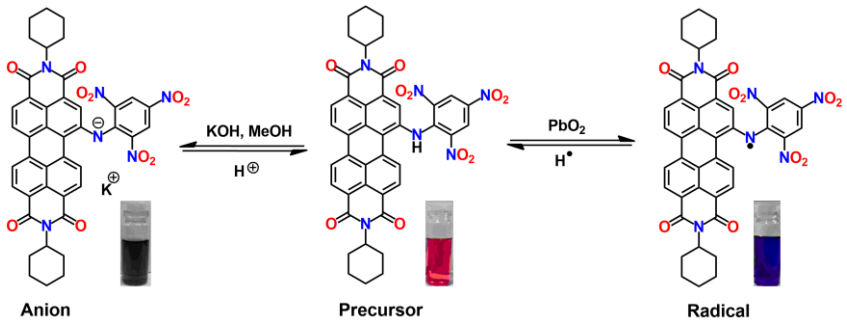

Scheme1. The reversible conversion between precursor, corresponding anion and neutral radical.

Ambient stable organic radicals have received tremendous attention from chemists because of their unique optical, electronic, and magnetic properties.[1-2] Such materials have been utilized in a range of applications, from conducting to magnetic films, to organic spintronics, biological probes for magnetic resonance experiments, in organic synthesis to photochemical and as electrode active materials as well as for development of next-generation of batteries.[3-4] The stability of the neutral radical can be modifiedutilizing steric effect and delocalization of spin density.Naphthalene tetracarboxylic diimides (NDIs) and perylene tetracarboxylic diimides (PDIs) are well-known organic scaffolds with extended π-surfaces and provide access to substitutions via its axial-, core- and shoulder positions, which make them suitable scaffolds for stabilization of neutral radicals. We earlier reported NDI/PDI based stable radical anion, radical cation and zwitterionic species in which the spin density is delocalized over the NDI/PDI scaffolds.[5-6] Herein, we wish to report the synthesis and characterisation of PDIbased ambient stable neutral radical and their corresponding switchable states. The neutral radical was prepared by the oxidation of PDI-Picryl with lead dioxide **(Scheme 1).** Here we would discuss the interesting optical and redox properties of this stable radical and corresponding multiple switchable states.

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P-140: Natural herbs (Neem, Curry and Mint) - based Extracellular Vesicles hold potential in delivery applications.

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Extracellular vesicles (EVs) are the double membrane-bound nanoparticles found to be released by almost all types of cells (**1**). In the last few years, mammalian, EVs evolved into promising drug delivery vehicles (**2**) yet they suffer from immunogenicity issues. EVS derived from natural herbs might alleviate these concerns, but they are notably neglected as delivery agents. In this study, we have highlighted the potential of extracellular vesicles derived from Neem, Mint and Curry leaves as nano-carrier delivery agents for breast cancer therapeutics. We developed a protocol to isolate the herb-based natural EVs using differential ultracentrifugation. Next, we performed the characterization of the EVs using DLS, Zeta Potential, microscopy (SEM for morphology and dimensional analysis) and FT-IR spectroscopy. Following the characterization, we prepared the two types of conjugates using EVs, namely complex of EVs with chitosan, a sugar molecule and complex of EVs, chitosan and PEGylated graphene oxide (GO-PEG). We analyzed the effectiveness of these complexes as dual delivery agents (siRNA molecules and Fluorescein) in the breast cancer cell MCF7. These herbs-based EVs offer lower cytotoxicity and enhanced cellular uptake as evident from our cellular imaging experiments.

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P-141: Aza[7]Helicene: Overcoming the Synthetic Bottleneck, Chiral Resolution and Modulating the Chiroptical properties.

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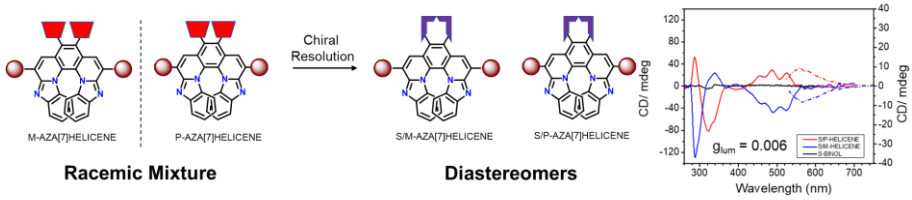

Helicenes are known over a period of nearly 100 years and continues to be in spotlight to date owing to its fascinating chiroptical properties. Helicene belong to class of polyaromatic compounds wherein the aromatic rings are ortho-fused adapting a chiral topology. Although, several synthetic methodologies such as Diels-Alder, Friedel-Crafts reaction for synthesis of helicene were developed, but over the years photochemical reaction continues to be preferred. Photochemical reactions are often limited by their requirement of highly diluted conditions so as to prevent [2+2] intermolecular cycloaddition and long reaction time.[1] Otani et al., reported a two-step synthesis of aza[7]helicenes wherein the intramolecular NH/CH intramolecular coupling is mediated by hypervalent iodine.[2] In terms of photoluminescence properties, moderate fluorescence quantum yield arises due to the weak oscillator strength owing to C_2 symmetry. The chiroptical properties quantified in terms of dissymmetry factor (g) is controlled by both the electric and magnetic transition dipole moments. With suitable substitution at various positions the $|g_{CPL}|$ can be varied from 0.006 to 0.013, thereby exhibits 20 fold enhancement.[3] Herein, a facile Knoevenagel type condensation reaction with a suitable active methylene group and aldehyde followed by intramolecular cyclization under both thermal and photochemical conditions was developed as an efficient and robust synthetic pathway. Moreover, by the incorporating suitable functional moieties, easy resolution of the racemic mixture of (P/M)-Helicenes can be achieved by reacting with suitable chiral resolving agents. Modifying the active methylene group with suitable substituents, allows the tuning of fluorescence and circularly polarised luminescence from visible to NIR region.[4]

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P-142: Exploring 4-hydroxy-3,5-dinitropyrazole as a precursor for the synthesis of *N*-methylene-C bridged insensitive energetic materials

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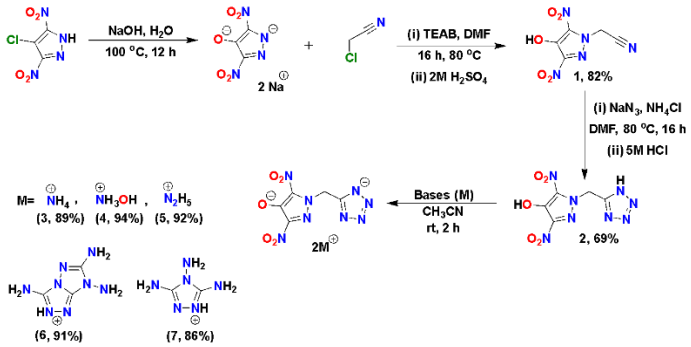

High Energy Density Materials (HEDMs) have found various applications in all walks of life (both civil and military fields). Due to several incidents related to accidental initiation of conventional explosive RDX, there is a requirement for the synthesis of safer explosives, which can withstand accidental stimuli, and are stable for storage, transportation as well as usage. The challenge lies in synthesis of high-performing insensitive explosives due to the inverse relation between physical stability and energetic performance. To tackle this challenge, modern-day explosives based on nitrogen ring heterocyclic rings like pyrazole, oxadiazole, tetrazole, etc. have been explored vastly due to their high heats of formation and density, as well as environmentally friendly nature. In this work, we have synthesized a series of insensitive compounds based on 4-hydroxy-3,5-dinitropyrazole and tetrazole energetic scaffolds, connected via *N*-methylene-*C* bridge. The presence of hydroxy functionality in between nitro groups on the pyrazole ring promotes physical stability via inter and intramolecular hydrogen bonding, as well as contributes to increasing the overall oxygen balance, which supports higher energetic performance. Two nucleophilic sites facilitate dicationic energetic salts formation, which provides a pathway for further enhancement of stability via electrostatic interactions. By pairing with various nitrogen-rich cations, fine-tuning of the energetic performance is also feasible. It was found out that the dihydroxylammonium salt of the neutral compound is thermally stable (T_d = 221 °C), insensitive towards impact and friction (IS > 40J, FS > 360N), and shows detonation properties comparable to RDX (D_v = 8627 m/s).

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P-143: Copper Corrole Immobilized onto Reduced Graphene Oxide: An Efficient Catalyst for Hydrogen Evolution Reaction (HER)

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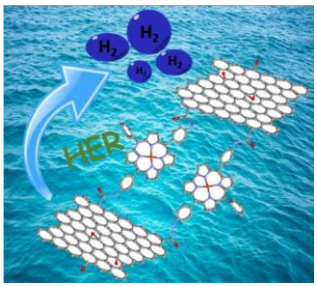

The consequences of the increased use of fossil fuels are putting our habitat at greater risk, thus there is a global need to find an alternative which is sustainable, renewable, and environmentally friendly[1]. One such clean alternative is to use hydrogen and it can be obtained by catalytic water splitting[2]. To date, platinum is one of the most efficient catalyst for hydrogen evolution reaction (HER) however, its earth-scarcity and high cost restrict its widespread use[3]. Therefore, there is an urgent demand to develop inexpensive and earth abundant 3d-transition metal based hydrogen evolution catalysts. Corroles, the contracted tetra-pyrrrolic macrocycles structurally similar to the corrin ring in vitamin B12 and it exhibits unique properties that make it more curious over porphyrin[4]. Due to inherent acidity of the three inner cavity protons, corroles can stabilize the central metal ions in their higher oxidation states compared to that of the dianionic porphyrins. Graphene oxide is a unique single layer material comprising sp^2-hybridised conjugated carbon atoms remains a material of choice because it acts as a supporting material for catalysts which improves the stability and electro-catalytic efficiency in HER[5]. Here, we show that a A2B copper corrole with para-aminophenyl and pentafluorophenyl groups at the meso- positions and functionalization of the copper corroles on reduced graphene oxide act as efficient catalyst towards hydrogen evolution reaction.

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P-144: Coordination-driven Opto-electroactive molecular thin films in electronic circuits

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Surface chemistry of nanoscale molecular thin films are highly desirable for understanding the interfacial phenomenon. The coordination-based oligomer film is used for optoelectronic and electrical applications. Here, we take advantage of simple yet classical layer-by-layer (LBL) method to assemble the Fe(II), Co(II)-bis-terpyridyl (bis-tpy) oligomer or heterostructures on tpy/ITO surface.[1] The assembly of tpy-NH_2 on ITO has been done through electrochemical deposition.[2,3] On templet layer using different transition metal ion and bis-terpyridine ligand step-wise for assembling symmetrical thin film. The molecular thin film on conductive transparent ITO electrode was further utilized for optical, electrochemical, electrical, and electrochemical impedance spectroscopy (EIS) to explore the possibility of a molecular electronic device. Here, we utilized the gel electrolyte to prepare a molecular electronic device. We placed the gel electrolyte in between ITO/tpy-[Fe(bis-tpy)]$_5$ and ITO/tpy-[Co(bis-tpy)]$_5$ to mimic the molecular electronic device configuration to measure the current-voltage response (I-V). Electrical impedance spectroscopy was used to experimentally deduce charge transfer resistance, contact resistance, and capacitance value followed by the circuit modeling.[4] The circuit model was further validated by building up a real electronic circuit using individual electrical components. Near vertically aligned molecular thin films can be suitable for various applications in optoelectronics,[5] electrochromic, and molecular electronics.

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P-145: Synthesis of Cotarnine Based Scaffold for Oral Cancer

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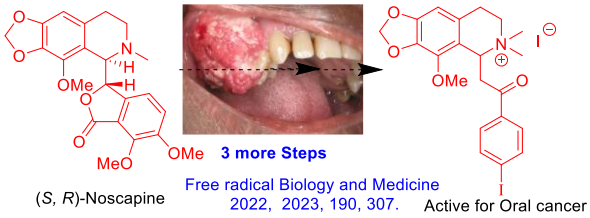

Members of the privileged tetrahydroisoquinoline family of alkaloids display a wide range of biological properties such as antitumor and antimicrobial activities.[1,6,7] Of particular significance within this family, cotarnine analogues were less explored derived cheaply from noscapine (Opium alkaloid).[2-5] We have synthesized a novel inhibitor of M Mitrochondrial protein-18 using cotarnine scaffold, which was found to induce SIMH and activated apoptosis. Interestingly, the target compound inhibited MTP18-mediated mitochondrial fission, along with increased mitofusin expression in oral cancer cells. It induced autophagy. Interestingly, this molecule-mediated SIMH resulted in the loss of mitochondrial membrane potential, leading to the consequent generation of mitochondrial superoxide to induce intrinsic apoptosis. Further, the above molecule, in combination with FDA approved anticancer drugs, exhibited higher apoptotic activity and decreased cell viability, suggesting the MTP18 inhibition combined with the anticancer drug could have greater efficacy against cancer. The details of synthesis and biological activity will be discussed.

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P-146: Metal-Free Straightforward Synthesis of β,β-Di-aryl Esters: A Cascade Strategy towards 3-Aryl-1-indanone Cores

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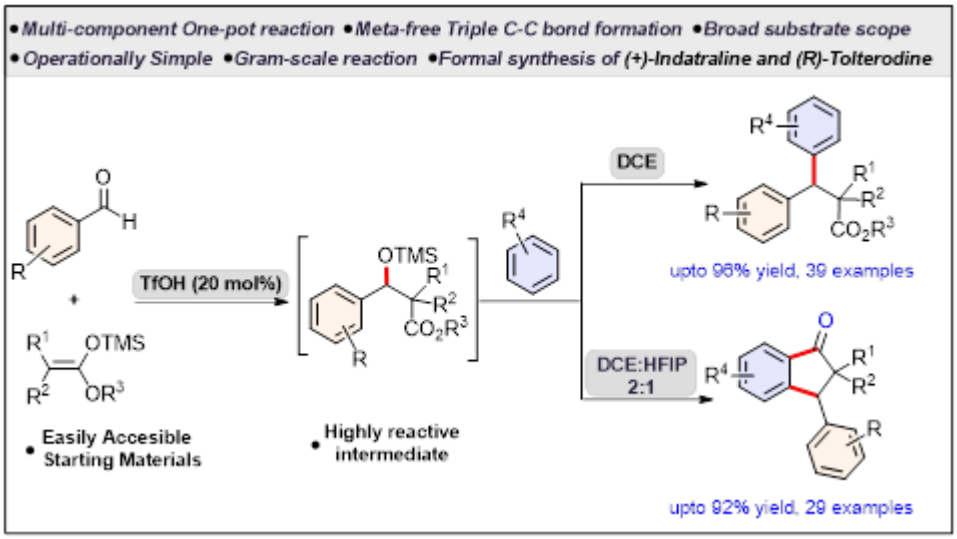

A multicomponent, solvent-dependent, one-pot Brønsted-acid catalyzed reaction of benzaldehydes, silyl enolates, and arene nucleophiles for the synthesis of potential drug candidates 3-aryl-1-indanones has been developed. This methodology possesses three C–C bond formation, broad substrate scope, facile scalability, and high regioselectivity. The b-O-silyl ethers produced *in-situ* were subjected to acid-catalyzed benzylic arylation with strong and weak nucleophiles, and the resulting b,b-di-aryl esters can undergo intramolecular cyclization to form the indanone products. Detailed mechanistic insight leads to a feasible reaction pathway. This practical and adaptable approach enables synthetically valuable transformations for the synthesis of medicinally valuable (*R*)-*tolterodine* and (+) indatraline.

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P-147: Regioselective Synthesis of Oxadiazolyl and Triazolopyridyl BODIPYs for Sensing of Mercury Ions and pH Sensors

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Fluorescence sensing is one of attractive area of current research due to its versatile utilities in analyte-detection, biolabeling, disease diagnostics, industrial products, environmental pollutants and drug delivery systems.[1, 2] In recent past, various types of fluorescent based sensors and probes have been reported including BODIPY, rhodamines, fluorescein and naphthylamide derivatives.[3] BODIPY (4,4-Difluoro-4-bora-3a,4a-diaza-*s*-indacene) exhibits interesting photophysical properties such as high molar absorption coefficients and fluorescence quantum yields, narrow emission bandwidths and high stability in physiological conditions.[4] The photophysical and electrochemical properties of BODIPY dyes can be easily tuned by functionalization at different positions of BODIPY core..[5] In our efforts to develop BODIPY-based probes[1], very recently we have developed a sequential one-pot synthesis of oxadiazolyl and triazolopyridyl-BODIPY derivatives by employing iodine(III)-promoted oxidative cyclization of BODIPY hydrazide-hydrazone; readily accessible from the reaction of formyl BODIPYs with arylhydrazides. Prepared BODIPY derivatives displayed red shifted absorption and emission maxima as compared to BODIPY. The β-triazolopyridyl BODIPY exhibited good binding affinity ($1.8 \times 10^4\ M^{-1}$) towards Hg^{2+} ions with detection limit upto 2.1 μM. Under acidic conditions, dimethylamino- and triazolopyridyl-BODIPYs exhibited blue shift in absorption (10-15 nm) and emission spectra (7-34 nm). Detailed synthesis and photophysical studies of the synthesized BODIPY derivatives will be presented during the conference.

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P-148: Visible Light Catalyzed PCET of Quinazolinones/ Benzothiadiazines as Amidyl/Aminyl Radical Precursors for Controlled Cascade Cyclization

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Quinazolinones/benzothiadiazines were used as amidyl/aminyl radical precursors for cascade cyclizations via a photoredox-catalyzed proton-coupled electron transfer (PCET) process for the first time. A controlled synthesis of isoindole-fused quinazolinones/benzothiadiazines was carried out via quinazolinone amidyl/benzothiadiazine aminyl radical addition to the C−C triple bond under mild conditions. This transition-metal-free method provides an efficient and broad substrate scope for the synthesis of isoindole-fused quinazolinones/benzothiadiazines with step economy and atom efficiency.

Key words: Aromatic compounds, Cyclization, Disulfides, Hydrocarbons, Proton coupled electron transfer, Visible light.

P-149: Development of BINOL-Ru Catalyst Covalently Immobilized on MSNs and Their Application in Asymmetric Hydrogenation

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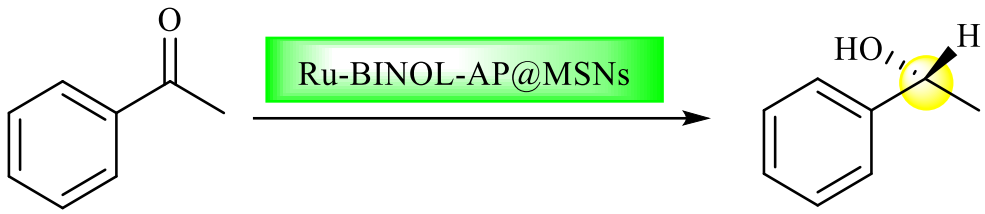

Scheme: Asymmetric transfer hydrogenation reaction catalysed by Ru-BINOL-AP@MSNs

The immobilisation of a chiral 1,1′-Bi-2-naphthol ligand (BINOL) on amine functionalized mesoporous silica nanoparticles (MSNs) via an amine linker (AP@MSNs). The resulting Bi-2-naphthol ligand onto the silica matrix (BINOL-AP@MSNs) was converted into a ruthenium complex (Ru-BINOL-AP@MSNs) without use of protecting or deprotecting groups. The final catalyst was characterized using Powder X-Ray diffraction, FE-SEM, HR-TEM, XPS, FTIR, Solid-state ^{13}C CP MAS NMR, BET, and TGA techniques as well as ICP-AES elemental content measurements substantiating that the Bi-2-naphthol ligand was successfully grafted onto the amino group of (3-aminopropyl)trimethoxysilane-functionalized silica matrix. The interest of this method increases when opportune catalytic precursors are able to perform the transformation in an asymmetric fashion, generating enantiomerically enriched chiral alcohols. The catalytic competence of the catalyst was successfully used in the asymmetric hydrogenation reaction and found to be having a good catalytic efficiency, leading to 84.38% conversion with enantioselectivity > 90% of the *R*-isomer for stereoselective transfer hydrogenation reaction. Additionally, the as-synthesised catalyst was able to be recycled five consecutive times without loss of activity, thus reducing solvent waste, and loss of precious metal and or ligand.

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P-150: Theory and Experiment for migration-diffusion controlled reversible electron transfer reaction

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We developed a novel semimicroscopic theory for diffusion and migration-controlled oxidative and reductive charge transfer. Theory is elaborated for fully and partially supported systems under DC bias on a planar electrode. The electric field-induced asymmetrical migration contribution of oxidized and reduced species in the electric double layer (EDL) region is accounted for using our jellium-dipole-underscreened-diffuse-layer model for the electric double layer. The essential nonlinearity that appears in the Nernst− Planck equation is circumvented through a novel approach by projecting migration contributions to modified Nernstian boundary constraint. Our formulation also accounts for the ionic strength-dependent anomalies in the interfacial electric field due to ionic underscreening, electrostatic interaction on diffusivity, the ion size effect of supporting electrolyte, and the charge of electroactive species in the migration current. The formula is derived for the current transient, and it accounts for the influence of the supporting electrolyte, electroactive species, solvent, electrode through jellium, and applied potential. The extent of migration−diffusion coupling is characterized by a dimensionless coupling number δ^{α}_{M} ($0 \leq \delta^{\alpha}_{M} < 1$). A smaller magnitude represents a weak coupling regime with a limiting ideal Cottrell behaviour, and $\delta^{\alpha}_{M} \sim 0.5$ represents a strong coupling regime. The theory elucidates that δ^{α}_{M} is dependent on the potential at IHP, OHP, diffuse electric double layer, ion size-corrected screening length, interfacial diffusivity, the charge on electroactive species, and the operative resistance from bulk to interface. Finally, we validate the theory with experiments and show that migration has a significant influence on the chronoamperometric and impedance response at all time scales.

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P-151: Alcohols as the Alkylating Agent under Base Metal Catalysis: Applications and the Underlying Mechanistic Landscape

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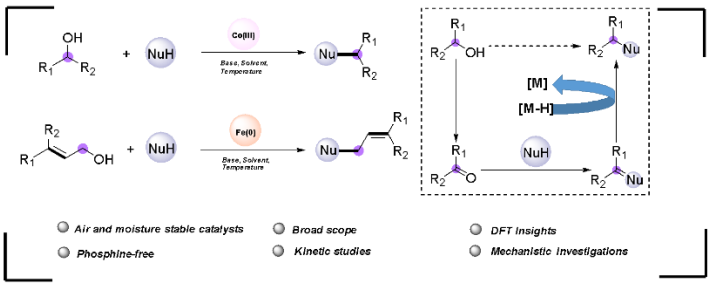

An atom-economical methodology for upgrading small molecules into higher order products are dehydrogenative reactions, wherein, the initial dehydrogenation reaction reveals a more reactive organic synthon that can undergo tandem functionalization reactivity.[1][2] Although significant advances using noble metals have been made, use of cost effective and environmentally benign base metals guides this methodology towards a new dimension. In this regard, we have described the use of high valent Cp*Co(III) system in one-step alkylation reactions with secondary alcohols.[3][4] DFT and experimental investigations sheds light on the involvement of a new paradigm in the oxidative activation of alcohols unlike its high-valent noble metal analogues.[5] In our recent work, we have developed a biomimetic C-allylation reaction using terpenols using knölker type Fe-catalytic system to obtain terpenylated products regioselectively in a single step.[6] Also, rationalization of the catalytic pathway *via* in-depth mechanistic investigations was achieved.

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P-152: Regioselective C-5 Halogenation of 8-Aminoquinoline by Ni-Catalyst and Co-Catalysed Chelation Assisted ortho-Iodination of Aromatic Sulfonamides with Molecular Iodine

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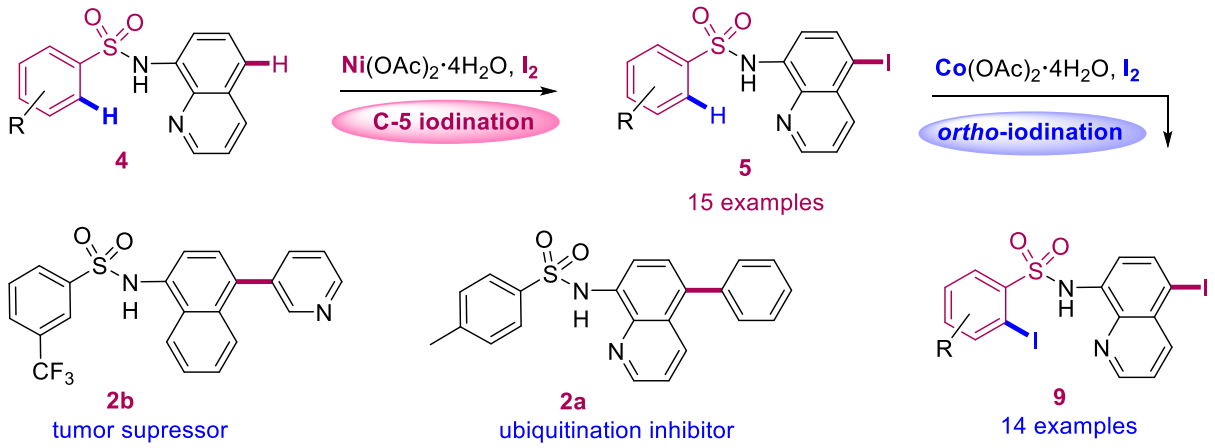

Transition metal-catalyzed C-H functionalization have a marvellous impact in the area of industrial organic chemistry. Furthermore, transition metal-catalyzed C-H halogenation for the development of aryl halides has been established as an alternative to conventional procedures, such as the Sandmeyer reaction, electrophilic aromatic substitution or directed lithiation.[1,2] A Ni(II)- and Co(II)-catalyzed sequential C-5 and *ortho*-iodination of sulfonamides using economical and milder molecular iodine (I_2) as an iodinating reagent is described for the first time. The 8-amino-5-iodoquinoline segment prepared via nickel catalysis act as a directing group for *ortho*-iodination by chelation assisted cobalt catalysis yielding in *ortho*-iodinated arylsulfonamide products. This methodology has been involved to various value added products by coupling reactions.[3]

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P-153: Catalytic synthesis of energy-rich fuel additive levulinate esters from levulinic acid using modified ultra-stable zeolite Y

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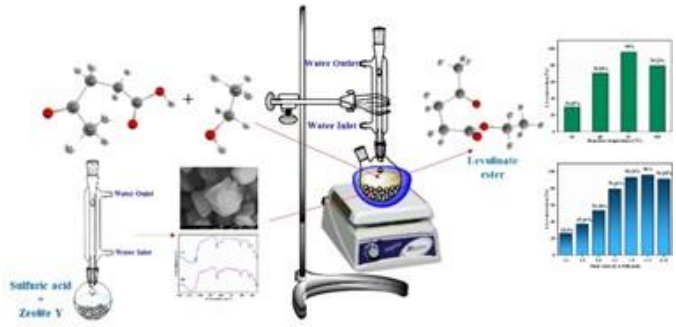

Esters of levulinic acid can be obtained by catalytic esterification of levulinic acid with alkyl alcohol such as methanol, ethanol, butanol gives respective alkyl levulinates in the presence of acidic catalyst either homogeneous or heterogeneous catalysts. Usage of homogeneous catalysts causes serious problems related to the environment, such as handling and transportation, toxicity, equipment corrosion, disposal, and regeneration. Due to these drawbacks of homogeneous catalysts, environment-friendly heterogeneous catalysts were developed, with considerable catalytic activity with renewability and stability in reaction medium. In the present investigation, the esterification reaction of levulinic acid with ethanol was performed using sulfuric acid-modified zeolite Y catalyst to synthesize ethyl levulinate. Characterization of zeolite catalysts was performed using SEM-EDS, XRD and FTIR techniques. The experiments were performed to find the optimum reaction parameters to obtain the maximum yield of 96% of the product, levulinate ester by varying catalyst concentration (2-12 wt %), levulinic acid to ethanol mole ratio (1:1 to 1:13), reaction temperature (40℃- 100℃). A maximum of 96% of levulinic acid conversion with 96% yield was achieved over 10 wt% catalysts, 1:11 levulinic acid: ethanol mole ratio, and reaction temperature of 80℃. The esterification of levulinic acid with ethanol followed pseudo-first-order reaction kinetics. The activation energy for this reaction was found to be 19.570 $KJmol^{-1}$.

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P-154: The temperature-induced phase transition generates the thermosalient effect in an organic salt.

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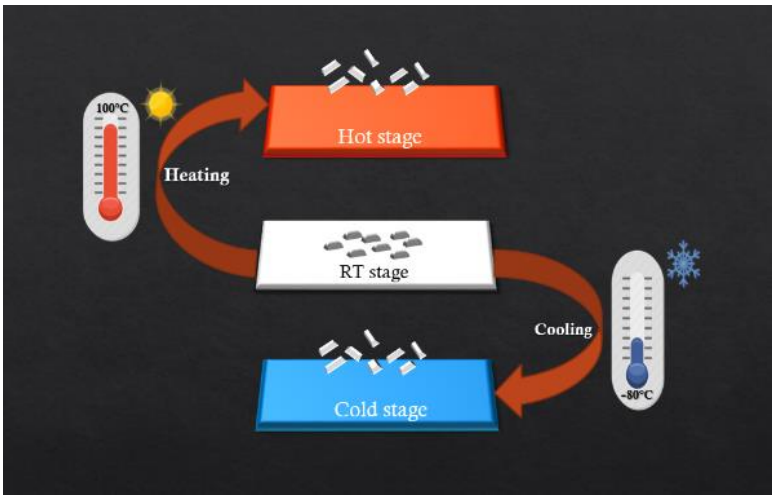

The word "salient" describes the crystal's propensity to show sudden jumping or movement in response to external stimuli. The term "Thermosalient Effect" is used when a jump occurs due to temperature[1]. The main cause of this phenomenon that we are currently aware of is phase transitions or strain created in the molecules as a result of temperature changes[2]. In this topic it is interesting to see how changes in structural parameters at the microscopic level can impact the compound's properties at the macroscopic level.

Herein, we discuss the organic salt form by grinding squaric acid and imidazole, which jumps at about -80 °C on cooling and over 100 °C on heating. DSC (differential Scanning Calorimetry) analysis explains that temperature induce a phase transition in the organic salt crystals. Structural analysis of SCXRD data explains that salt has a layer structure, and change in the distance between the layers is what causes the shearing in the crystal, which leads in crystal jumping.

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P-155: Dansyl Based Molecular Rulers for Probing Depth-Dependent Solvation Properties at Charged-Lipid/Water Interface

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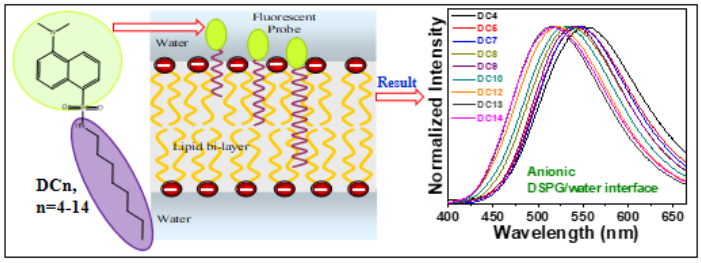

Biologically important phenomena like molecular interaction, charge transfer, signal transduction, drug transport etc. occur at the membrane/water interfaces. These processes are predicted to be strongly affected and controlled by the depth-dependent local hydration state, H-bond availability, dynamics and lipid ordering across the lipid/water interfaces.[1-3] Thus, precise knowledge of depth dependent static and dynamic properties at lipid/water interfaces is very essential not only to explain their role in membrane biology, but also to develop efficient drug delivery systems (DDSs) and drug detoxification systems.[1-4] With this objective, we have synthesized a new class of solvatochromic dansyl-based fluorescent probes (molecular rulers) by attaching alkyl chains of different lengths. A series of steady state and time-resolved spectroscopic studies of the dyes with the various saturated and unsaturated artificial lipids, both zwitterionic and anionic lipids, suggest that dansyl-based molecular rulers can *specifically* be utilized to probe the depth-dependent solvation properties across the lipid/water interface of *anionic* lipid bilayer at gel-phase (see Figure 1). Fluorescence studies also imply that longer the alkyl chain-length of the lipid, larger the variation in position of the dye in the anionic lipid bilayer. Confocal imaging of the dansyl dyes in human lung A549 cell line clearly signify that dansyl molecular rulers can be used to monitor lipid-droplets inside the living cell. All atom molecular dynamic simulation is also explored to explain the molecular picture of the depth-dependent positions of the rulers as well as the local hydration state at the lipid/water interface.

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P-156: TFA-Mediated One-Pot Tandem Regioselective Synthesis of 3-Substituted-1-Aryl-1H-Pyrazolo-[3,4-b]quinolines from Anilines and Pyrazolones Using DMSO as one Carbon Source

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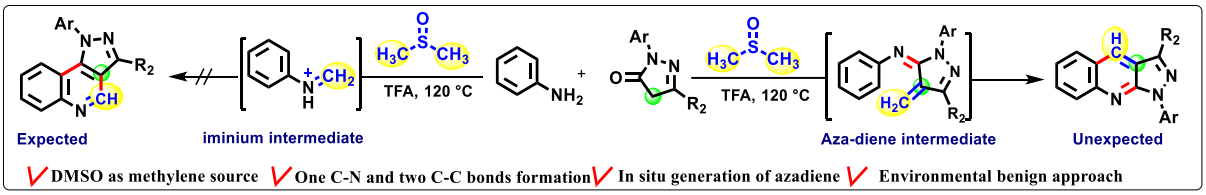

An acid-mediated and DMSO participant one-pot tandem synthesis of 3-substituted-1-aryl-1H-pyrazolo-[3,4- b]quinoline from readily available anilines and pyrazolones was achieved. This method enables regioselective construc-tion of the valuable heterocycles under transition-metal and oxidant-free conditions in which DMSO acts as a methine source as well as solvent making this process an environmentally benign approach. A broad range of diversely substituted aryl amines and pyrazolines are successfully employed in this reaction to access a series of pyrazolo[4,3-c]quinolones through a novel cascade mechanism. Furthermore, the application and mechanistic studies of the present methodology also demonstrated.

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P-157: Spontaneous self-assembly of macrocycles to extended nanostructures

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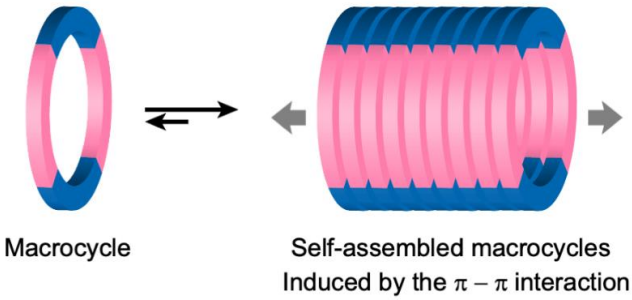

Figure 1: Schematic representation of p - p interaction-induced self-assembly of macrocycles.

Predictable and spontaneous self-assembly of macrocyclic molecules is of fundamental interest to understanding a wide range of chemical and biological problems and their underlying functions. These self-assembly processes are induced by one or several noncovalent interactions. Particularly rigid macrocycles with large p-surfaces are prone to self-assemble in nanotubes containing inner pores, usually with defined diameters. Such self-assembling nanopores are increasingly attractive for molecular recognition, catalysis, and mass transport. Also, the extended long-range p-stacking in those nanostructures is appealing to the field of organic electronics and material chemistry. We have synthesized several rigid-extended macrocycles that employ anthracene, pyrene, chrysene, and an aromatic dicarboxylic acid linker through several known reactions. Owing to their large p-surface, they spontaneously self-assemble in the solution to give an ordered nanostructure. The self-assembly processes have been thoroughly investigated using several analytical and spectroscopic techniques. Interestingly, we have found that relatively flexible macrocycles are less prone to self-assembly than their rigid counterpart and capable of a guest binding. In this contribution, we will demonstrate some of these results in detail.

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P-158: Regioselective Carbosulfonylation of Alkynes: Metal free Approach to Access β-Carbo Vinylsulfones

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The sulfone functionality is widely employed in organic chemistry and vinylsulfone containing motifs exhibit a variety of biological activities such as HIV-1 inhibitors,[1] cysteine protease inhibitors[2] and covalent protease inhibitors.[3] Sulfonylation of alkynes with simultaneous formation of C-C bond[4] provide one of the simplest method for producing highly substituted and stereoselective carbo vinylsulfones. Most of the carbosulfonylations requires a two-step procedure e.g halosulfonylation of the alkyne followed by a Pd-catalyzed cross-coupling to obtain the intermolecular product.[5,6] Wu et al proposed one-step procedures for perfluoroalkylsulfonylation of terminal alkynes but this methodology can only yield sulfonyl hydrazide derivatives with fluoroalkyl groups.[7] Nickel-catalyzed carbosulfonylation of alkynes utilising sulfonyl chlorides and boronic acids is another method by which such compounds can be prepared with high stereoselectivity but the use of expensive boronic acids & free radical initiators, toxic metal and additives make the route economically unsuitable.[8] With our ongoing interest in the synthesis of medicinally relevant molecules,[9,10] we became interested in di-functionalisation of alkynes. During the course of this study, we achieved one-pot regioselective intermolecular carbosulfonylation of alkynes using sodium sulfinates and cyclic 1,3-diones in the presence of iodine and potassium carbonate under mild condition. This strategy is utilised to a variety of terminal alkynes, sodium sulfinates, and cyclic 1,3-diones to synthesize β-carbo vinylsulfones in good yields.

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P-159: Cationic Ruthenium(II)-CNC Pincer Complexes with Multiple NHC Ligands: Catalytic Application in Hydration of Nitriles under mild Condition

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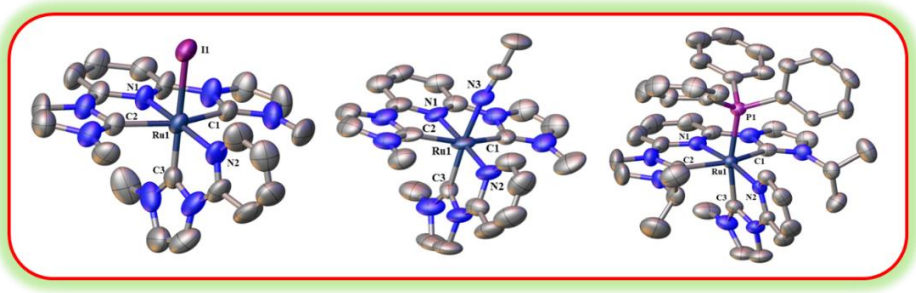

Figure 1: Molecular structure of Ru(II)-CNC pincer complexes with multiple NHC ligands

NHCs ligand serves as excellent ancillary ligands for the synthesis of a variety of homogeneous catalysts. A series of novel Ru(II) pincer complexes, $[Ru(CNC^{R})(CN^{Me})I]PF_6$, $[Ru(CNC^{R})(CN^{Me})(CH_3CN)]2PF_6$, and $[Ru(CNC^{R})(CN^{Me})(PPh_3)]2PF_6$ [where (R = Methyl, Isopropyl, Cyclohexyl) (CNC = 2,6-Bis(imidazole-2-ylidene)-pyridine), and (CN^{Me} = 2-(3-methyl imidazole-2-ylidene)-pyridine)] have been synthesized and characterized by multinuclear NMR, HRMS, and solid-state single-crystal X-ray crystallography (Figure **1**). The $[Ru(CNC^{R})(CN^{Me})I]PF_6$ have been synthesized by the reaction of NHC ligand precursors and a Ru(III)-NHC complex $[Ru(CN^{Me})Cl_3(H_2O)]$ recently developed in our group, as a precursor. The reactivity of halide complexes were investigated by the reaction of CH_3CN and PPh_3 in which quick substitution of these ligands occurred, indicating the lability of the iodide ligand. The UV-Vis spectra of these complexes exhibited the hypsochromic shift by exchanging anionic I^- ligand to neutral CH_3CN and PPh_3 ligands. The catalytic activity of these complexes were explored for the hydration of nitriles under an aqueous condition with a catalytic amount of base. Comparing the catalytic activity for hydration of nitriles from these complexes shows that $[Ru(CNC^{iPr})(CN^{Me})I]PF_6$ has excellent reactivity as compared to all other analogous complexes. In contrast, CH_3CN and PPh_3 complexes show poor reactivity as compared to similar iodide complexes.

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P-160: Inverse Electron Demand Diels Alder Reaction of Aza-o-Quinone Methides and Enaminones: Accessing 3-Aroyl Quinolines and Indeno[1,2-b]quinolinones

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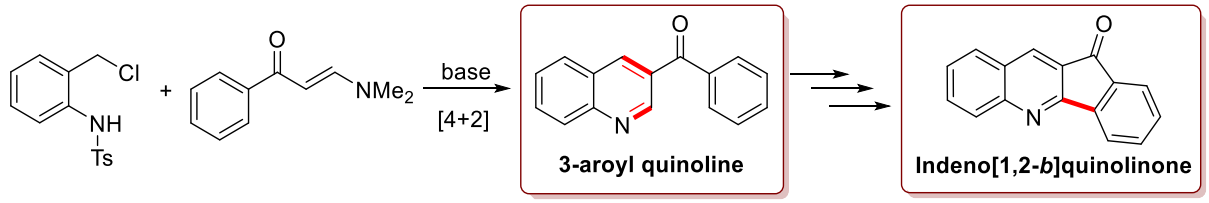

Scheme 1. Inverse electron demand Diels Alder reaction of aza-*o*-quinone methides and enaminones

Quinolines are a class of heterocycles which are of utmost importance in medicinal chemistry and industry. Quinoline derivatives exhibit a wide range of biological activities such as antibacterial, antioxidant, anticancer, anti-inflammatory, antifungal, and antileishmanial. We have developed an Inverse Electron Demand Diels Alder cycloaddition route toward 3-aroyl quinolines from enaminones and *in situ* generated aza-*o*-quinone methides. The reaction was found to be general with a range of substituted enaminones and aza-o-quinone methides, and we could validate the applicability of the methodology in gram scale. We also demonstrated a one-pot strategy toward 3-acyl quinolines starting from the corresponding aliphatic ketones. Finally, we utilized the 3-aroyl quinolines for synthesizing indeno[1,2-*b*]quinolinones *via* a Pd-catalyzed dual C−H activation approach.

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P-161: Photoredox/Palladium Dual Catalysis for Visible-Light Mediated C-H Functionalization of *N*-protected carbazoles

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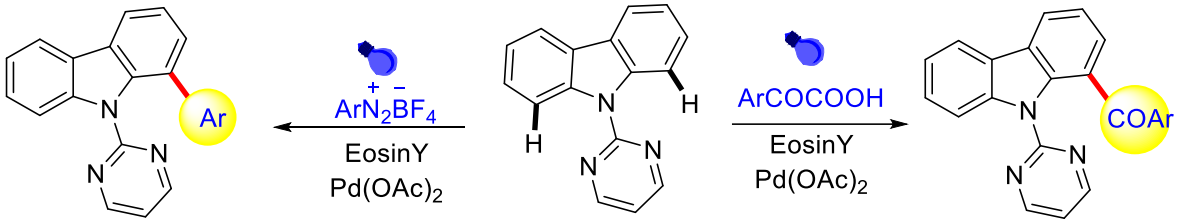

* Single site selective C1 arylation and acylation
* Inexpensive organophotocatalyst
* Wide substrate scope
* No thermal activation
* Moderate to good yield

A mild and efficient site-selective C-1 arylation/acylation of *N*-protected carbazole derivatives with diazonium salts/glyoxalic acid derivatives has been developed in visible light by a dual catalytic system comprising of Eosin Y and palladium acetate. The methodology has good functional group tolerance, excellent site selectivity and furnishes the desired products in moderate to good yields.

P-162: Synthesis, Spectral and Redox Properties of Barbituric Acid appended N-Confused Sn(IV) Porphyrin and its Utilization in Photodynamic Therapy

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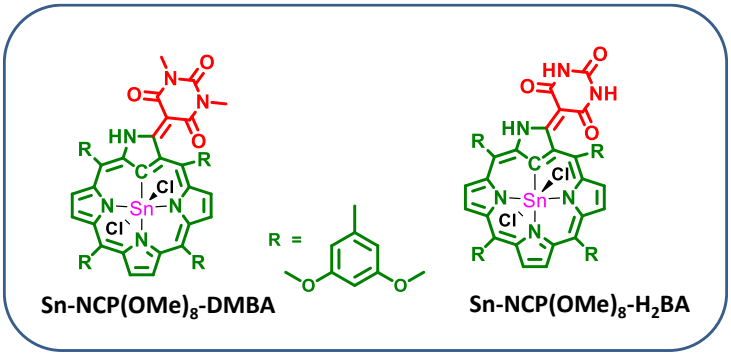

Fig. 1. Molecular Structures of N-Confused Porphyrins used in this study.

N-Confused Porphyrin (NCP) is an analogue of porphyrins in which one of the pyrrole ring is twisted toward outside and connected to *meso*-carbons at α and *β* positions.[1] This inverted pyrrole is responsible for the change in many photophysical and chemical properties. In general, NCPs have solvent-dependent spectral features since there are having two stable tautomeric forms.[2] In polar solvents, an externally protonated (2H) form is favoured due to hydrogen bonding, while in nonpolar solvents an internally protonated (3H) form is usually more stable. N-Confused porphyrin has a wide range of applications in the field of photodynamic therapy (PDT), nonlinear optics (NLO), catalysis, sensing etc.[3] Keeping this in mind, we decided to synthesize *β*-functionalized tin-based N-Confused Porphyrins for PDT application. Herein, we report the synthesis and characterization of tin metallated dimethyl barbituric acid (Sn-NCP(OMe)$_8$-DMBA) and tin metallated barbituric acid (NCP(OMe)$_8$-H$_2$BA) appended NCP. These NCPs exhibited red-shifted electronic spectral features compared to the free base NCP and have absorption in the NIR region. In this presentation, we will describe the synthesis, spectral and electrochemical redox properties of tin metallated barbituric acid appended NCP and their derivatives and their utilization in PDT in detail.

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P-163: Hypervalent Iodine(III) Mediated Synthesis of Isoxazoline *via* Oxidative of cyclization of Aldoximes

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Hypervalent iodine reagents have gained much attention in the field of organic synthesis because of their non-toxic, eco-friendly, mild reactivity, easy handling, and availability. Isoxazoline moiety belongs to a noteworthy class of compounds and occurs in several natural products. As this moiety has great biological significance, various methods have been developed for the synthesis of isoxazolines. These compounds have been prepared by using metal, oxidant or base mediated protocols in the past few years. This unit is also important in synthetic chemistry as a precursor for many useful compounds. In this context, we have established an efficient approach to access substituted isoxazolines via a metal-free and base-free protocol by employing aldoximes, styrene, acrylonitrile, and other dienophiles as reaction partners. This strategy employs readily available organohypervalent iodine reagent as an oxidant for the construction of isoxazoline under mild reaction conditions. The results of our approach will be presented.

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P-164: Recent Development Towards Green Synthesis of Anticancer Molecules

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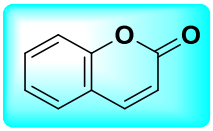
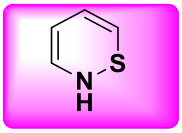
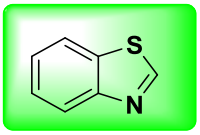


Coumarin



Thiazine



Benzothiazole

Cancer is acknowledged as the most common cause of mortality from the list of significant health-related problems and is brought on by unchecked cell development.[1] In coming Future cancer mortality will surpass that from cardiovascular illnesses. In order to combat the spread of cancer globally, it is need of hour for medicinal chemists to develop some unique medication.[2] A well-planned strategy is unavoidably needed for the development of innovative chemotherapeutic medicines with assumed potency, reduced toxicity, and high selectivity.[1] Heterocyclic compounds, viz coumarin, thiazine, and benzothiazole, invade a specific position to demonstrate the relationship between chemical structure and pharmacological activity in medicinal science.[3-5] Therefore, the efficient synthesis of drug-like heterocyclic compounds using greener approaches is an important task among medicinal chemist and chemical biologist.[6,7] The details of recent developments of these molecules using greener approaches will be presented therein.

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P-165: A new Naphthalimide based fluorescence probe for selective detection of Picric Acid

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A new naphthalimide-tetrabenzimidazole based fluorescent probe, **5** has been designed and synthesized. The photophysical properties of the probe 5 was examined in solvents of different polarity. The absorption maxima and fluorescence intensity shift toward high wavelength region upon increasing the polarity of the medium. Upon increasing water fraction (*fw*, 10-70%) in the medium the intensity of probe initially decreased significantly. However when the water fraction was further increased (*fw*; 80-90%) aggregation induced emission was observed with a blue shift. In 90% aqueous-THF medium probe upon interaction with different class of ions and explosive molecules showed high sensitivity and selectivity for picric acid (PA) in which relative fluorescence intensity quenched (switched – *Off*) significantly. Jobs plot analysis, based on emission titration data revealed a 1:1 binding stoichiometry between probe, **5** and PA. The limit of detection (LOD) was estimated and found to be 1.6×10^{-8} M (16 nM). The practical application of the probe has been demonstrated on test paper strip to detect PA with naked-eye sensitive response. Further, the mechanism of sensing was confirmed by ^{1}H, ^{13}C NMR, FTIR and Mass spectrometric analysis.

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P-166: A highly selective fluorescent sensor for Fe^{3+} based on covalently linked derivative of two naphthalimide unit

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A 2,2'-(((anthracen-9-ylmethyl)azanediyl)bis(ethane-2,1-diyl))bis(6-(piperidin-1-yl)-1H-benzo [de]isoquinoline-1,3(2H)-dione) as potential fluorescence probe has been designed, synthesized and its optical behavior were examined in different medium. The photophysical behavior of probe and its affinity toward different metal ions have been analysed in aqueous medium (90% aq. HEPES buffer in 10% ACN), protein medium and live cells. Its fluorescent sensor activity towards biological active ions like (cations, anions, NPPs) was carefully investigated. Probe showed excellent selectivity toward Fe^{3+} over other competitive metal ions. In the presence of Fe^{3+} naked-eye sensitive bright brown color developed in the medium (switched – *off*). In neutral and alkaline pHs (7-14) fluorescence enhancement observed however, in the acidic medium (pH, 6-1) fluorescence quenching was observed. All experiments were carried out at pH 7.4. The binding stoichiometry indicated that a 1:1 complex was formed between probe and Fe^{3+}. The binding mechanism was studied by ^{1}H NMR titration, FTIR and HRMS. The real-time application of Fe^{3+} was demonstrated in test paper-based detection.

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P-167: HFIP Promoted Metal-free Homodimerization of Styrene Diols: An Efficient Approach toward the Synthesis of 2-Phenylnaphthalenes

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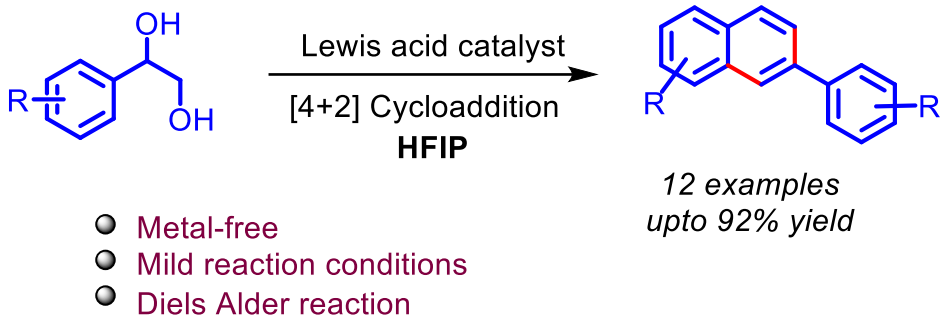

Due to its potent estrogen receptor (ER-β) agonistic properties the privileged 2-phenylnaphthalene molecule has received significant interest. Under mild conditions, herein, we have described a metal-free, straightforward, efficient strategy for the synthesis of 2-phenylnaphthalenes from 1-phenylethane-1,2-diols. In this present synthetic protocol, 1,1,1,3,3,3-hexafluoro-2- propanol (HFIP) is utilized as a solvent that stabilizes the reaction intermediate. We have performed an *in situ* IR experiment for mechanistic aspects that has revealed that the reaction proceeds through the formation of phenylacetaldehyde. The process involves an intermolecular [4+2] Diels–Alder reaction. HFIP as a solvent helps to stabilize the reaction intermediates for this cycloaddition. Moreover, this dimerization works under mild conditions with inexpensive catalysts, and it provides excellent yields. Several control experiments were carried out to gain mechanistic insights into the reaction.

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P-168: Solvent Induced Conversion of a Self-Assembled Gyrobifastigium to a Barrel and Encapsulation of Zinc-Phthalocyanine within the Barrel for Enhanced Photodynamic Therapy

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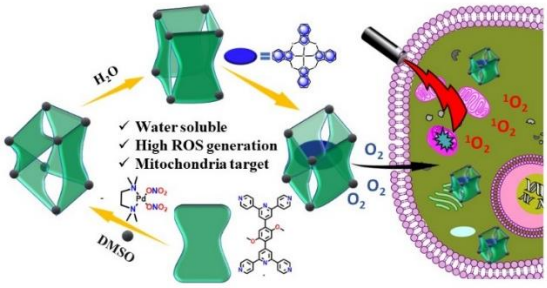

Selective formation of less symmetric architecture in the self-assembly of cis-blocked square planar Pd(II) or Pt(II) acceptors with tetratopic N-donor ligands are challenging. Herein, we report the exclusive formation of rare gyrobifastigium- geometry (**GB**) via coordination-driven self-assembly of the tetradentate donor (**L**) with cis-Pd(II) acceptor. The gyrobifastigium with the narrow windows was converted to a tetra-facial barrel (**MB**) with large windows by solvent induction. The interconversion from gyrobifastigium to tetragonal barrel opens an avenue for encapsulating water-insoluble photosensitizer; zinc phthalocyanine (**ZnPc**). The **ZnPc** has shown great potential applications as a photosensitizer (PS) in photodynamic therapy (PDT) owing to its strong absorption in the red-light region (660-720 nm) and biocompatibility. However, suboptimal PDT performance is observed for **ZnPc** due to the poor solubility and tendency to form aggregates in aqueous media. In this present study, the effective solubilization of **ZnPc** in aqueous media is achieved through the encapsulation of **ZnPc** within a water-soluble barrel (**MB**). The confinement of the **ZnPc** within the cavity of the **MB** (**Zn ZnPc⊂MB**) enhanced the singlet oxygen quantum yield in water. The enhanced cellular uptake and cytotoxicity of **ZnPc⊂MB** compared to **ZnPc** in HeLa cells showed that encapsulation of **ZnPc** within a water-soluble cage is an efficient method for the enhancement of PDT.

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P-169: Ratiometric and colorimetric "naked eye" selective detection of CN^- ions by electron deficient Ni(II) porphyrins and their reversibility studies

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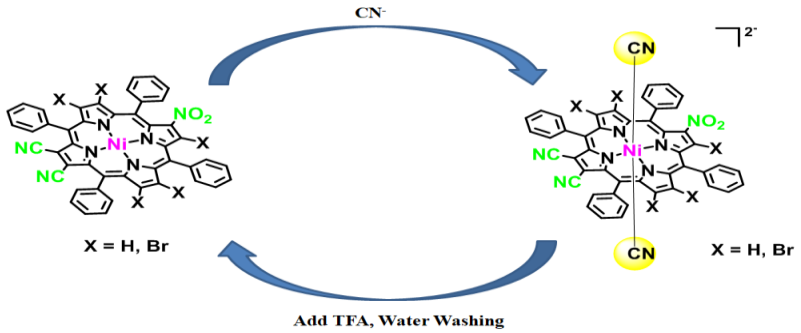

In general, square planar Ni (II) porphyrins exhibited very weak axial ligation and extremely low binding constants with nitrogenous bases. We are showing an easy, rapid, reusable, selective and sensitive 'naked eye' colorimetric cyanide ion sensing by highly electron deficient planar and nonplanar *β*-substituted Ni(II) porphyrins with good binding constants through coordinative interactions.[1] Highly electron deficient *β*-substituted Ni(II) porphyrins were synthesized and utilized as novel sensors for selective rapid visual detection of CN^- ions. This work describes the electronic spectral and electrochemical redox properties of these sensors. The ratiometric and colorimetric responses of these porphyrins were monitored by the change in optical absorption spectra. These sensors were found to be highly selective for cyanide ions with very good binding constants through axial ligation of CN^- ions and are able to detect the CN^- ions concentration in ppm level. This sensors can be recovered from $2CN^-$ adducts by acid treatment and reused without loss of sensing ability. CN^- binding strongly perturbs the redox properties of the parent porphyrin π-system. The applicability of this porphyrin as practical visible colorimetric test kits for CN^- ions in aqueous and non-aqueous media has also been explored. The mode of binding was confirmed by spectroscopic studies and DFT calculations.[2-3]

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P-170: Photocatalyzed Hydroxy-Arylation of Olefinic Double Bond in Visible Light: Synthesis of 3-Benzyl-3-hydroxyisoindolin-1-ones

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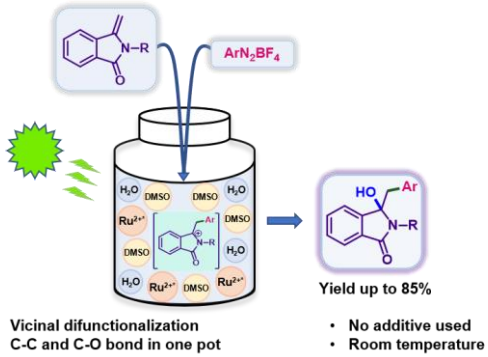

N-Substituted 3-hydroxyisoindolin-1-ones are useful structural scaffolds found in numerous bioactive natural products (Chilenine and Fumadensine) and pharmaceutical agents (CRR-228 and CRR-271) and used as a Raf kinase inhibitor and MEK protein kinase inhibitor.[1] Typically, 3-hydroxyisoindolin-1-ones are useful synthons[2] as they can be dehydrated to 3-methyleneisoindolin-1-ones or deoxygenated to bioactive isoindolin-1-one derivatives. In view of the profound biological importance of 3-hydroxyisoindolin-1-ones, various synthetic routes have developed over the years. We explored the feasibility of photocatalyzed synthesis of 3-benzyl-3-hydroxyisoindolin-1-ones in visible light. We anticipated that a Meerwein-photocatalytic approach might work on *N*-substituted 3-methyleneisoindolin-1-ones as starting materials and enable difunctionalization at the double bond. The entitled work describes a ruthenium-catalyzed and visible light-assisted hydroxy-arylation of the terminal double bond of *N*-substituted 3-methyleneisoindolin-1-ones. The reaction takes place with aryl diazonium salt as the arylating reagent and water as the hydroxyl source in visible light at ambient temperature. The strategy entails vicinal difunctionalization of alkene and enables construction of 3-benzyl-3-hydroxyisoindolin-1-one heterocyclic scaffolds in moderate to good yields. C−C and C−O bonds are formed in one pot without any external additive and oxidant through an in-situ generation of a carbocation intermediate in green light. The catalysis initiates via a radical pathway and involves a carbocation intermediate. The strategy provides an easy access to these molecules with potential medicinal chemistry applications.

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P-171: Femtosecond Laser-Induced Thermal Spectroscopy for Investigating the Molecular Interactions in Liquids

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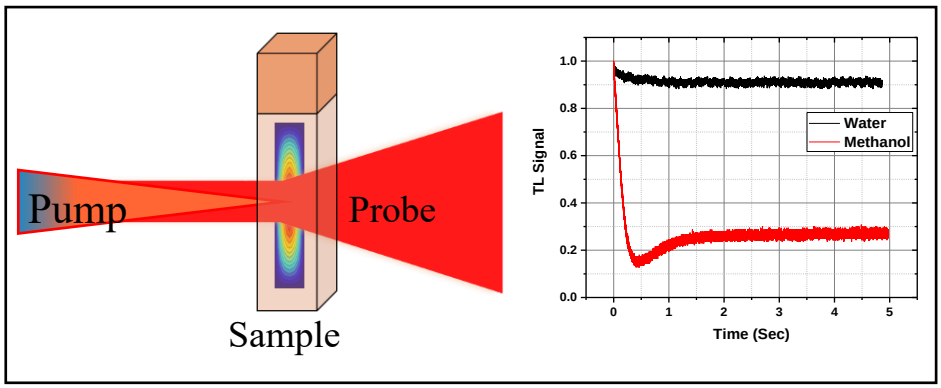

Femtosecond laser-induced thermal spectroscopy is a highly sensitive photophysical spectroscopic technique used for characterizing the physical and chemical properties of liquids, colloidal mixtures, nanoparticles, thin films etc. The thermally induced lensing effect is exhibited by the samples due to the localized heating by high repetition rate femtosecond lasers. In this technique, a temperature gradient, leading to a refractive index gradient is formed inside the sample. Heat accumulated inside the sample is dissipated into the bulk through the conduction and convective heat transfer process. From the steady-state and time-resolved thermal lens measurements, it was found that the molecular heat convection process in alcohols is strongly dependent on various molecular characteristics viz. molecular shape, size, chain length etc. In the case of binary mixtures of mono, di and tri-hydric alcohols with water, it is found that the convection heat transfer process is strongly affected by intermolecular hydrogen bonding interaction.

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P-172: Design and Synthesis of POM-MOF Hybrid Materials

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The polyoxometalates (POM) possess unique properties such as strong acidity, redox- and catalytical-activity. The metal organic frameworks (MOFs) are ideal hosts for a POM as a guest because they (MOFs) possess large surface area, ordered structure, high stability and tenable pore size.The POM-MOF hybrids show synergistic properties of POM and MOF. These POM-MOF hybrid materials have wide applications in catalysis, sorption, electrochemistry, magnetism, medicine etc. Encapsulation of POM into the pores of MOF is one of the method to synthesize the hybrid materials. Post synthetic modification is one of the important concept used for modification of metal organic frameworks. In this work, amino terephthalic acid is used as one of the ligand for the post synthetic modification. Various MOFs with amino-terephthalic acid ligand are functionalized with polyanions through electrostatic interaction via protonation of amino groups. The resultant POM-MOF hybrid materials are characterized by FTIR- and UV-DRS spectroscopy, PXRD studies, electrochemical- and gas adsorption-studies.

Keywords: Polyoxometalate, metal organic framework, hybrid materials, catalysis, gas adsorption.

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P-173: Molecular simulations of temperature and concentration dependence of structure and ionic mobility in diglyme-based Sodium-Ion electrolytes

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Glyme-based sodium salt solutions exhibit excellent electrochemical properties as battery electrolytes since they could enable the co-intercalation of sodium into graphite [1,2]. For example, solutions of $NaPF_6$ in glyme show exceptional chemical stability and better thermal stability than alternative carbonate-based electrolytes. The oxygen atoms present in the glyme molecules coordinate with the Na^+ ion in an octahedral manner, which can also be referred to as solvated ionic liquids of the form $[Na(glyme)]^+$---$anion^-$, with an electrochemical window of 4V and ionic conductivity of 1mS/cm [3]. The understanding of the solvation behavior of these electrolytes requires molecular-level exploration.

We perform computer simulations based on classical molecular dynamics and plane-wave density functional theory to mimic atomic interactions and ionic mobility.[4] Unlike the previous experimental and theoretical works which usually explore only a 1 M concentration of liquid electrolytes, we have studied the structure and ion dynamics over a range of concentrations of $NaPF_6$ in diglyme. The nature of the atomic interactions and the strength of these interactions were studied using radial distribution functions and uninterrupted lifetime analysis. The formation ion clusters were elucidated using the cluster analysis and dimer distribution function profiles suggesting that the Na^+ ions mostly exist as solvated ions that are coordinating with solvent molecules (free ions or solvent-separated ion pairs). Also, some fraction exists as contact ion pairs, and very few as aggregated ion pairs those increasing slightly with temperature and more with ion concentration. The self-diffusion coefficients of Na^+, PF_6^- ions, and the diglyme molecules were calculated using Einstein's relations from the mean-squared displacement of the respective species. The ionic mobility of Na^+ and PF_6^- ions were modelled using both Nernst-Einstein's and correlated Nernst-Einstein's relations was validated with experiments.

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P-174: A Turn-Off CRISPR/Cas9 System for Precision Genome Engineering Applications

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Targeted protein degradation (TPD) has emerged as a promising therapeutic strategy with the potential to eliminate disease-causing proteins. Proteolysis targeting chimeras (PROTACs) work with the principle of hijacking the body's own regulatory mechanisms i.e., ubiquitin-mediated proteasomal degradation. The strategy has the potential to target proteins that are undruggable with traditional small molecules. From the structural point, an E3 ligase binding ligand, a target protein of interest binding ligand, and a linker covalently connecting these two molecules is the basic necessity of PROTAC design. These heterobifunctional molecules form a ternary complex by simultaneously binding to TOI and E3 ligase substrate (CRBN), resulting in the ubiquitination of the TOI and eventually its proteasomal degradation. Even with the growing applications of CRISPR-Cas9 in genome engineering and gene therapy, its Spatiotemporal regulation to eliminate off-target activities remained the bottleneck. We have developed a turn-off gene editing system with novel heterobifunctional protein degraders that selectively remove TOI (Cas9) via ubiquitin-proteasome degradation. This work provides insight into regulating CRISPR/Cas9-based genome engineering systems via PROTAC technology.

P-175: Nanotrap Grafted Cationic Hybrid Composite Material for Effective Toxic Chemical Segregation from Water

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Oxoanions made of metals are potentially harmful contaminants that seriously pollute the water. As a result, the separation of these species has recently drawn a great deal of research interest. Several excellent adsorbents have been used to manage chemicals effectively, but their restricted microporous nature, non-monolithic applicability, relatively sluggish kinetics, and lower selectivity prevented their widespread real-time use. In this study, we developed an innovative anion exchangeable hybrid composite aerogel material (IPcomp-6), which combines a stable cationic metal-organic polyhedron with a hierarchically porous metal-organic gel that is programmed with specific oxoanions trapping moieties. Even when there was a 100-fold excess of other coexisting anions, the composite scavenger was able to segregate different hazardous oxoanions from water, including, $HAsO_4^{2-}$, SeO_4^{2-}, ReO_4^-, CrO_4^{2-}, and MnO_4^- Even at low concentrations and considerably below the As(V) limit for drinking water set by the WHO, the material was able to selectively remove traces of $HAsO_4^{2-}$. Moreover, the hybrid material can successfully eliminate arsenate from natural drinking water samples and simulated industrial wastewater samples, in both batch and dynamic column exchange sorption experiment. The mechanistic role of multifunctionalities of IPcomp-6 towards efficient arsenate capture was further investigated by numerical flow-velocity experiments along with theoretical calculations.

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P-176: Arylation of Maleimide *via* Weakly Coordinating Acetamide Assisted Cross-dehydrogenative Coupling

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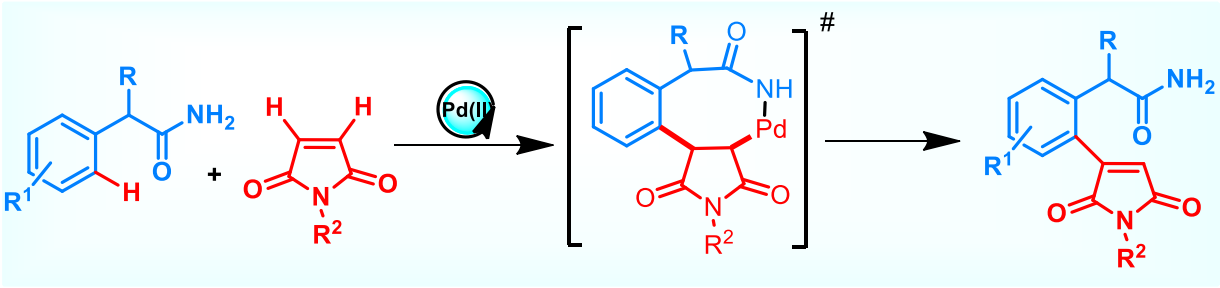

Maleimides are an important class of organic molecules present as a core moiety in various natural products and biologically active compounds. They also serve as an important synthetic precursor for various organic transformation reactions.[1] However, maleimides have been rarely employed as coupling partners for the direct synthesis of 3-aryl substituted maleimides *via* oxidative Heck-type reaction, due to the lack of b-hydrogen at the syn-periplanar position.[2] Therefore, herein, we report an efficient and highly selective synthesis of 3-arylacetamide incorporated maleimides through the cross dehydrogenative coupling process using the simple and native primary acetamide as a weakly directing group with Pd(II)-catalysis conditions. This reaction furnishes 3-arylated maleimide derivatives in good yields with high functional group tolerance. Furthermore, 3-arylated maleimides were transformed into synthetically important derivatives.[3] Based on preliminary control experiments, a probable reaction mechanism has been proposed for the distal C-H bond functionalization reaction. In addition, the photophysical properties of the synthesized products were also explored to give some useful insight about their characteristics.

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P-177: New Insights into Proteasome Inhibition Strategy for Enhanced Specificity and Cellular Toxicity

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The Proteasome is a multi-catalytic enzyme complex found in the nucleus and cytoplasm of all eukaryotic cells. It is the primary intracellular proteolytic system involved in intracellular proteolysis. The destruction of a protein is initiated by the covalent attachment of a consisting of several copies of ubiquitin chain (more than four ubiquitin molecules) through the concerted actions of a network of proteins, including the E1 (ubiquitin-activating), E2 (ubiquitin-conjugating), and E3 (ubiquitin-ligating) enzymes.[1] The ubiquitin-proteasome pathway is essential for the regulated degradation of intracellular proteins in eukaryotic cells. The Proteasome degrades damaged, oxidized, or misfolded proteins and plays a vital role in regulating proteins that control the cell cycle, transcription factors, and cell growth. Therefore, the continued health of the malignant cells, as opposed to normal cells, may depend on the degradation of damaged proteins. So, proteasome inhibition is a targeted therapy for cancer to promote cell cycle arrest or apoptosis. Bortezomib is the first selective, reversible, and only proteasome inhibitor for treating multiple myeloma. But bortezomib displays severe side effects due to non-specific cytotoxicity towards healthy tissue.[3] So, there is a clear need to develop new proteasome inhibitors with improved safety and efficacy profiles.

In this research, we have developed azobenzene based proteasome inhibitors which has photo switchable activity in proteasome and thus increasing the specificity of proteasome inhibitor, having better inhibition activity than known proteasome inhibitors. The results obtained from the theoretical and experimental studies will be shown in the poster.

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P-178: Mechanoresponsive Heptagon-Containing Non-planar Heteronanographenic Molecules

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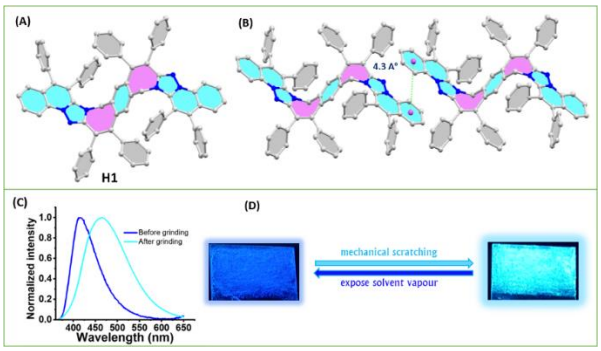

Figure 1. (A) Crystal structure and (B) crystal packing showing π-π stacking of a representative heptagon-containing nonplanar π-conjugated nanographenic compound **H1**. (C) Solid-state emission spectra before grinding and after grinding of the compound **H1**. (D) Digital photographs of a thin film of **H1** on a glass surface showing reversible mechanochromism.

Polycyclic heteroaromatic compounds (PHACs) have been recognized as potential organic materials for many applications in materials science because of their amazing features.[1] Among them, PHACs with heptagonal rings have drawn the attention of researchers due to their dynamic behavior, electronic properties, aromaticity, and solid-state packing. Heptagon incorporation can not only induce negative curvature within the scaffolds but also confer significantly altered properties through interaction with adjacent non-hexagonal rings. Despite the reports of several beautiful examples in recent years, synthetic approaches to heptagon-embedded molecules remain relatively limited due to the inherent difficulties of heptagon formation and incorporation into heteroaromatic frameworks. Here, we describe a rhodium-catalyzed efficient annulative π-extension (APEX) strategy that delivers variety of heptagon-containing π-extended nonplanar polycyclic heteroaromatic scaffolds from simple azolium units.[2] This class of fascinating nonplanar π-conjugated nanographenic compounds exhibited excellent solubility in organic polar solvents, tunable visible range emission with good quantum yield, and reversible mechanochromism property (**Figure 1**).

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P-179: An Anomalous Phase Transformation of Three Different Co-crystals of Citric Acid and 1,2-*bis*(4-pyridyl)Ethene in Solution and Solid-State Along with [2+2] Photochemical Reactivity

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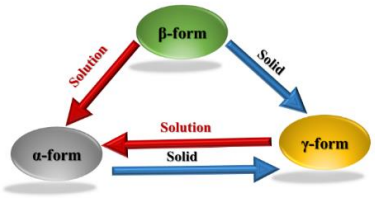

The design and preparation of multi-component solids, which are referred to as co-crystals, have been pursued, extensively, in recent times, for the development of a myriad of supramolecular assemblies with tailor-made properties, due to the ability of such co-crystals to alter the material properties with ease and find varied applications in the domains of pharmaceutics, materials sciences, *etc*. For example, pharmaceutical co-crystals, a subset amongst different types of co-crystals, having at least one of the co-formers as an Active Pharmaceutical Ingredients (API), offer enhanced bioactivity compared to their native drugs and in material science properties like photoluminescence, mechanical strength, *etc*., can be improved by crystallization, due to the enhanced purity of the material. Furthermore, the co-crystals also facilitate template-directed targeted covalent synthesis, enabling the non-reactive species to undergo a [2 + 2] photochemical cycloaddition reaction. In this regard, morphology, crystal growth in terms of kinetics, and thermodynamics play a significant role in the development of the desired materials. Herein, we present a system that has been thoroughly analysed on those fundamental aspects by employing the co-crystallization process on citric acid and 1,2-bis(4-pyridyl)ethene (*bpyee*), which provides an unusual formation of three different co-crystals, with varied molecular compositions, from a one-pot crystallization batch from a solution of 1:1 co-formers, showing different stability in solution and solid-state as shown in Scheme 1. Furthermore, all the forms undergo [2 + 2] photochemical reactivity upon UV-irradiation, due to the favourable Schmidt's photoreactive distance between the adjacent *bpyee* molecules.

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P-180: Anti-Markovnikov Palladium-Catalyzed Oxidative Acetalization of Activated Olefins

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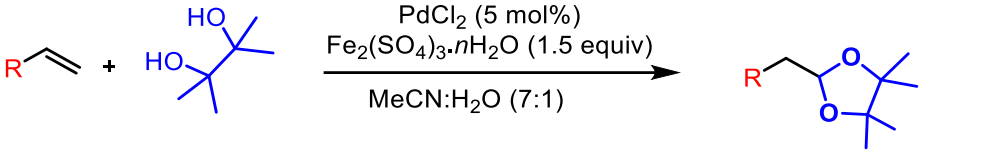

- ✓ Mild and benign reaction
- ✓ anti-Markonikov's selectivity
- ✓ Wide substrate scope

***anti*-Markovnikov product**
55 examples

In order to produce highly regioselective *anti*-Markovnikov compounds, an effective palladium-catalyzed oxidative acetalization of triggering olefins was established. In this approach, Fe(III) sulphate[1] has served as the sole reoxidant. *Anti*-Markovnikov acetals were developed using a variety of olefins, including aryl or benzyl acrylates, homoallylic alcohols, aryl-allylethers, and vinylarenes. Pinacol has been proven to be the superior diol for oxidative acetalization via the *anti*-Markovnikov pathway, competing against internal ketal or methyl ketone synthesis.[2] A range of 1,2-diol and 1,3-diols were also investigated in this methodology for potential terminal acetal emergence. The bulky ligand pinacol enabled the regioselectivity to be accomplished. [3] With adequate substrates, the cyclic acetals can be used as orthogonally functionalized 1,3- or 1,4-dicarbonyl or deoxygenated compounds, which were involved in the efficient synthesis of natural products. [4]

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P-181: Anion-templated programmable Chiral Self-Sorting in Pd_2L_4 Cages and the switching between chiral and achiral isomers

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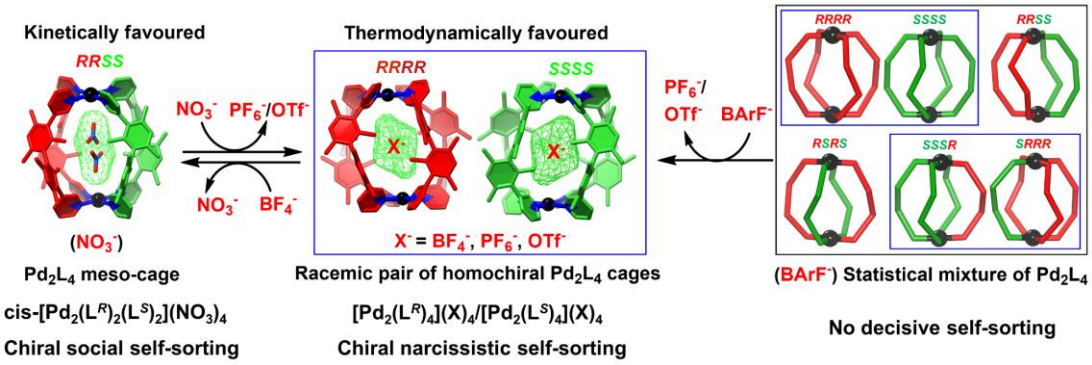

Chiral self-sorting is one of the fundamental molecular features with relevance to the origin of life and many biological functions. When a racemic mixture of building blocks is allowed to undergo self-assembly to form discrete molecules of increasing complexity, they can undergo social or narcissistic chiral self-sorting. The control over outcome of such chiral self-sorting, whether narcissistic or social leading to homochiral or heterochiral, is never been achieved in coordination-driven self-assembly to form metal-organic cage. Herein we report anion-induced chiral self-sorting of $[Pd_2L_4]$-type metal-organic cages, where the outcome of chiral self-sorting can be controlled by varying the counter-anions. NO_3^- anion encapsulation resulted a heterochiral meso-cage, {cis-$[Pd_2(L^R)_2(L^S)_2](NO_3)_4$}, through chiral social self-sorting. Encapsulations of BF_4^-, OTf^-, PF_6^- anions offered the racemic mixture of homochiral cages, {$[Pd_2(L^R)_4](X)_4/[Pd_2(L^S)_4](X)_4$}, through chiral narcissistic self-sorting. Bulky $BArF^-$ anion, which cannot be encapsulated within the $[Pd_2L_4]^{4+}$ cages afforded all possible diastereomers without any selective self-sorting. Anion exchange enabled structural transformations between homochiral and heterochiral cages. The kinetically favored product of NO_3^- encapsulated heterochiral meso-cage can be transformed into a racemic mixture of homochiral cages upon exchange with PF_6^- and OTf^- anions, but not by BF_4^- anion. Even the thermodynamically favored product of the racemic mixture of homochiral cage, included with BF_4^- anion, can be converted into the kinetic product of the meso-cage upon exchange with NO_3^- anion. The lack of selective chiral self-sorting associated with $BArF^-$ anion can be driven into high-fidelity chiral self-sorting upon exchange with PF_6^- or OTf^- anions.

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P-182: Photochemical Properties of Polyoxometalate Supported Transition Metal Complexes

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Polyoxometalates (POMs) compounds exhibit interesting redox properties. The redox properties of POM can be tuned by making hybrid materials with transition metal coordination complexes (TMCs).[1] The transition metal coordination complexes can act as counter cation in numbers of POM based organic-inorganic hybrid compounds. The POM hybrid materials with coordination complexes of the redox active ligands are not well explored. The 1,1'-[1,4-phenylene-bis(methylene)]bis(4,4'-bipyridinium) ligand have good electron accepting ability, redox activity and also one of the interesting photochromic material.[2] Therefore design and synthesis of POM-TM-bis-bipyridinium compounds will exhibit synergistic properties. In this work, we present synthesis and characterization of POM supported transition metal complex with 1,1'-[1,4-phenylene-bis(methylene)]bis(4,4'-bipyridinium). The resultant hybrid materials are characterized by FT-IR, DRS, TGA, PXRD studies and unambiguously by single crystal X-ray diffraction.

Keywords: Polyoxometalates, Transition metal complexes, Bipyridinium derivative ligand, Photochromic meterials etc.

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P-183: Tungsten Based Tin Oxide Nanoparticles: Role of Sacrificial Agents in Degradation of Organic Toxic Dye

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Water is the most essential natural resource. Gradually increase in the water contaminants due to speedy growth in the anthropogenic activities causes water pollution which affected its ecosystem and aquatic life [1]. Many studies have been conducted regarding the degradation of dye from which photocatalytic degradation seeks attention because it is eco-friendly and without any secondary contamination it provides total degradation of soluble organic pollutants from water and soil [2]. SnO_2 semiconductor having a wide band gap that can be easily modify by doping of impurities. It is used as a photocatalyst due to its ease of band gap engineered and excellent stability. To enhance the photocatalytic efficiency of pure SnO_2, the lattice of SnO_2 nanoparticles is engineered by doping of tungsten atom. Photocatalytical degradation efficiency towards organic toxic dye is checked by using sacrificial agents such as Methanol, ethane-1,2-diaminetetracetic acid, and Triethanolamine.

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P-184: Hydrogen Production from Formic Acid over Ruthenium Catalysts in Water

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It is supposed that world energy demand will continuously increase in the next few decades. Therefore, it is very important to accept the challenge of supplying sustainable energy to the world in near future. Hydrogen is supposed to be an efficient chemical energy carrier that allows for matching the increasing energy demand with the reduction of greenhouse gases. Its high-energy combustion or use in fuel cells produces water as the only byproduct. The physical and chemical properties of hydrogen gas do not consider as an ideal energy vector. With a limited volumetric energy density, it must be either compressed at very high pressure (350-700 bar) or liquefied at a very low temperature. Hydrogen gas is highly flammable and can diffuse through several materials. Thus, the chemical storage of H_2 in solid or liquid compounds is currently intensively investigated. In recent years, formic acid has been used as an important fuel either without reformation or with reformation. Formic acid could serve as one of the better fuels for portable devices, vehicles, and other energy-related applications in the near future. In addition, formic acid is an important platform C-1 chemical that is produced on a bulk scale in the industry. The low cost, the ready availability of formic acid and the favourable thermodynamics for hydrogen generation from aqueous formic acid make it an ideal candidate for the on-demand production of hydrogen gas using a suitable catalyst under ambient reaction conditions. Now, we have focused on recent developments in the use of formic acid as a liquid organic hydrogen carrier (LOHC) by using molecular catalysts.

Keywords: CO-free system; formic acid; hydrogen gas; molecular catalyst; water;

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P-185: Novel Route to Synthesize 1,4- Dihydroquinoline Derivatives by Nitrene Insertion Using Five Membered Heterocyclic Rings as Diene Precursor for [4+2] Cycloaddition with Benzyne

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Nitrogen heterocycles having wide range of applications forming not only an important building block of many naturally and synthetically available bioactive compounds but also act as synthetic precursors of nitrogen-containing compounds having pharmaceutical and industrial importance. 1,4- Dihydroquinoline derivative, a Nitrogen containing heterocycle can be used as reactant as well as reagent in synthesis of various types of biologically and pharmaceutically important compounds like ciprofloxacin, ofloxacin, sparfloxacin etc. [1] Because of these wide range of applications, 1,4- dihydroquinoline are subject of intense research. [4+2] Cycloaddition reaction is an important tool for the synthesis of various 1,4- dihydroquinoline derivatives. In continuation of our ongoing efforts to develop synthetically useful heterocyclic frameworks via nitrene transfer strategy,[2,3] we have synthesised various 1,4- dihydroquinoline derivatives.[4] Operational simplicity, no by-product formation, ambient temperature, atom-economy and high stereoselectivity are crucial features of the present protocol, which would enhance the scope of chemical and pharmaceutical applications of Quinolines.

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P-186: Fluorescent Copper conjugated Curcumin cystine nanoprobe for selective determination of Fe^{3+} and G-quadruplex DNA

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We are here to report the synthesis of fluorescent copper-curcumin-cysteine (Cu-CC) as a sensing platform. The synthesized probe has been confirmed by UV-visible spectroscopy, FT-IR, XRD, SEM, and TEM characterization techniques, respectively. The mechanistic aspects of selective sensing of Fe^{3+} and detection of different G-quadruplex DNA has been illustrated based on 'turn-off-on' concept of regeneratable fluorescence sensing probe. Interestingly, we have noticed a high selectivity to Fe^{3+} ion by as-developed Cu-CC sensing probe in comparison to other metal ions. Further, the restoration of fluorescence of sensing probe in the presence of different DNA sequence is illustrating a cost-effective, convenient and reliable detection methodology of DNA detection. The real-world sample analysis performance of regeneratable sensing probe for Pu27 DNA detection in the fresh human blood serum samples is showing a satisfactory result.

P-187: Liquid-liquid Phase Separation (LLPS) from Small Molecules and Their Fates

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Compartmentalization, by selectively localizing biomolecules in separated compartments, is an important characteristic of living cells. Cell uses a wide variety of protein-phase transitions to assemble and disassemble liquid-like focal bodies, within membranes and the cytoplasm, as a method to organize bioactivity. In recent years, liquid-liquid phase separation (coacervate) has emerged as a synthetic mimic to realize the formation of a particular class of dynamic compartments in cells, called membrane-less organelles (MLOs)[1]. To understand the physicochemical principles underlying MLO functioning such as their formation dynamics, aging, and impact on cellular processes, detailed studies are needed in both living cells and model systems. Although coacervates are made of long-chain nucleoside phosphates, oligonucleotides have been reported, but small molecule-based coacervates are seldom reported[2,3]. Herein, we introduced two different strategies to create small molecule based LLPS and tried to mimic their unique properties. In our first approach, inspired by MLOs meta-stable nature[4] (after performing their function, trends to transform into aggregate which sometimes causes diseases such as Parkinson, Alzheimer), we introduced the complementary charge in single molecule by changing pH of the solution to create dynamic LLPS. Interestingly, they are meta-stable in nature and temporally transform into thermodynamically stable hierarchical micron-sized fibers. In our next approach, inspired by non-equilibrium nature of the MLOs, we tried to create a reaction-driven transient LLPS with the help of boronic-ester dynamic covalent chemistry (between boronic acid and glucose). The LLPS formation is highly selective towards glucose and the lifetime of LLPS can be tuned by changing glucose and deactivator concentration (here lactone). All these systems can act as sequesters to the incoming guest molecules and shows excellent reversibility. We believe these reports will open pave towards new directions to explore small molecule based coacervate and their limitless functional properties.

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P-188: A micellar catalysis strategy applied to the Pd-catalyzed C–H arylation of indoles in water

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The creation of environmentally friendly catalytic methods is an ongoing interest and a topic in demand because of the environmental damage caused by the production of fine chemicals and pharmaceuticals. This initiative's main thrust is to replace volatile organic solvents (VOSs) with green reaction media because VOSs are the primary source of environmental pollution due to their widespread use (more than 85% of the total mass utilisation of a chemical process) and insufficient efficiency of recovery.

Simple access to functionalized indoles would be made possible by the selective control over a number of rival C-H sites. Here, we describe a modular and selective C-H arylation of indoles following the micellar catalysis approach by using the third generation "designer" surfactant SPGS-550-M in the presence of 1 mol% of [(cinnamyl)[PdCl]$_2$under mild conditions. The nature of the phosphine ligands was found to be critical for achieving site selectivity, DPPF and DPPP are the two forms of the phosphine ligand that were discovered to be essential for promoting the arylation at C3-H and C2-H respectively. The reaction can be scaled and offers high regio (C3 vs C2) and chemo (C vs N) selectivity with a broad functional group tolerance. Without sacrificing quality, the surfactant aqueous solution can be recycled and used again without compromising on product yields.

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P-189: Coupling of Single –Ni-Atom with Ni-Co Alloy Nanoparticles for PEM Fuel Cell Application

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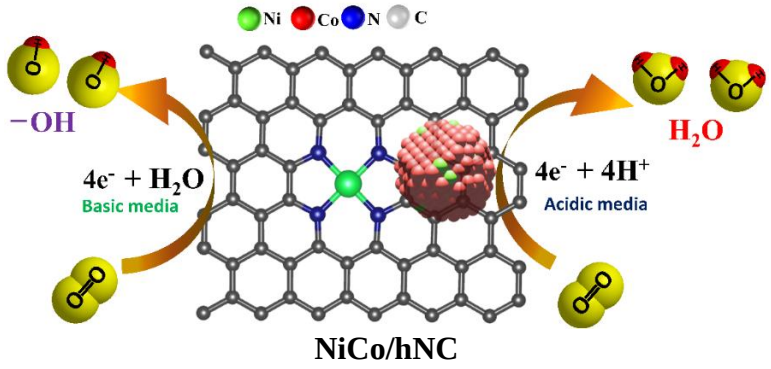

Figure 1. Schematic illustration shows ORR in basic (left) and acidic media (right) using as-synthesized NiCo/hNC electrocatalyst.

The development of a precious metal free electrocatalysts for proton exchange membrane fuel cell (PEMFC) with high activity and excellent stability for oxygen reduction reaction (ORR) remains an important challenge. Herein, highly efficient, and robust earth-abundant electrocatalyst is reported in both alkaline and acidic media, that are made up of metal-organic framework-derived Ni-N_4 sites and highly dispersed NiCo-alloy nanoparticles doped in unique hollow nitrogen doped mesoporous carbon denoted as NiCo/hNC. The synergistic interaction between NiCo alloy nanoparticles and Ni-N_4 sites in NiCo/hNC exhibits outstanding ORR activity at a half wave-potential of 0.925 V in alkaline media and 0.78 V in acidic media versus the reversible hydrogen electrode. Density functional theory and X-ray absorption spectroscopy suggested the strong interaction between Ni-N_4 site and NiCo-alloy nanoparticles. NiCo-alloy partially transferring electrons to the single Ni-site of NiCo/hNC and tune the adsorption free energy for ORR intermediates to facilitate the reduction of O_2. The PEM fuel cell test reveals NiCo/hNC catalyst shows excellent performance in H_2/O_2 and H_2/air and stable up to 24 hours for single cell operation.

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P-190: Deciphering the Role of Metal-Thiol Bond on the Excited State Relaxation Process of BSA Protected Metal Nanoclusters

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The protein scaffolds have drastically improved the quantum yield of Nanoclusters. Regardless of possessing tremendous properties like bright fluorescence, biocompatibility and high quantum yield, the fluorescence mechanism still remained unexplored.[1] To probe the same, we investigated the relaxation pathways of bovine serum albumin (BSA) protected group XI metal (Au, Ag and Cu) NCs, in the presence of electron donating (Trolox) and accepting (Methyl Viologen) groups. Through steady state and time resolved spectroscopic studies, we have determined the optical response of all the clusters to donors and acceptors. It was observed that the extent of covalent nature of M-S bond dictate the generation and stability of the LMCTs via triplet state in the clusters. The BSA-Ag NCs lacked these LMCT pathways due to weak M-S interactions, while BSA-Au and BSA-Cu NCs exhibited strong LMCT dependent luminescence with a distinct difference in between them.

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P-191: Ruthenium (II)-Catalyzed Redox-Neutral C−H Alkylation of Arylamides with Unactivated Olefins

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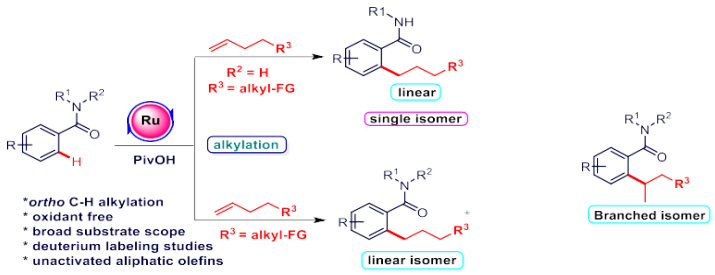

The transition-metal-catalyzed chelation aided selective C-H alkylation of substituted arenes with olefins has fascinated considerable devotion in modern organic synthesis. By using this approach, *ortho* alkylation of substituted aromatics was effectively synthesized in a highly regioselective manner.[1] Typically, the low valent metal complexes are sensitive to air and inert conditions are required. To overcome this issue, researcher have been trying to develop an efficient protocol for the C-H alkylation *via* the deprotonation pathway.[2] However, this type of alkylation reaction is very challenging and difficult to succeed. Generally, in the deprotonation pathway, substituted arenes react with olefins affording alkenylated products owing to the facile *β*-hydride elimination. Thus, only few reports are available on the alkylation of substituted arenes with olefins *via* a deprotonation pathway.[3] In this symposium, we are presenting a highly challenging weak chelation group aided redox-neutral C-H alkylation of arylamides with unactivated olefins catalyzed by a ruthenium complex *via* the deprotonation pathway. This protocol has broad substrate scope with high functional group tolerance. Remarkably, the reaction was well-suited with various substituted arylamides including secondary and tertiary and functionalized/unfunctionalized unactivated alkenes. In this reaction, anorganic acid (PivOH) acts as a proton source in protonation step and the corresponding acetate group deprotonates the *ortho* C-H bond of arylamides. A plausible reaction mechanism involves the C-H bond activation/insertion followed by protonation was presented and reinforced by the H/D exchange experiment.

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P-192: Continuous-flow Fe-Zeolite catalyzed temperature directed synthesis of bioactive tetraketones and xanthenes using epoxide and cyclic-1,3-diketone via Meinwald

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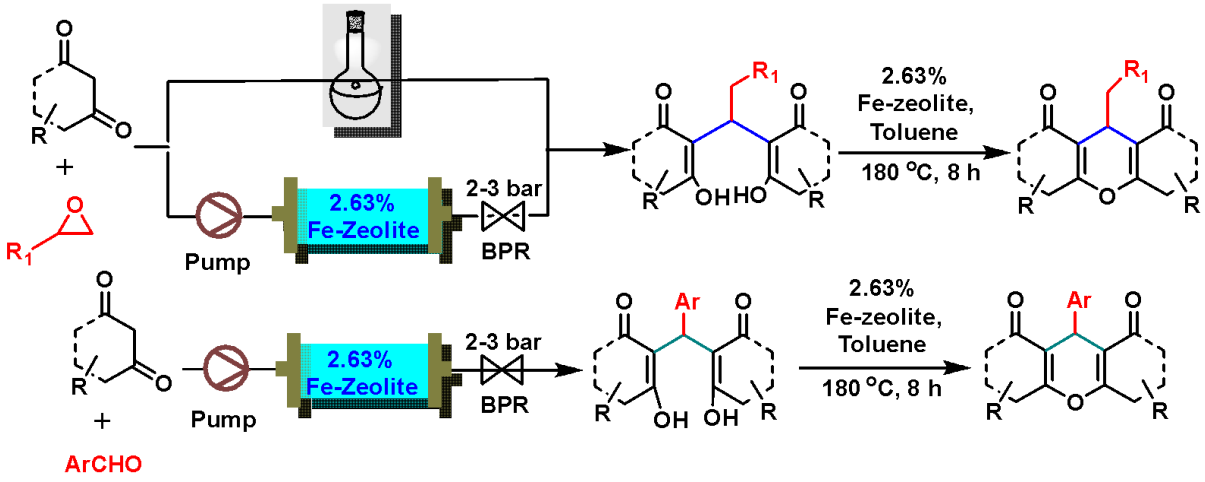

Tetraketones and xanthenes are important class of bioactive compounds.[1-3]A sustainable approach for the bioactive tetraketone synthesis using epoxides and cyclic-1,3-diketones in the presence of Fe-zeolite as a catalyst via Meinwald rearrangement has been developed under batch and continuous flow module. Further increasing the temperature to 180 °C, these tetraketones undergoes cyclization reaction in the presence of catalytic Fe-zeolite to afford xanthene derivatives. Moreover, this Fe-zeolite catalyst is also useful for the reaction of aldehyde and cyclic 1,3-diketone affording the tetraketone in high yield. Advantageously, the present approach offers gram scale synthesis in batch as well as in continuous flow. This approach is sustainable to generate many bioactive tetraketones and xanthenes, which does not produce any waste. The Fe-zeolite used in this process is easy to synthesize in multigram-scale, inexpensive, and easy to recover, and recyclable.

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P-193: A Protective Metal-Organic Framework with Multiple Donor Site for an Efficient Surface Coating Application Supported by Optical Spectroscopic and DFT Studies

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As electroless and electrodeposition of Cu composite coatings on various substrate surfaces have improved, so as the interest of researchers in metal deposition processes developed enormously. It was made possible by numerous recent applications of Cu based coatings because of their improved functional characteristics. This article discusses how organic additive affect an electroless copper bath while coating the surfaces. While coating Glycine and sodium hypophosphite were the two reducing agents used in copper bath; a non-toxic natural tri-sodium citrate was used as a complexing agent and sodium hydroxide as electrolyte for Anti-Corrosion studies. The accelerating effect of organic additives depends on the throwing power, thickness uniformity, surface tension, control of the grain structure, and deposit properties. Concentrations of 1 ppm and 10 ppm of organic additives were optimized and studied at 72 ^{o}C and a pH range of 4.7 to 5.2. The physico -chemical parameters were computed using weight gain, anodic, and cathodic polarisation techniques to test the stabilising effects of organic compounds in 1% NaCl. When the amount of Cu was reduced in the solution bath, atomic force microscopy (AFM) studies of the deposits revealed a granular structure of the electrodeposited thin films of metal-organic framework. Quantum mechanical indices like E_{HOMO}, E_{LUMO}, energy gap (E), and dipole moment (μ) were used to determine the effects of the stabilisers' adsorption on copper. The theoretical structural elucidation of the newly synthesized thiophene appended benzothiazole hydrazone and band gap of the copper coordinated organic framework have also been determined using DFT Calculations.

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P-194: A practical, Metal and additive free regiodivergent synthesis of polysubstituted indolizines

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Indolizine moiety is a worthwhile nitrogen-containing heterocycle that is the structural motif of various biologically active natural products such as swainsonine, castanospermine, lamellarine, camptothecin[1] as well as the synthetic compounds possessing anticancer, anti-tubercular, anti-inflammatory, antiviral, antioxidant, phosphatase inhibitor, analgesic, etc activities.[2] In view of such a wide range of biological activity of indolizine based compounds, various research groups are working on developing new synthetic routes for the construction of privileged indolizine moiety *via* C-H bond activation,[3] cross-coupling of pyridine and alkenes,[4] *trans* annulations of pyridotriazoles with alkynes,[5] cycloisomerizations of propargylic pyridines and alkynylpyridines[6] along with some multi-component approaches.[7] The usage of expensive and toxic metals like rhodium, ruthenium, palladium, gold, silver, platinum, etc., and complex starting materials make these synthetic routes less impactful. To avoid these complicated methodologies, herein, we have developed a metal and base free, atom-economic method for the regiodivergent synthesis of crucial six or eight substituted indolizine from *meta*-amide substituted pyridine and alkyne *via* a [2+2+1] cycloaddition under ambient conditions. The reaction proceeds through the cleavage of the carbon-carbon triple bond and regioselectivity of this cycloaddition is controlled *via* a hydrogen bond, which is supported by DFT studies.

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P-195: Pd-catalyzed site selective and Chemoselective CH functionalization towards Polyring Fused N-heterocycles

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For the last couple of decades, the functionalization of unactivated C-H bonds bonds at will for the strategic introduction of bonds or functionalities have been a matter of extensive investigation. Herein, we have unraveled an interesting Pd-catalyzed site selective C-H functionalization on 5-benzoyl-pyrrolo[2,1-*a*]isoquinoline scaffold, in which three different functionalizable C-H bonds were identified that could be judiciously transformed towards multiring fused *N*-heterocycles. The experimental and theoretical investigations have shown that there is a preference for Pd-catalyzed cross dehydrogenative coupling towards 8*H*-indeno-pyrrolo[2,1-*a*]isoquinolinone derivatives. Later, we identified a hitherto unknown oxygen induced palladium catalyzed selective C-H amination in 5-benzoyl-pyrrolo[2,1-*a*]isoquinoline towards a pentacene *viz*., 9*H*-indolo-pyrrolo[2,1-*a*]isoquinoline. Finally, we came across an unexpected site selective C-H amination towards the formation of multiring fused benzazepine while using a substrate bearing a NO_2-group on the benzoyl moiety of starting substrate. This result can be attributed to the stability and higher electron density at the reaction centre on isoquinoline ring.

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P-196: Aminium radical-cation catalysed S_N2 type Nucleophilic Ring Opening of Activated Azetidines with Arenes and Heteroarenes: Synthetic Route to Tolterodine

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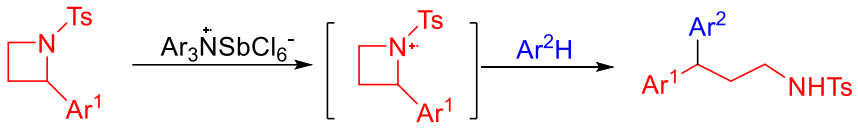

Ar^2= aryl, heteroaryl. Yield up to 98%

- Optimum reaction condition
- Low catalyst loading
- Transition metal-free
- Excellent yield
- Broad substrate scope
- Gram-scale synthesis

Aminium radical- cation mediated S_N2-type nucleophilic ring-opening of various 2-phenyl-*N*-tosylazetidines with electron rich arenes and heteroarenes to afford various 3,3-diaryl/heteroaryl propylamines with excellent yield (up to 98%) is reported. This synthetic route is utilised for the synthesis of tolterodine.

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P-197: Cadmium-metal-organic framework: Synthesis, characterization and fluorescent studies towards nitroaromatic explosives

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From the last two decades, metal-organic frameworks (MOFs) have gained significant attention due to their potential applications in different domain.[1,2,3] Here, we have synthesized a novel [Cd(7-ANDS)(bpa)$_{1.5}$]2H$_2$O MOF (Cd-MOF) (7-ANDS = 7-aminonaphthalene-disulphonate; bpa = 1,2-bis(4-pyridyl)ethane) through a solvothermal reaction, and successfully characterized *via* elemental analysis, FT-IR, PXRD, TGA, single crystal X-ray diffraction techniques. Through single crystal X-ray diffraction, it has been observed that the resulted MOF consists of two-dimensional framework. Moreover, this Cd-MOF exhibits the excellent luminescent properties and shows the capability for the selective detection of DNP among the numerous nitroaromatic analytes that make it potential chemosensor.

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P-198: Stereoselective Synthesis of Functionalized Succinimides by Radical Cascade Sulfonation, Cyclization, and Concomitant Thiolation/Selenation of Aza-1,6-Enynes.

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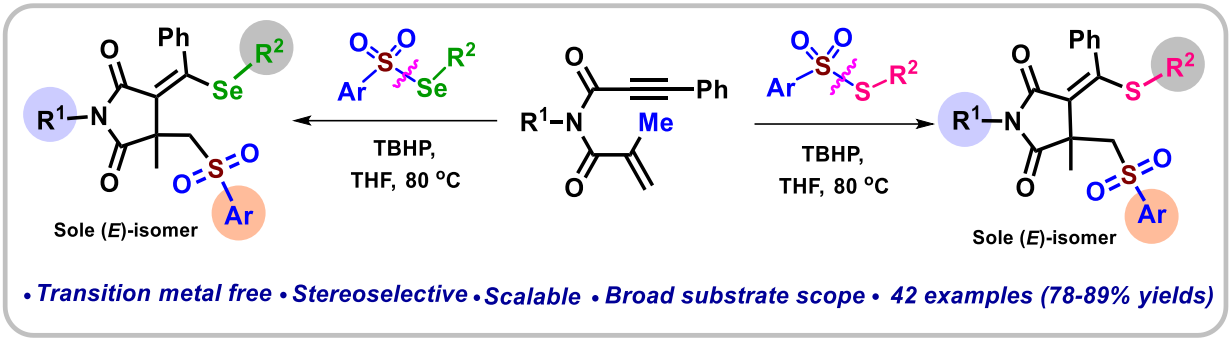

A metal-free radical cascade seleno/thiosulfonation of aza-1,6 enynes has been developed to access seleno/thiosulfonated succinimides. The developed method allows the stereoselective synthesis of highly decorated succinimides under mild reaction conditions in good to excellent yields. The proposed radical pathway for the reaction is well supported by the control experiments.

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P-199: Bay expanded Terrylene Diimide exhibiting Room Temperature Phosphorescence

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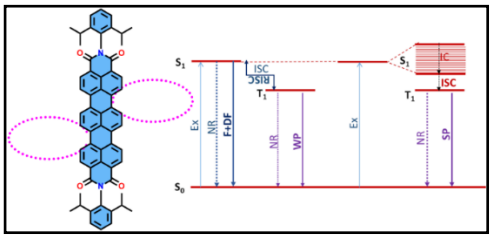

The fine-tuned opto-electronic and photophysical properties of rylene diimide (RDI) derivatives make them suitable candidate for the applications in Organic Field Effect Transistors (OFETs), Organic light Emitting Diodes (OLEDs), Organic Photovoltaics (OPVs), bio-imaging and sensors.[1] One such strategy is the expansion of the RDI core using arene/heteroarene as a fusion unit along the shorter molecular axis. The expanded molecules have distinct properties from their parent RDI along with the inherited properties like thermal and photochemical stability, high molar extinction coefficients. [2] The number and position of the fused rings plays a critical role in finetuning their properties. In this direction, we have synthesized a p-expanded terrylene diimide (TDI) with the fusion of heteroarene having 10 fused rings along the shorter axis. This expansion has resulted in the intense p- p stacking owing to the increased planarity. It is believed that stacking quenches the fluorescence emission. However, it can drastically enhance the phosphorescence.[3] Contrary to the expectation, despite of the p- p stacking, the synthesized molecule showed enhanced emission much higher than the parent molecule. The emission persisted for 2 milliseconds at room temperature. The achievable triplet state and enhanced ISC efficiency obtained from their phosphorescence spectra hinted towards the involvement of the delayed emission along with the prompt fluorescence. Thus, expansion of the TDI core has been proved to be an excellent strategy for the achievement of room temperature phosphorescent (RTP) molecule along with enhanced emission that are demanded for the cutting-edge application such as phosphorescent-OLEDs and biological electronic materials for gated-imaging and bio-sensors.

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P-200: Classifying deep eutectic solvents for polymer solvation *via* intramolecular dimer formation

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Deep eutectic solvents (DESs) have emerged as versatile and inexpensive solubilizing media with widely varying physicochemical properties.[1,2] Establishing characteristics of a novel solvent milieu for polymer dissolution is an important exercise. Assessment of two DESs constituted of H-bond acceptor (HBA) choline chloride (ChCl) and H-bond donors (HBDs) glycerol and urea named ChCl:Gly and ChCl:Urea, respectively, as solvents for polydimethylsiloxane (PDMS) solvation is carried out *via* investigation of intramolecular dimerization by pyrene (Py) end-tagged PDMS of MW 3100 (Py-PDMS-Py) as a fluorescent probe in the temperature range 293.15–363.15 K. The outcomes are compared with those in liquid PDMS of average MW 2000 (PDMS2000) and in glycerol. While the intramolecular dimerization by Py-PDMS-Py happens exclusively in the excited-state in liquid PDMS2000, wavelength-dependent fluorescence excitation spectra along with excited-state intensity decay kinetics reveal presence of ground-state interactions between pyrenyl moieties in ChCl:Gly, ChCl:Urea and glycerol. [3] This leads to the proposition that PDMS prefers to stay in predominantly coiled form in DESs and glycerol as opposed to that in PDMS2000, where PDMS-PDMS contact is maximized leading to the absence of ground-state heterogeneity. Thus, while the liquid PDMS2000 is characterized as a "good" solvent, DESs ChCl:Gly and ChCl:Urea along with glycerol may be designated as "bad" solvents for PDMS dissolution.

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P-201: Visible-light-driven Photoredox and Palladium dual catalysis: a route to directing group assisted decarboxylative site-selective benzoylation of N-phenyl-7-azaindoles

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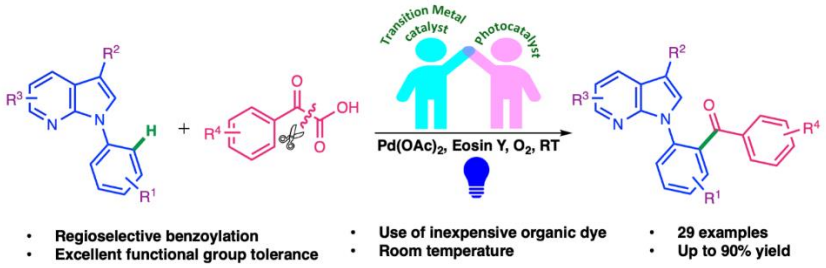

Figure 1: Directing group assisted decarboxylative ortho-benzoylation of N-aryl-7-azaindoles with α-keto acids.

Directing group assisted C-H activation plays a significant role in functionalizing specific C-H bonds and helps in the construction of diverse molecular scaffolds by employing transition metals,[2] they do possess certain limitations in terms of cost, harsh reaction conditions, and broad general applicability. Some of these challenges have been addressed by invoking dual catalysis approach assisted by photocatalyst in visible light. Such dual catalytic systems have resulted in an organic metamorphosis, allowing distinct activation modes inaccessible through single catalytic system, and offering complementarity to traditional organic reactions. The entitled work describes the directing group assisted decarboxylative *ortho*-benzoylation of *N*-aryl-7-azaindoles with α-keto acids by synergistic visible light promoted photoredox and palladium catalysis. Detailed mechanistic studies suggest that the decarboxylative photoredox cycle of Eosin Y with Pd proceeds via a radical process. 7-azaindoles are useful scaffolds found in many pharmacologically active compounds. Various methods for selective *ortho*-functionalization of *N*-phenyl-7-azaindoles under thermal conditions have developed in recent years.[3]

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P-202: A Photophysical Insight into the Mode of Action of Polyphenols as Protein Aggregation Modulators in The Ultrafast Timescale

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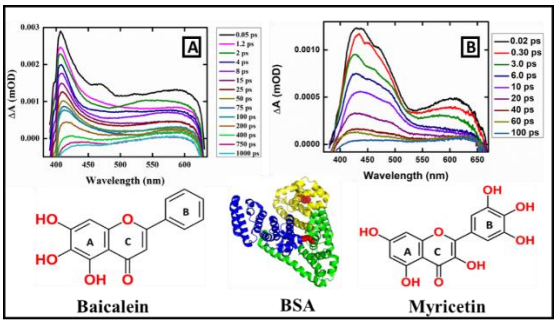

Figure 1: Transient Absorption Spectra of BSA bound to (A) Baicalein and (B) Myricetin

Misfolding has been shown to give rise to protein aggregates that serve the major triggering factors for several debilitating neurodegenerative diseases starting, namely Alzheimer's Disease and Parkinson's Disease, to name a few. Extensive research is being carried worldwide out in discovering suitable drugs that can prevent such diseases by either inhibiting aggregation or breaking up pre-formed aggregates[1]. Non-lethal, naturally occurring polyphenols have stood out to be one of the crucial antidotes. Apart from their anti-oxidant properties, they can exhibit both irreversible covalent and reversible non-covalent interaction with protein aggregates thereby, preventing protein self-association, redistributing oligomers into non-toxic ones, reducing damage due to free-radical formation and dissolving protein aggregates[2]. But the mechanism of how the polyphenols (baicalein, myricetin, and EGCG) modulate the fibrillation is still not clear. These biologically active compounds are well primed to exhibit excited state intramolecular protein transfer (ESIPT) which might play an important role in the aggregation modulation process. To probe the ESIPT process, we have studied the excited state photo physics of the polyphenols in the ultrafast timescale in neat solvents (to mimic the hydrophobic interior of protein aggregates) as well as in surfactants (both pre and post-CMC) and in presence of evolving aggregates as a function of the incubation time. The difference in the evolution of the spectral properties of these compounds as a function of protein aggregates provides significant insights into the possible modes of action of these polyphenols.

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P-203: Water enabled, nickel-catalyzed highly chemoselective C-allylation of (NH)-indoles employing alcohols

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The first 'in-water' nickel-catalyzed chemoselective C3-allylation of (NH)-indoles employing allylic alcohols under mild conditions is reported here. Different indoles and allylic alcohols were found compatible with excellent chemo-, regio-, and stereo-selectivity and functional group tolerance. The use of water not only provides sustainability by eliminating the need for organic solvent as reaction media but it also activates allylic alcohols via hydrogen bond networking and stabilizes the consequent hydroxide ion (strong solvation effect) resulting in facile oxidative addition, and thereof the formation of electrophilic π-allylNi complexes leading to C3-allyl indoles. The study further highlights the first Hydrogen-bond assisted intermolecular N → C allylic migration via π-allylNi complexation and reports the first synthesis of allyl indoles using allylamine as electrophilic precursors.

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P-204: Cobalt (II)-based spin crossover materials with twisted PDI dianion

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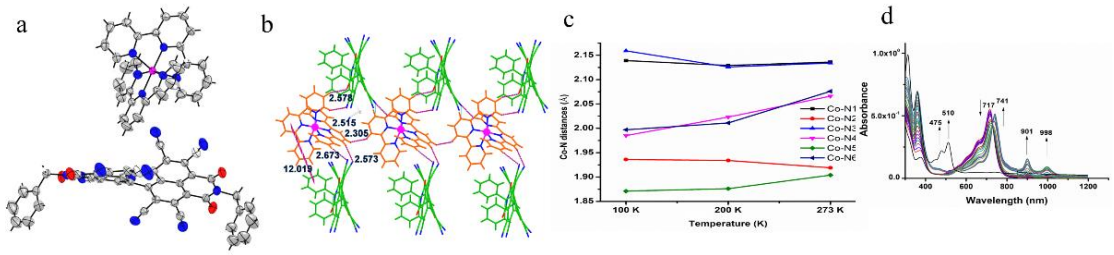

Fig. 1: a) Crystal structure of metal complex; c) Supramolecular interactions and crystal packing along ac-plane at 273 K.; c) Plot of variation of metal-ligand bond lengths with temperature; d) UV-Visible spectrum- titration of metal complex with oxidising agent.

Hybrid organic-inorganic materials are intriguing due to their flexibility in fine tuning of functionalities leading to their applications in memory-based storage devices, transistors, magnetoelectric supramolecular switches, magnetic and conducting materials. A spin crossover complex (SCO) showing electronic transitions from low spin (LS) to high spin (HS) state capable of showing hysteresis is a perfect example of such application[1,2].

Herein, we wish to report the synthesis and characterisation of $[Co(terpy)_2]$ [Benzyl-PDI-CN_8] complex through different analytical techniques. Perturbation by temperature, external stimuli induce changes in the supramolecular interactions between the twisted redox switchable helical perylene diimide (PDI) counter anion and the terpyridine (terpy) bound cobalt which further results in the variable metal-ligand bond lengths.

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P-205: Influence of C–H•••S Hydrogen Bonds on Thermal Expansion Studies in Two Concomitant Co-crystals of Ethionamide and 2-Thiobarbituric acid

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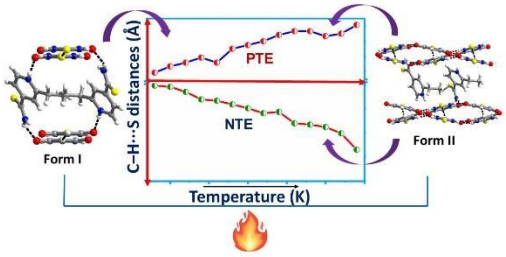

Thermoresponsive materials have drawn tremendous attention in recent times, as these materials can be used as thermochemical actuators or sensors.[1] Thermal expansion is a physical property of any material which can be classified into three categories, positive thermal expansion (**PTE**, increase in dimension upon heating), negative thermal expansion (**NTE**, decrease in dimension upon heating), and zero thermal expansion (**ZTE**, no change in dimension upon heating).[2] In any material, **PTE** is most frequently observed whereas **NTE** and **ZTE** are rarely observed. The most demanding materials are those that exhibit either **NTE**, **ZTE**, or both upon heating in any direction.

Thermal expansion studies on purely organic materials having non-covalent interactions are usually show **PTE** whereas organic assemblies having **NTE** or **ZTE** are not well explored.[3-4] So, development of organic materials with potential properties of **NTE** or **ZTE** has garnered much attention to address currently growing societal demands for the novel materials. In this context, we present here comparative thermal expansion studies on two organic concomitant co-crystals (Form I and II) of Ethionamide (**ETH**) and 2-Thiobarbituric acid (**TBA**). Variable temperature single crystal X-ray diffraction (**VTSCXRD**) study reveals that both Forms have significant **PTE**, **ZTE** and more interestingly, one of the co-crystals shows significant **NTE**. Complete structural analysis of the two co-crystals reveals that **PTE** as well as **NTE** are solely governed by weak C–H···S hydrogen bonds which is not too far documented in the literature. We describe also in this presentation, vividly, the efficacy and influence of C–H···S hydrogen bonds towards the thermal expansion in both forms.

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P-206: Synthesis, Spectral and Electrochemical Studies of Dicyanovinyl Substituted Porphyrins for Excited State Charge Transfer Dynamics

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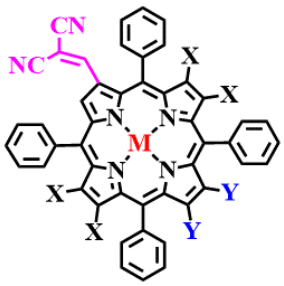

X = H, Y = H, M = 2H, Ni^{II}, Cu^{II}, Co^{II} and Zn^{II}
X = H, Y = Ph, M = 2H, Ni^{II}, Cu^{II}, Co^{II} and Zn^{II}
X = Ph, Y = H, M = 2H, Ni^{II}, Cu^{II}, Co^{II} and Zn^{II}

Figure 1. Molecular structures of synthesized porphyrins.

Dicyanovinyl substituted porphyrins having different number of phenyl groups were synthesized and characterized by UV-Vis, Fluorescence, NMR spectroscopic techniques and MALDI-TOF mass spectrometry. These porphyrins were prepared by Vilsmeier-Haack formylation, Suzuki reaction and Knoevenagel condensation.[1] The dicyanovinyl substituted porphyrins are utilized in the various fields such as nonlinear optics (NLO) and chemodosimeters for ratiometric and colorimetric sensing of cyanide ions.[2] These systems also depicted effective π-conjugation between the pyrrole ring and its olefinic substituent which is reflected in the UV-vis absorption spectra as the red-shifting of both Soret and Q-bands compared to precursors and also it exhibited tuneable redox properties and high dipole moment due to push-pull *β*-substituents. DFT studies showed nonplanar and saddle shape conformation. In this presentation, we discuss the synthesis, spectral and electrochemical redox properties of these porphyrins and their utilization in detail.

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P-207: Cu-Catalyzed and Iodine Assisted Domino Synthesis of Thioaurones through C-S Bond Formation using Xanthate Surrogate

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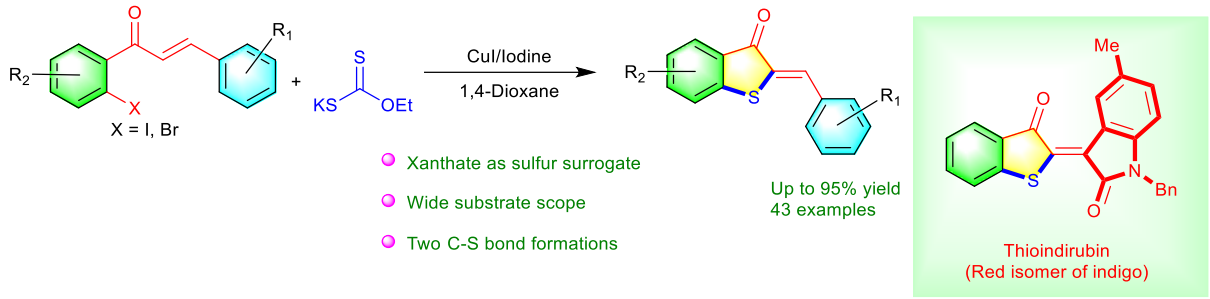

Scheme 1. Domino synthesis of thioaurones using xanthate as a sulfur source.

Due to numerous biological activities and widespread applications, the synthesis of sulfur-containing heterocyclic compounds has become an important tool in synthetic organic chemistry.[1] Specifically, thioaurones are useful synthetic intermediates for biologically important and fused heterocyclic compounds.[2] In addition, thioaurone has been used as a precursor for thioindigo dyes and photoswitchable biomolecules.[3] Therefore, considering the importance of thioaurones, recently we have reported the synthesis of thioaurones using odorless xanthate sulfur surrogate and iodine as a reagent. The reaction proceeds *via* in-situ C-S bond generation followed by C=C reduction of α, β-unsaturated, and α-iodination of saturated ketones. Iodine plays a dual role in this reaction as a reducing agent and halogen source in iodination. Synthesis of thia-analog of indirubin the red isomer of indigo was also achieved.[4]

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P-208: Hydroxamate-Directed Access to β-Kdo Glycosides

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The reaction repertoire for forming short-term aziridinone or azaoxyallyl cation from α-halohydroxamate is conceptually extended to design Kdo-glycosyl donor by installing hydroxamate moiety at anomeric centre which shown to be highly effective for stereoselective access to β-Kdo glycosides. Pivotal roles of hydroxamate over amide is disclosed in control experiments. Among the 2-keto-3-deoxy sugar acid family, 3-deoxy-D-manno-oct-2-ulosonic acid (Kdo) represents an eight-carbon keto-sugar acid present in bacterial polysaccharides through glycosidic linkage. [1] α-Glycosidic form of Kdo is present in Gram-negative bacteria as constituent of lipopolysaccharide (LPS) core region which is crucial for maintaining structural integrity of the bacterial membrane. On the other hand, Kdo β-glycoside residue is present in the repeating unit of capsular polysaccharides (CPS) of both Gram-positive and Gram-negative bacteria [2-3] for example, β-Kdo oligosaccharide linker can be found in the reducing end terminus of the CPSs of Escerichia coli, Kingella kingae or Neisseria meningitidis. Cytidine monophosphate, a sugar nucleotide that is processed by Kdo glycotransferase, cites another example where β-glycoside residue of Kdo is present.

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P-209: A Bidirectional Iterative Approach to Sequence-Defined Unsaturated Oligoesters

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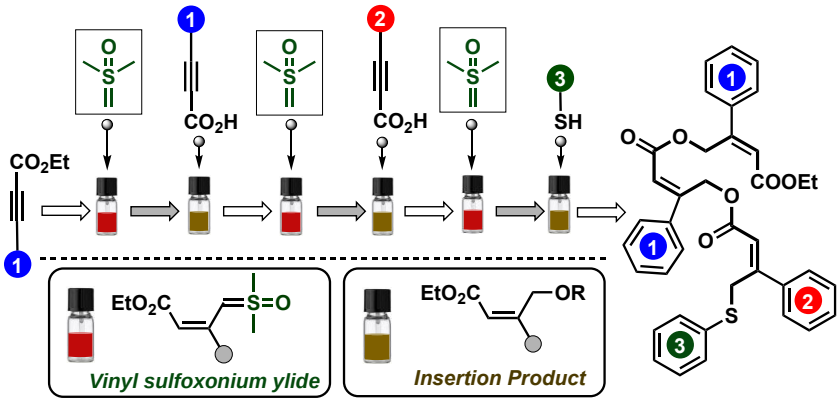

We have developed a metal and reagent-free strategy for the synthesis of unsaturated oligoesters via sequential insertion of vinyl sulfoxonium ylides into the O−H bond of carboxylic acid. Like two directional coupling of amino acids (N- to C- terminal and C- to N- terminal) in peptide synthesis, the present approach offers a strategy in both directions to synthesize oligoesters. The sequential addition of the vinyl sulfoxonium ylide to the carboxylic acids (acid iteration sequence) in one direction and the sequential addition of the carboxylic acids to the vinyl sulfoxonium ylide (ylide iteration sequence) in another direction yield (Z)-configured unsaturated oligoesters. To perform this iteration, we have developed a highly regioselective insertion of vinyl sulfoxonium ylide into X−H (X = O, N, C, S, Halogen) bond of acids, thiols, phenols, amines, thiols, indole, and halogen acids under metal-free reaction conditions. The insertion reaction is applied to a broad range of substrates (> 50 examples, up to 99% yield) and eight iterative sequences. Mechanistic studies suggest that the rate-limiting step depends on the type of X−H insertion.

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P-210: Probing the effect of glycation on the esterase activity of Human Serum Albumin: A spectroscopic study

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Human Serum Albumin (HSA) is the most abundant protein of blood plasma involved primarily in the transport of a multitude of compounds such as fatty acids, hormones etc. (1) It is a multifaceted protein and apart from maintaining the fluid distribution in blood capillaries, it also possesses multiple lesser-known enzymatic properties. (2) The esterase activity of the protein results from its ability to hydrolyze an ester bond in p-nitrophenyl acetate which in turn has the HSA protein acetylated. (3) We have investigated the effect of glycation of HSA on its esterase activity. The glycation of the protein has been achieved with glucose, fructose and ribose. The ester of interest is p-nitrophenyl acetate (PNPA) and the hydrolysis process and kinetics were studied via UV-Vis spectroscopy whereby the formation of the product, p-nitrophenol was monitored through its characteristic peak at ~400nm. Ribose is known to possess the highest ability to modify HSA, followed by fructose and glucose. (4) We observe that the esterase activity of the protein is reduced following glycation when compared to non-glycated HSA. In addition, it was observed that HSA glycated with ribose exhibited the least extent of esterase activity. This suggested that the modifications of the protein following glycation with ribose affected the enzymatic function of the protein to a higher extent compared to fructose and glucose modified HSA.

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P-211: Green Synthesis of Biologically Active Spiro Heterocyclic Compounds

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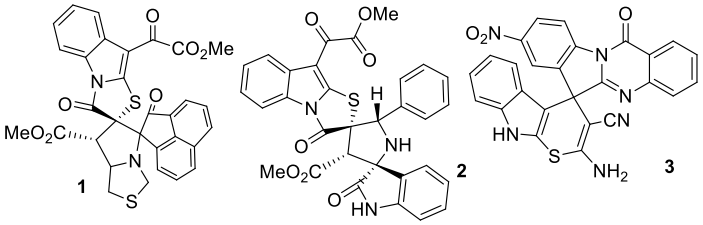

Functionalised heterocyclic molecules are popular for their wide pharmaceutical applications.[1] In particular, spiro heterocyclic moieties are structurally relevant in the field of drug design and are ubiquitously present in natural products and many biologically active compounds.[2] Dispiro pyrrolidine analogues are building blocks for fighting cancer and microbial infections.[3] Work in our laboratory had resulted in a new methodology for the nucleophilic ring opening of thieno[2,3-*b*]indole in presence of dimethyl acetylenedicarboxylate which led to the synthesis of a thiazolo[3,2-*a*]indole derivative. The latter was found to act as an excellent dipolarophile in the 32CA reaction with azomethine ylide (AY) derived from carbonyl compounds and various *α*-amino acids yielding biologically relevant dispiroheterocycles such as 1.[4] AY generated *via* iminium route from isatins and 1,2,3,4 tetrahydroisoquinoline/benzyl amines were also found to cycloadd stereoselectively to the dipolarophile yielding compounds such as 2.[5] Tryptanthrin based thiopyrans, synthesized by electroorganic method, were found to possess anti-staphylococcal therapeutic effect; the nitro-substituted hybrid molecule 3 was found to be most promising against *S. aureus* ATCC 29213 with a high selectivity index.[6] Further, AY generated from tryptanthrin were used for 32CA reaction with isatylidenes.

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P-212: Effect of methyl substituent on thermal expansion in imidazolium-p-hydroxybenzoate Salt

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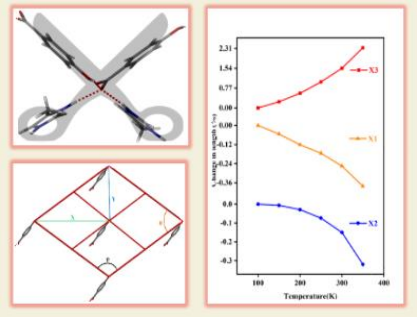

Materials with negative and zero thermal expansion property have drawn significant attention to the researchers in material science. These materials are widely employed as actuators, sensors, heat-shield materials and other devices.[1] Negative thermal expansion in the multicomponent organic crystalline materials is relatively less studied.[2,3] Recently, Das *et al*. have reported uniaxial colossal negative thermal expansion (NTE) and positive thermal expansion (PTE) of an organic salt (**IMD-HBC**) of imidazole and *p*-hydroxybenzene carboxylic acid induced by scissor motion of flexible hydrogen bonded structure with a coefficient of thermal expansion **(**CTE) -115 MK^{-1} and +210 MK^{-1} along crystallographic *b* axis and approximately along crystallographic *a* axis respectively within the temperature range of 100 K to 350 K.[4] Small PTE (CTE: 19 MK^{-1}) along the principal axis X2 has been observed in **IMD-HBC** salt.[4] Here, we report biaxial NTE in an organic salt (**4-MIMD-HBC**) of 4-methylimidazole with *p*-hydroxybenzene carboxylic acid with CTE -15 MK^{-1}, -12 MK^{-1}, and 92 MK^{-1} along the principle axes X1, X2 and X3 respectively from 100 K to 350 K. Methyl substituent in imidazole has pronounced effect in the overall thermal expansion property of the salt. Although scissor motion has been also observed in the crystal structures of **4-MIMD-HBC** which explains NTE along the principal axis X2, the change of intermolecular interactions due to methyl substituent induces NTE along the other principal axis X1. This study explains the effect of methyl substituent for tuning of thermal expansion property of organic imidazolium salt which can lead to design of new materials for desired thermal expansion property.

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P-213: Control of Spin Coupling Through Bridge in Bimetallic Porphyrin Dimer

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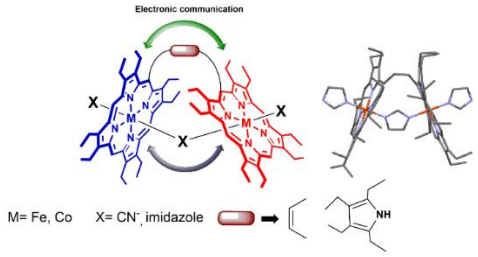

Metalloporphyrins are known to be excellent candidates having large planar π ligands and two axial coordination sites, which potentially allow electronic/magnetic interaction between metal ions. Electronic and magnetic interactions between transition metal ions have been interesting from theoretical and experimental viewpoint in order to design high conducting and paramagnetic materials. Imidazole and imidazolate are excellent donating ligands to iron and other transition metals like cobalt and they allow electronic/magnetic interaction between metal ions. The existence of strongly interacting metal sites in bi- and tetranuclear metalloproteins such as hemocyanin, copper oxidases, hemerythrin, superoxide dismutase, and cytochrome *c* oxidase provides an additional importance for gaining an understanding of the coordination chemistry principles which are unique to multi metal system. Antiferromagnetic coupling mediated by imidazolate, cyanide and oxo-bridging ligands is of particular interest as is the concept of binuclear catalysts. Explication of the electronic structure of metalloporphyrins draws significant attention in order to understand the function and the catalytic activities of the naturally occurring heme proteins. In the present investigation, we wish to report the synthesis and characterization of cyanide/imidazolate bridged bimetallic porphyrin dimers linked by rigid *cis*-ethene and flexible diethyl pyrrole spacers which shows a unique electronic communication through bridging ligand by varying the metal (M=Fe, Co), spacers as well as redox non innocent bridging ligand. [1-4]

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P-214: Oxygen Bridged Bimetallic $BaCu_2O_3.4H_2O$ Nano Catalyst For *C-O* Cross-Coupling Reaction

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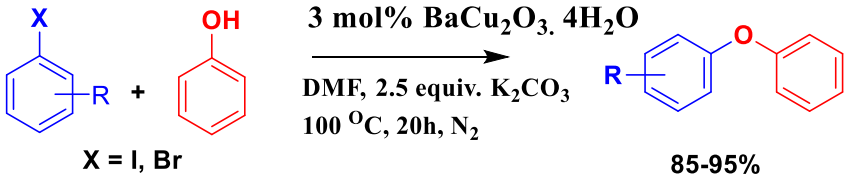

Scheme 1: Standardised reaction condition for *C-O* cross-coupling of phenol with haloarenes

The oxygen bridged bimetallic catalysis takes special interest now a days for its higher catalytic activity which arises due to a proficient effect called synergistic effect. Our group previously reported two oxo bridged bimetallic $CuMoO_4$ and $BaMoO_4$ nano catalysts for *N*-arylation and *S*-arylation reactions. [1-4] Since transition metal catalysed *C-O* cross-coupling reaction plays a significant role in biologically active drug molecules and pharmaceuticals [5-6], it takes our attention to develop some new bimetallic catalytic system for this *C-O* cross-coupling reaction.

Herein, for the first time we reported the synthesis of oxygen bridged bimetallic $BaCu_2O_3.4H_2O$ nano catalyst and applied this catalyst for *C-O* cross-coupling reaction. The catalyst is efficient and recyclable. The reaction proceeds with ligand free condition and shows high functional group tolerance.

Keywords: Bimetallic, Oxygen bridged, $BaCu_2O_3.4H_2O$, *C-O* cross-coupling

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P-215: Synthesis and investigation of backbone modified squaramide dipeptide self-assembly

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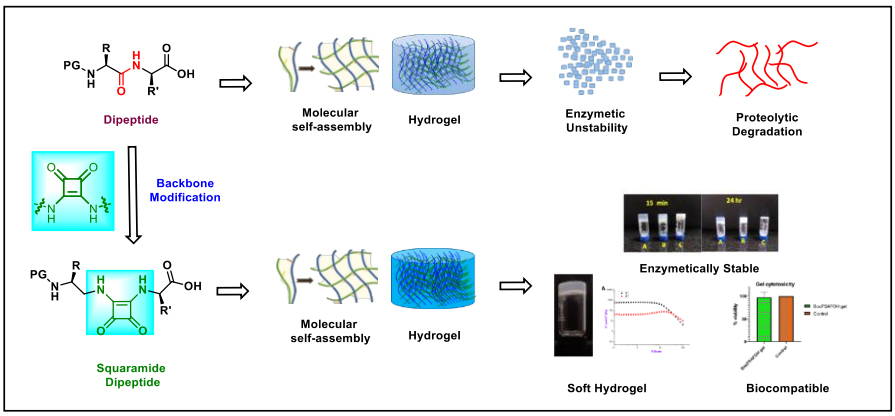

Dipeptides are minimalistic peptide building blocks that form well-ordered structures through self-assembly. Self-assembled structures are propelled by cooperative non-covalent interactions such as stacking, hydrogen bonding, ionic, and hydrophobic interactions. One of the most intriguing self-assembled Phe-Phe (FF) motifs has been extensively explored as a low molecular weight hydrogel for drug delivery, tissue engineering, imaging, tectonics, etc. The backbone of the dipeptide is crucial for extending secondary structures in the self-assembly structure, and a subtle change in the backbone structure hugely affects the macromolecular arrangement. The squaramide (SQ) motif has the unique advantage of hydrogen bonding, which can promote self-assembly. We integrated an SQ unit into the FF backbone in this work. The resulting carbamate-protected backbone modified dipeptide (BocFSAF-OH) exhibited self-assembly with a fibrillar network. The dipeptide was found to possess excellent enzymatic stability and high cytocompatibility. The resulting matrix has a hydrogel character when combined with the polysaccharide-based biopolymer sodium alginate. As a low molecular weight hydrogelator with excellent enzymatic stability, this dipeptide may find applications in a variety of fields, including drug delivery and tissue engineering.

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P-216: Regioselective synthesis of 5,6,7,8-tetrahydroindolizine *via* 1,1,2-trifuctionalisation of alkynes

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Tetrahydroindolizine structural motif is present in a range of naturally-occurring and synthetic bioactive molecules. Tetrahydroindolizine scaffold has been utilized as key intermediates for the synthesis of indolizidine alkaloids.[1] They show excellent antimicrobial, antifungal, anticancer activities and used for the treatment of human cytomegalovirus (HCMV) infections. In view of their importance in synthetic and medicinal chemistry plethora of synthesis methodology for the preparation of tetrahydroindolizine has been reported in recent years. Sulfones are another class of compounds that has gained importance due to their role in drug discovery programs, as sulfone containing compounds and their derivatives have been used for the treatment of dermatitis, herpetiformis, leprosy and tuberculosis. They show an array of application in cosmetics, agrochemicals and pharmaceutical industry.[2] Construction of tetrahydroindolizine core *via* Annulation of 2-Formylpiperidine and 1,3-Dicarbonyl compounds, partial reduction of indolizine, Brønsted acid-catalyzed dehydrative cyclization of Pyrroles N-tethered with Allylic alcohols, along with some multicomponent reaction are known however use of expensive and toxic metal catalysts, complex starting materials, multistep synthesis, low overall yields, poor regioselectivity and limited substitutions are serious limitations of the aforementioned methods. Herein, we designed tetrahydroindolizine fused sulphones, a hybrid molecule and a facile synthesis of 5,6,7,8-tetrahydroindolizines *via* 1,1,2-trifuctionalisation of alkynes so as to investigate their biological activities.

References:

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P-217: Base Promoted C-3 Chalcogenylation of Indolines with Dichalcogenides

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A new and efficient method for the C3-chalcogenylation of indoline at room temperature has been achieved by base mediated promoter. The present protocol exhibited a broad functional group tolerance with high yields and regioselectivity. This base promoted chalcogenation features the use of metal free and iodine free condition with simple operation and easy to handle the reaction that reduction and C-H functionalization occurs in one step. Through this easy and eco-friendly protocol allows access to wide range of C-3 chalcogenide of indoles.

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P-218: Palladium anchored N-Heterocyclic Carbene on a Porous Polymer – An Efficient Heterogeneous Composite Catalyst for Eco-Friendly Suzuki-Miyaura Coupling

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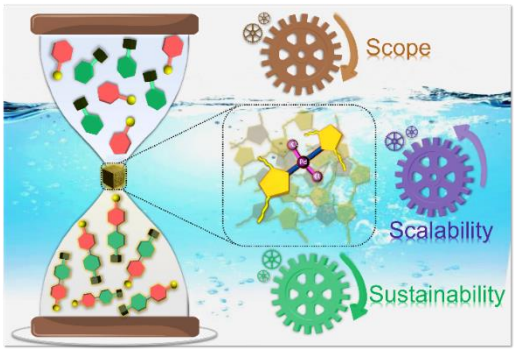

Aggregation induced catalyst deactivation during the reaction in supported metal catalysts prevail as one of the pitfalls toward their practical implementation.[1] Herein, homogeneously dispersed palladium coordinated N-Heterocyclic carbene was strategically integrated inside a microporous hyper-cross linked polymer (HCP) via post-synthesis structural modulation. Successful immobilization of spatially isolated Pd (II) units onto the polymer scaffold yielded highly robust heterogeneous catalysts 120-MI@Pd NHC & 120-EI@Pd NHC, respectively. 120-EI@NHC Pd (4.41 wt% Pd loading) illustrated remarkable catalytic potency (yield up to >99%) toward eco-friendly Suzuki-Miyaura coupling reaction (SMC) at room temperature. The superior catalytic efficiency of 120-EI@Pd NHC is further highlighted from its excellent functionality tolerance over 42 substrates bearing electronic diversity and TOF value reaching up to 4.97×10^3 h^{-1} at a very low catalyst dosage of 0.04 mol%. Pertaining to heterogenization, the polymer catalyst could be easily reused with intact catalytic efficiency for at least 10 cycles. The catalytic competence of 120-EI@NHC Pd in terms of scope, scalability and sustainability advocates its proficiency while processability was achieved by crafting 3D aerogel monolith. The conceptual feasibility was further investigated by devising a cup-based nano-reactor with gram-scale product isolation over 3 catalytic cycles.[2]

References:

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P-219: Synthesis of meso-tetracyanobutadiene-Appended Porphyrin for NLO Application

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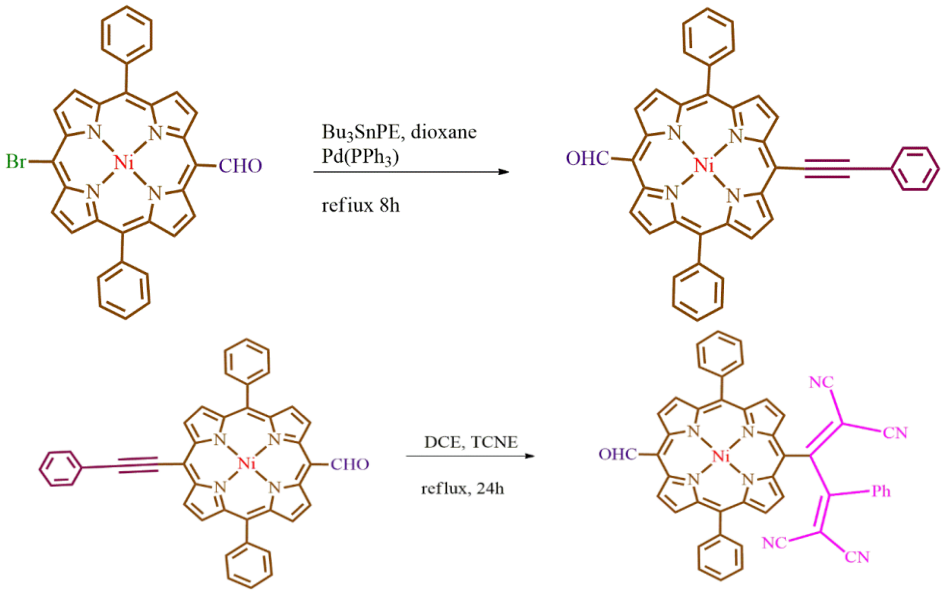

Figure 1. Molecular structures of synthesized porphyrins.

A donor-acceptor conjugated porphyrin with TCBD (1,1,4,4-tetracyano-buta-1,3-diene) chromophore at meso positiona and its metal analogue, NiTCBD was synthesized from (5-phenylethynyl-10-formyl-10,20-diphenylporphyrinato) nickel, H2-PE(CHO). The synthesized porphyrins are characterized by UV-Vis, NMR spectroscopic techniques and MALDI-TOF mass spectrometry. The reaction proceeds via [2 + 2] cycloaddition and retroelectrocyclization reactions of tetracyanoethylene (TCNE) with H2-PE(CHO). These porphyrins were prepared by halogenation, Vilsmeier-Hack formylation, Stille reaction and [2+2] cycloaddition reaction. Tetracyanoethylene (TCNE) acts as a powerful dienophile for electron-rich alkenes and alkynes and form donor–acceptor (D–A)-appended π-conjugated chromophores.

The TCBD substituted porphyrins are utilized in the various fields such as nonlinear optics (NLO), electrical conductivity.[2] In this presentation, we discuss the synthesis, spectral and electrochemical redox properties of these porphyrins and their utilization in detail.

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P-220: Nanoencapsulation of Ru(*p*-cymene) Complex Bearing Ginger-based Natural Product into Liposomal Nanoformulation to Improve Its Cellular Uptake and Antiproliferative Activity

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The organometallic compounds are prospective candidates in the row of developing metallochemotherapeutics with the aim of overcoming the limitations of platinum drugs. In order to explore the anticancer properties of organometallic compounds with natural medicines, two Ru(II)-p-cymene complexes containing the natural products, viz., 6-gingerol (6G) and benzylated-6-gingerdione (B-6GD) have been synthesized and characterized well.[1] The phenolic group of the Ru(6G) complex facilitates its higher cell-free antioxidant activity than its analog complex. Also, the same complex shows higher cytotoxicity toward A549 lung and HeLa-S3 cervical cancer cells than the Ru(B-6GD) complex but lower cytotoxicity toward A2058 metastatic melanoma cancer cells. Both complexes are shown to easily accumulate in melanoma cancer cells, and their degree of cytotoxicity in the same cells is found to be positively correlated with cell uptake. The cytotoxicity of complexes arises from their intracellular activity, mainly due to the induction of singlet oxygen production in cancer cells. The subcellular fractionation study shows that mitochondria and ER-Golgi membranes might be their predominant targets. Also, the mechanistic investigation revealed that Ru(B-6GD) induces caspase-dependent non-apoptotic cell death whereas Ru(6G) can induce caspase-independent non-apoptotic cell death. Furthermore, both complexes are found to moderately alter the adhesion properties of cancer cells, which is beneficial for antimetastatic treatment. Despite the potential pharmacological activity, Ru(6G) is encapsulated into polymer-supported liposomes to reduce its toxicity and further improve its anticancer potency. The π-conjugated yne–ene chain of polydiacetylene aids in the development of a stable nanoformulation, which achieved a slow release of the complex.[2-3] Most importantly, the cancer cell uptake of the liposome-encapsulated Ru(6G) complex is 20 times enhanced, and the total ROS formation in cancer cells is significantly increased compared to the non-encapsulated complex. However, the nanoformulation does not alter the antimetastatic potency of the encapsulated complex.

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P-221: Recent Advancement in Synthesis of Organo-Catalysed Antitubercular Agents

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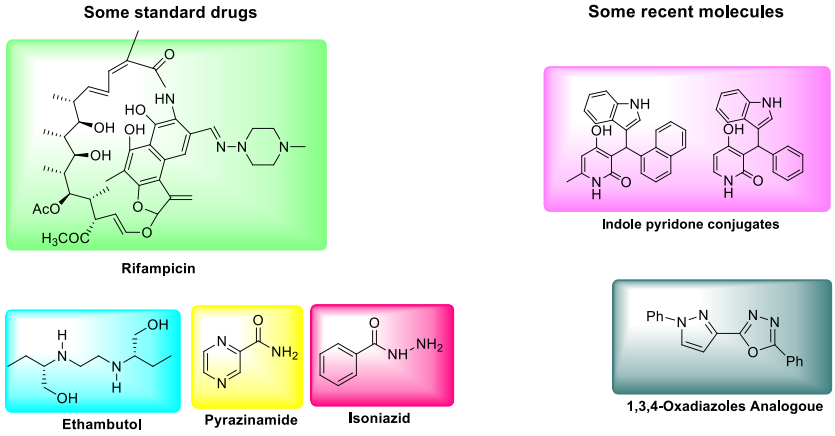

Tuberculosis (TB) is an infection registered by all civilizations for generations. Tuberculosis is caused by the bacillus *Mycobacterium tuberculosis* (*M. tuberculosis*) and it is a major cause of death in the developing world.[1] There are large number of cases and deaths recorded due to decreasing efficiency of four first-line drugs; Rifampicin, Isoniazid, Pyrazinamide, and Ethambutol.[2] New drugs with innovative modes of action must be developed to combat Tuberculosis. Here we discuss some anti-tuberculosis agents which are synthesized by using organocatalysts. Organocatalysts-mediated synthesis is environmentally benign and highly compatible. Numerous anti-Tuberculosis agents are synthesized utilising organocatalysts and tested for their *in vivo* and *in vitro* anti-mycobacterial activity against *Mycobacterium tuberculosis* pathogens. Some of them showed promising potency. [3, 4]

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P-222: "Naked eye" colorimetric sensing response of benzothiazole-based imine chemosensor towards copper (II) ion detection: synthesis, characterization and theoretical investigations

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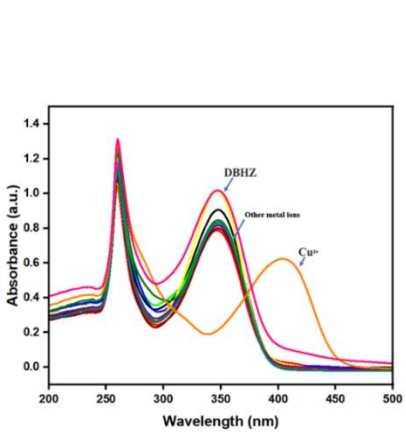

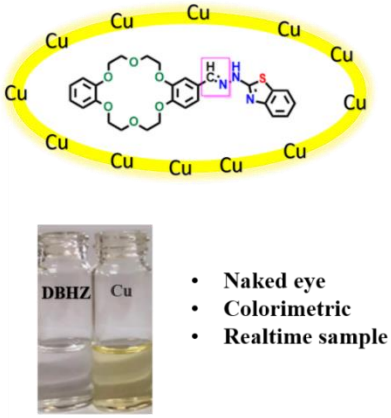

A highly selective and sensitive Cu^{2+} ion receptor (E)-2-(2-((6,7,9,10,17,18,20,21-octahydrodibenzo[b,k][1,4,7,10,13,16]hexaoxacyclooctadecin-2-yl)methylene)hydrazinyl) benzo [d]thiazole **[DBHZ]** was designed, synthesized, and characterized via standard techniques such as FT-IR and H^1, C^{13} NMR spectroscopy and HRMS. Dibenzocrownether with benzothiazole moiety showed a large bathochromic shift (57 nm) and a definite colour response from colorless to yellow irrespective of presence of other cations. **DBHZ** can detect Cu^{2+} ions with low LOD and also be used to determine Cu^{2+} ions in the real samples. Binding ratio of **DBHZ** and Cu^{2+} turned out to be a 2:1 with the analysis of Job plot. The sensing mechanism of **DBHZ** for Cu^{2+} was illustrated as the combination of metal-to-ligand charge transfer and intramolecular charge transfer via theoretical calculation. Computational DFT study was performed on the free ligand **DBHZ** and complex with Cu^{2+} to investigate the interaction site, to calculate the energies of the frontier molecular orbitals and to support some of the experimental results. The highlight of this work is that the receptor is effective as a naked-eye sensor for Cu^{2+} ions.

Keywords: Benzothiazole, Naked eye, Cu sensing, Realtime, DFT.

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P-223: Aminium Radical-Cation Catalyzed S N 2-type Ring-Opening Reactions of Aziridines with O/S/N/C-Nucleophiles: Formal Synthesis of (R)-Halostachine

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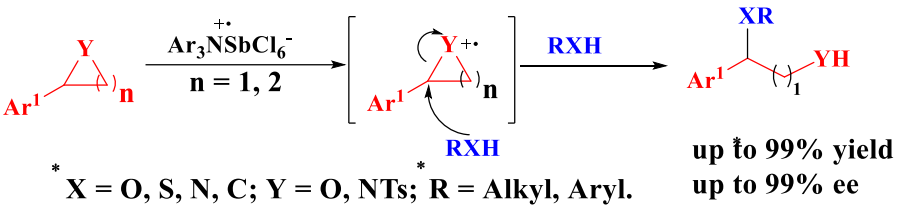

* X = O, S, N, C; Y = O, NTs; * R = Alkyl, Aryl.

- ü Optimum reaction condition
- ü Low catalyst loading
- ü Transition metal-free condition
- ü No Use of additive to controle the racemization of aziridines
- ü High yield & high ee
- ü Broad substrate scope
- ü Gram-scale synthesis

Aminium radical-cation catalyzed, highly enantio- and regioselective S_N2-type nucleophilic ring-opening of various 2-phenyl-*N*-tosylaziridines with *O*/*S*/*C*-nucleophiles to afford the corresponding various amino/thio ethers with excellent yield (up to 99%) and enantioselectivity (up to 99%) has been reported. This atom-economic protocol was extended for the synthesis of the (*R*)-Halostachine alkaloid.

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P-224: Regio- and Chemoselective [4+2]-Annulation of Aromatic Sulfoxonium Ylides with 1,3-Diynes *via* Cp*Co(III) Catalysis

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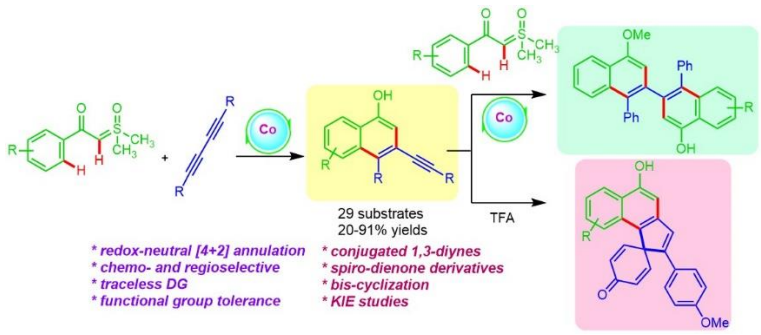

Transition-metal-catalysed chelation-aided cyclization of substituted aromatics with π-components through C-H functionalization is a powerful approach for the synthesis of cyclic compounds.[1] This type of cyclization reaction is achieved with 1,3-dienes, 1,3-enynes, and 1,3-diynes, which encompasses an extra alternative conjugated π-system with the regio, chemo-selectivity[2,3] and bis-annulation[4] as challenging issues. Sulfoxonium ylide has recently been accepted as a traceless directing group for metal-catalyzed cascade annulation with carbon-carbon components to construct cyclic organic molecules in a redox-neutral pathway in the absence of an external oxidant. In this conference, we will present an earth-abundant, air-stable, and cost-effective cobalt(III)-catalyzed redox-neutral [4+2]-cyclization reaction of aromatic sulfoxonium ylides with 1,3-diynes affording highly useful 1-naphthol derivatives having internal alkyne at the C3-position in moderate to excellent yields.[5] 1-Naphthols containing internal alkynes were efficiently converted into highly significant, biologically active spiro-dienone derivatives and useful *bis*-annulated poly-carbocyclic molecules. A possible reaction mechanism is proposed based on detailed mechanistic investigation such as kinetic isotopic effect and deuterium labelling studies.

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P-225: Metal- and catalyst-free photoinduced radical cascade reactions to achieve thioalkylation of quinoxalin-2(1H)-ones: an efficient synthesis of β-heteroaryl thioethers

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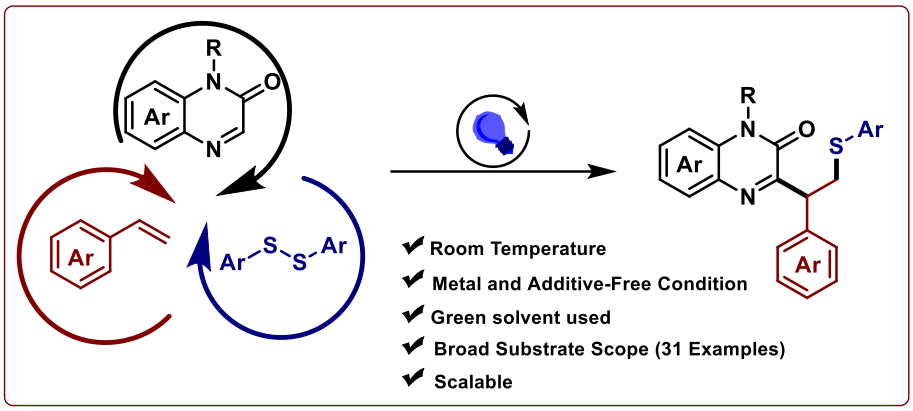

Cascade reaction being a viable solution for manufacturing complex organic frameworks in a step-economic fashion, has been extensively studied. Still, utilization of pharmaceutically-important heterocycle to cascade reaction for its regioselective functionalization remains less explored. This research article discussed the light-driven cascade reaction for thioalkylation of quinoxalin-2(*1H*)-one with alkene and aryl disulfide. This greener approach eliminates the requirement of any external photocatalyst to generate the key radical synthons from various aryl disulfides. This protocol also manifests compatibility with alkyne providing the regioselective vinylated quinoxalin-2(*1H*)-one. The practical applicability of this methodology was illustrated by scale-up experiments and late-stage modification of pharmaceutically active compounds. Detailed mechanistic experiments were conducted using several spectroscopic studies to corroborate the hypothesis of quinoxalin-2(*1H*)-one as a photosensitizer.

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P-226: Deciphering a Membrane-bound Hydrocarbon Producing Metalloenzyme

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The increasing concerns about global warming due to the use of fossil fuels have triggered enormous interest in developing renewable and eco-friendly Biofuels. Since hydrocarbons such as alka(e)nes are the major components of fossil fuels, their biosynthesis in a sustainable fashion has gained tremendous attention in the past few decades. In this regard, a hydrocarbon-producing metalloenzyme (HPM) has gathered significant interest in the production of 1-alkenes. However, despite its importance, this enzyme remained enigmatic due to its membrane-bound nature. HPM, so far, could not be purified and has eluded biochemical and mechanistic investigation. Recently, we made efforts to decipher this enzyme's long-standing mystery. We purified the HPM for the first time to homogeneity. We thoroughly characterized the enzyme biochemically and investigated the mechanistic plot of this enzyme. We established the metal identity of the enzyme and identified the key residues essential for the activity of HPM. Further, we established that HPM is an oxygen and redox-dependent enzyme and have identified the optimal redox partner proteins to support the in vitro activity of HPM. We also determined the substrate specificity and Michaelis-Menten kinetics parameters of the enzyme. Moreover, we also obtained the first mechanistic insights of HPM. Further, we made efforts to engineer the HPM-system for the high titer production of 1-alkenes. Our results provide a robust framework for further characterization of HPM and also aid in evaluating the properties of HPM and engineering it for efficient biosynthesis of 1-alkenes that have a multitude of applications in various industries. Additionally, our approach to investigating HPM, a challenging integral membrane enzyme, will not only open new avenues to explore membrane-protein biochemistry but also direct the science toward utilizing such enzymes for the production of the next generation of biofuels.

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P-227: Biocatalytic Asymmetric Synthesis of Tetrahydro-1-Benzazepines using Imine Reductases (IRED)

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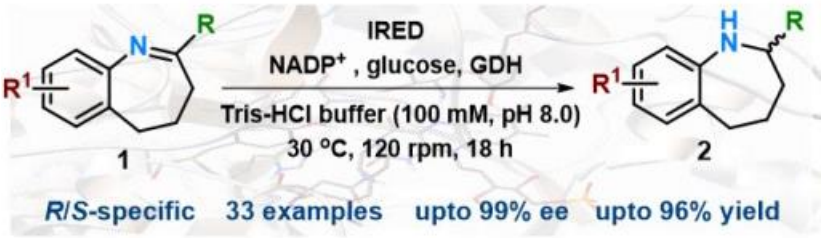

The benzannulated seven-membered heterocycles, which are often referred to as tetrahydro benzazepines are of great pharmaceutical importance as they are a part of several marketed drugs. Some of the prominent drugs with a tetrahydrobenzazepine scaffold are the natural product galantamine, used for the treatment of Alzheimer's disease[1], fenoldopam[2], an antihypertensive agent and epinastine used as an anti-allergic drug[3]. Although, only a few chemical methods are known for the asymmetric synthesis of chiral substituted tetrahydro-1- benzazepines, but no biocatalytic methods have been reported till date. Here we have developed a biocatalytic method for the asymmetric synthesis of substituted 1-benzazepines (2) by the reduction of corresponding cyclic imines using imine reductases (IREDs).

For this purpose, we have screened various imine reductases from different sources. Among them IR-1 from Kribbella catacumbae[4] and IR-2 from Cystobacter ferrugineus[5] gave the enantio-complementary tetrahydro-1-benzazepines by the reduction of cyclic imines in high yield and high enantiomeric excess. The synthetic versatility of this method has shown by the synthesis of various alkyl, aryl and benzo substituted tetrahydro-1-benzazepines in high yield (upto 96%) and excellent enantioselectivity (upto 99% ee). Such a method gave us facile and greener access to a large number of substituted benzazepines in enantiopure form with potential application in pharmaceuticals.

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P-228: Imperative Label-free distinctions between breast cancer and normal chromosomes

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An important indicator for the diagnosis and prognosis of cancer is epigenetic dysregulation, which includes DNA methylation and histone modifications (**1**). Here, we have used a few analytical techniques comprising FT-IR, UV-Visible, CD spectroscopy, and Cyclic Voltammetry, which are capable to differentiate cancer chromosomes from their normal counterparts by looking through the abnormal DNA methylation landscape and histone methylation. Our main concerns are with breast cancer chromosomes vs. the normal counterparts. Herein, we used breast cancer MCF-7 and normal breast epithelial MCF-10A cell lines for chromosome isolation and biophysical characterization. Hypermethylation has been reported in MCF 7 cancer cell-derived chromosomes in comparison to the normal ones (**2**). The changes that affect cytosine methylation (5-methylcytosine) levels certainly affect the DNA-protein interactions**.** Our data could provide insight into how cancer chromosomes differ from their normal counterparts in terms of their structure, conformations, and electron transport abilities. These data would be useful in the realization of biosensors for studying cancer microenvironments.

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P-229: Tuning of Thermal Expansion Properties of Mixed-Ligand MOF by Ligand Variation

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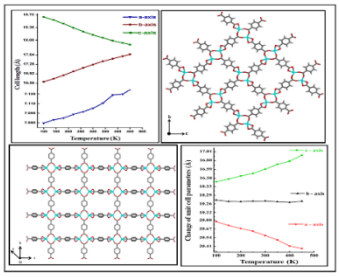

Negative Thermal Expansion (NTE) and Zero Thermal Expansion (ZTE) are two unusual phenomena that challenge the conventional concept of thermal expansion.[1] Both PTE and NTE may cause great damage in high precision instruments. Hence control over thermal expansion is necessary, which has been successfully achieved by preparing composites by particular stoichiometric combination of NTE and PTE.[2, 3] NTE in MOFs is closely associated with the flexibility of the framework which depends upon the ligands.[4, 5] Thermal expansion property in some MOFs have been tuned by absorption and desorption of volatile guest molecules.[6]

Colossal linear NTE and PTE of a two-fold interpenetrated MOF **([Co(Pz)(TPA)])** has been reported before. Further we have synthesized another MOF **([Co(Bpy)(TPA)])** with similar framework by replacing the ligand pyrazine (Pyz) in the **[Co(Pz)(TPA)]** MOF with 4,4'-bipyridine (Bpy). The new MOF has shown axial NTE, near ZTE and PTE along *a*, *b* and *c* axes respectively. Thermal expansion of both the MOFs has been studied by variable temperature single crystal X-ray diffraction (VT-SCXRD). Analysis of the crystal structures determined by VTXRD reveals 3D fencing motion in both the MOFs which explains NTE and PTE in 2D.

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P-230: First NHC Catalyzed Enantioselective Cycloaddition Reactions of Enals with α-Functionalized Vinyl Ketones

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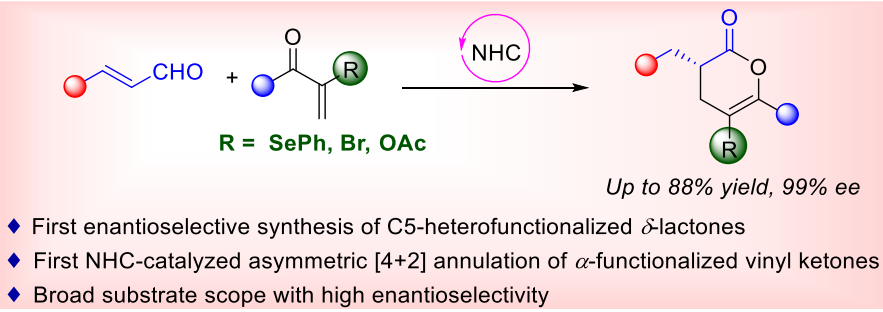

The functionalization of organic molecules with a heteroatom(s) often improves the activity of the parent compounds and opens new domains for applications through easy manipulations of these functionalities. On the other hand, dihydropyranones are the core structure of numerous pharmaceuticals and biologically active natural products. Therefore, an organocatalytic method for the preparation of hetero-functionalized dihydropyranes is highly desired. *N*-Heterocyclic Carbene (NHC) catalysis has emerged as a versatile organocatalyst for the preparation of δ-lactones using enals with chalcones. The asymmetric synthesis using α-substituted enones or vinyl ketones (β-unsubstituted enones) has yet remained challenging under NHC catalysis.

Herein, we report the first direct NHC organocatalytic asymmetric methods for the synthesis of C5-heterofunctionalized dihydropyranones *via* [4+2] annulation of α-functionalized vinyl ketones with enals. The dihydropyranones substituted with phenylselenide, bromo or OAc were obtained in high yield with excellent enantioselectivity. This direct access to functionalized δ-lactones is expected to further augment the bioactivity evaluation study.

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P-231: A Bronsted acid-catalysed regioselective carboxamidation of 2-indolylmethanols with isonitriles

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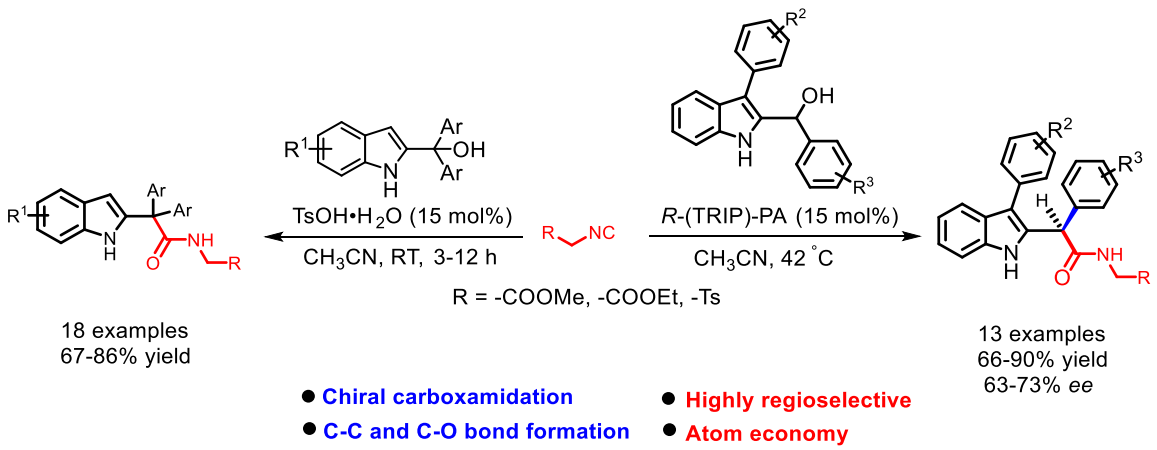

We report C2-selective direct carboxamidation reaction of 2-indolylmethanols with readily available isocyanoesters/cyanides. The reaction was catalysed by bronsted acid such as p-TsOH to deliver the regioselective amidation products in 67-86% yield at room temperature. The developed methodology provides an alternative access to traditional metal-free carboxamidation via C-C and C-O bond formation with high atom economy. Furthermore, the developed approach was diversified to synthesize chiral indole-2-carboxamide derivatives with a moderate enantiomeric excess (63-73% ee).

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P-232: Low-temperature hydrogen production from methanol

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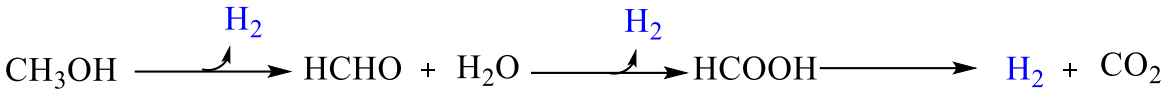

Hydrogen is a potential clean energy carrier, and when used in fuel cells, it only produces water as a by-product. Unfortunately, the presence of hydrogen gas in the earth's atmosphere is extremely low (≈1 ppm by volume). Therefore, one of the major hurdles in exploring the hydrogen economy with full potential is the safe production and storage of hydrogen gas. Notably, carrying big and heavy hydrogen cylinders with high pressure has critical safety and economical challenges. On the other hand, using liquid hydrogen storage materials (such as HCHO, CH_3OH, and HCOOH) in the fuel tank of existing vehicles (using petroleum products) to generate hydrogen on-board to supply to fuel cells is not only a viable concept but also very economical. In this context, methanol, which contains an appreciably high gravimetric content of hydrogen (12.5 wt%), is a promising candidate for on-board and off-board (stationary) large-scale production of hydrogen gas. Methanol reforming at a very high temperature (>200 °C) has been explored for hydrogen production. Here, we have tried to produce hydrogen production from methanol in water at low temperatures, which leads to a practical and efficient approach for low-temperature hydrogen production from methanol in water.

Keywords: water; hydrogen gas; *In-situ* catalyst; low-temperature; methanol

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P-233: Recent Synthetic Development on 2-Hydroxy-1,4-naphthoquinone (Lawsone)

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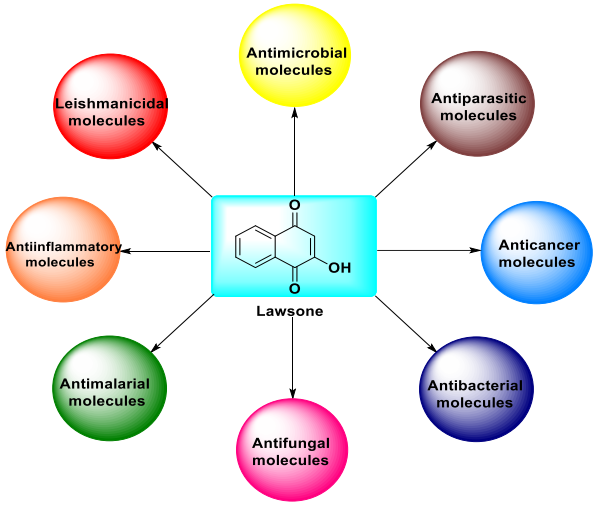

Lawsone is one of the simplest naturally occurring naphthoquinones. It is a unique naphthoquinone that has several uses in various domains of modern sciences.[1] In Chemical Sciences it has been utilised as a starting material for the synthesis of numerous biologically active molecules with intriguing features for many decades.[2] In addition to being a common naturally occurring and pharmaceutically relevant molecule, Lawsone has been investigated as a key precursor in the synthesis of bio-relevant materials.[3-4] they play a fundamental role in several living cells as electron carriers in the respiratory chain, as well as in blood coagulation and carboxylation of glutamates.[5] Due to the intimate relationship between 2-hydroxy-1,4-napthaquinone and the biochemical processes of cells, these compounds have been extensively explored in the synthesis of several bioactive compounds bio-relevent materials will be presented therein.

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P-234: Detection of cyanide in mainstream smoke of tobacco products through Naked-eye colorimetric, turn-on fluorescent Schiff base sensor and its theoretical studies.

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A newly designed pyrazole carbonitrile derived Schiff base [PS3] for "naked eye" colorimetric and turn on fluorometric cyanide ion sensing was synthesized by reacting 3-amino-1H-pyrazole-4-carbonitrile with 4-methylthiazole-5-carbaldehyde were comprehensively studied based on experimental and well supported theoretical calculations. PS3 showed high sensitivity of cyanide ions (CN^-) with a binding stoichiometry of 1:1 in acetonitrile solution. The PS3 sensor exhibited high specificity towards CN by interrupting its intramolecular charge transfer, resulting in a color change from colorless to yellow and remarkable ''turn-on" fluorescence emission. The detection limits for CN^- by UV-Vis spectrum is 0.38×10^{-7} M, respectively. The PS3 sensor can act as an efficient chemical sensor for detecting the CN^- ions under common environmental and physiological conditions (pH 5–12). Besides, the sensor can also detect CN in tobacco products (such as cigarette and cigar). PS3 is an excellent CN– sensor that exhibits some advantages, including easy synthesis, distinct fluorescence and color change, high selectivity, low detection limit, reversibility, and good anti-interference ability to analyze solution and tobacco product, together with fluorescence imaging. The optimized structure and electronic transitions were confirmed by DFT and TDDFT studies. The mechanism of the metal ion complex is proposed based on experimental and theoretical calculation (DFT). The aim of this study is focused on the determination of the HCN in mainstream smock of different brands of cigarette by naked eye calorimetric method.

Keywords: Schiff base, naked eye, ICT, CN detection, tobacco product, DFT.

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P-235: Effect of Hydrogen Bonding as a Latent Catalyst in Greener Substituted Benzoxazine and their Applications

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Many investigations have been separately conducted on green synthesis, and structural modification by substituting the oxazine ring and incorporating the latent catalytic effect within the Bz monomer to obtain a high-performance polybenzoxazine (PBz). To achieve all the benefits in one structure, we have developed a straightforward synthetic strategy to synthesize a genuinely biobased latest 4th generation Bz monomers with oxazine-ring substituted at the 2-position. The bio-derived chemicals *o*-vanillin (oV), vanillin (V), furfurylamine (fa), and benzaldehyde (ph) are utilized to obtain the monomers, oV-fa-[2]ph, oV-fa-[2]ov and oV-fa-[2]v, in a solventless microwave-assisted method at a lower temperature, time and in good yields over conventional method. To elucidate the inherent catalytic effect due to positioning of phenolic-OH (at *o*- or *p*-position in oV-fa-[2]ov and oV-fa-[2]v, respectively), compared to control monomer (without phenolic-OH, oV-fa-[2]ph), in ring-opening polymerization of monomers is established successfully by performing a comparative detailed study of inter- and intra-molecular H-bonding and solid structural evidence is provided. Among the series, the oV-fa-[2]v monomer showed the lowest polymerization temperature (T_p ~ 180 ºC), a higher degradation temperature (T_{max} = 370 ºC), and a faster polymerization kinetics (E_a = 88 kJ/mol), and poly(oV-fa-[2]v) showed glass transition temperature (T_g = 130 ºC), limiting oxygen index (LOI = 31.5), hydrophobicity (contact angle = 98º) and char yield (Y_c = 35 %) inferring installing -OH at *p*-position is crucial for better set of properties than at *o*-position. The monomers were explored as solventless low-temperature processable adhesive and lap shear strength (LSS = 51 kg/cm^2) was significantly improved by blending with the first generation simplest agro-waste cardanol-based monomer, a great combination of soft and hard segments in polymer network, in one-step is accomplished.

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P-236: Imine-based highly polar achiral unsymmetrical four-ring bent shaped liquid crystals: Design, synthesis and characterization

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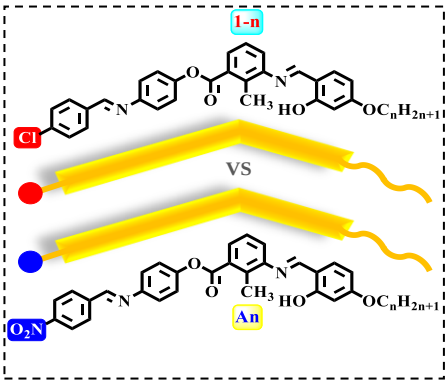

Hockey-stick-shaped liquid crystals are interesting due to their unusual physicochemical properties. The nematic phase observed in these materials has shown interesting properties like ferroelectric-like switching, ease of alignment in the coated cell, large flexoelectricity, etc. Polar moiety viz. F, Cl, NO_2 etc., in the molecular architecture of hockey-stick-shaped molecules originate permanent dipole moment that affects the phase structure and physical properties [1–3]. Herein, we have designed and synthesized a new series of four-ring-based hockey-stick-shaped molecules having polar Cl and NO_2 groups at one end and variable aliphatic chains at another end of the molecular long axis [1,2]. The four phenyl rings are attached via one ester and two imine linking groups. All the compounds exhibited enantiotropic mesomorphism. The lower homologs exclusively showed nematic phases and higher homologs exhibited nematic cybotactic and/or smectic A phase. A comparative approach for the two different analogs has been developed in this work. Small and wide-angle X-ray scattering (SAXS/WAXS) experiments have been performed that elaborated the internal arrangement of molecules in layers. The density functional (DFT) study confirmed that the molecules had a resultant dipole moment (~6 – 9 Debye) which in turn cancelled out when the molecules, in the bulk phase, were arranged preferably antiparallelly as a dimer.

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P-237: Studies on Photoluminescence Property of Silicon Dioxide Quantum Dots Anchored on Different Types of Carbonaceous matrix & their Application for Metal Ion Sensing

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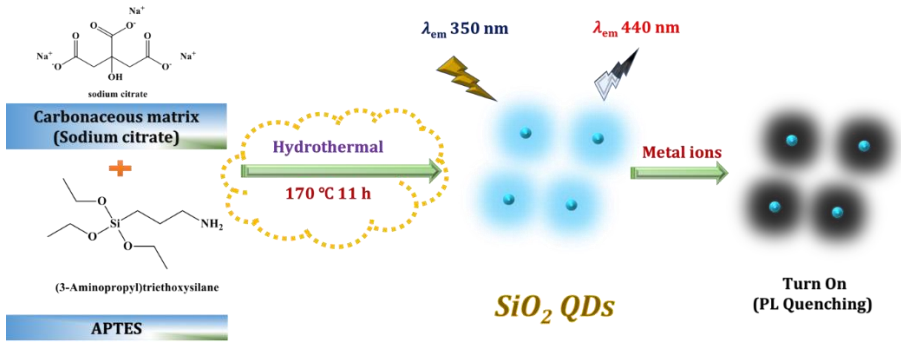

Hexavalent chromium, i.e., Cr(VI) is water soluble and carcinogenic in nature. There has been a consistent effort for developing simple yet sensitive and selective analytical method for detecting metal ions at ultratrace level concentration in water.[1] Among these methods, photoluminescence quenching is a promising method. Herein, we present development of silicon dioxide quantum dots (SiO_2 QDs) anchored on different type of carbonaceous matrix and their application from detecting Cr(VI) in water. Though SiO_2 QDs are mainly explored for light emitting and imaging applications,[2] but it has not been explored as a probe for detecting heavy metals. Herein, we present the study of photoluminescence property of SiO_2 QDs anchored on different carbon matrix (sodium citrate, amino acids) which were synthesized via a hydrothermal method. The first batch of SiO_2 QDs anchored on sodium citrate was prepared by hydrothermal treatment of APTES and sodium citrate in aqueous solution for 170 °C for 11 h. The as-synthesized SiO_2 QDs anchored on sodium citrate exhibited a strong blue photoluminescence, corresponding to maximum excitation and emission wavelengths at 350 and 440 nm, respectively. These QDs were characterized by UV-Vis, PL, XPS and HR-TEM, and were found to selectively detect Cr(VI) in aqueous solutions. The detailed photoluminescence study including SiO_2 QDs based on other carbonaceous matrix will be studied with their application for metal ion sensing.

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P-238: Visible light mediated Direct Activation of Benzoquinone for the Generation of Quinoxaline Derivatives

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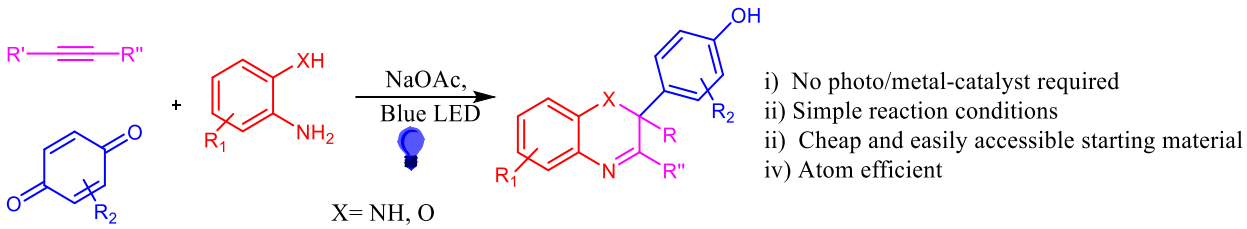

Visible light-driven and photocatalyst-free three-component coupling of benzoquinones, alkynes, and ortho-phenylenediamines/ortho-aminophenol is reported. The protocol provides a facile tandem route for synthesizing value-added 1,2-dihydroquinoxalines and Benzo-oxazines at room temperature from readily available starting materials in moderate to high yields. The bimodal absorption and emission changes in 1,2-dihydroquinoxalines upon protonation/deprotonation endow them with high sensitivity for amine detection, as well as fluorescent probes with PL efficiency up to 48%. The Benzo-oxazine derivatives synthesized are a core sturcture of commerically available drug Bisoxatin acetate.

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P-239: Unraveling topoisomerase IA gate dynamics in presence of PPEF and its preclinical evaluation against multidrug-resistant pathogens

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Type IA topoisomerases maintain DNA topology by cleaving ssDNA and relaxing negative supercoils. The inhibition of its activity in bacteria prevents the relaxation of negative supercoils, which in turn impedes DNA metabolic processes leading to cell death. Using this hypothesis, two bisbenzimidazoles, PPEF and BPVF are synthesized, selectively inhibiting bacterial TopoIA and TopoIII. PPEF stabilizes the topoisomerase and topoisomerase-ssDNA complex, acts as an interfacial inhibitor. PPEF display high efficacy against ~455 multi-drug resistant gram positive and negative bacteria. To understand molecular mechanism of inhibition of TopoIA and PPEF, accelerated MD simulation is carried out, and results suggested that PPEF binds, stabilizes the closed conformation of TopoIA with –6Kcal/mol binding energy and destabilizes the binding of ssDNA. The TopoIA gate dynamics model can be used as a tool to screen TopoIA inhibitors as therapeutic candidates. PPEF and BPVF cause cellular filamentation and DNA fragmentation leading to bacterial cell death. PPEF and BPVF show potent efficacy against systemic and neutropenic mouse models harboring *E. coli,* VRSA, and MRSA infection without cellular toxicity.

Keywords: Bisbenzimidazoles, Topoisomerase, Antibacterial Agents, Molecular dynamics simulation.

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P-240: Iodine(III) Catalyzed Unprecedented Direct Construction of (Hetero)functionalized Pyrazolines, Pyrazoles and Isoxazoles

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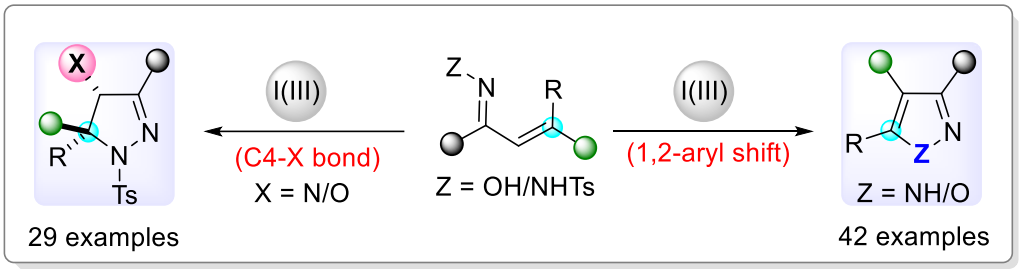

Pyrazolines and their analogous aromatic *aza*-heterocycles have a wide range of applications in pharmaceutical and agrochemical industries. Often, the functionalizing of the parent heterocycles with a heteroatom diversifies/improves its activity. This also offers new domains of reactivity in organic synthesis. However, a direct synthesis of heteroatom-functionalized pyrazolines as well as fully-functionalized pyrazoles and isoxazoles have remained challenging.

Hypervalent Iodine catalysis has recently emerged as one of the major areas of catalysis due to its several inherent properties and unique mode of activations. Herein, we have developed the first I(III)-mediated general method for the preparation of highly functionalized 4-oxyacylated- and 4-aminated pyrazolines from hydrazones. In addition, the reaction pathway from similar precursors could be controlled alternatively to produce 3,4,5-trisubstituted pyrazoles and isoxazoles *via* 1,2-aryl shift/aromatization cascade after intramolecular oxidative cyclization. One of the products is a key intermediate in the preparation of a marketed drug, Valdecoxib.

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P-241: Ruthenium Catalyzed Stereo- and Chemoselective Oxidative Coupling Reaction of Vinyl ketones and Acrylates: Application to Synthesis of FR252921

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FR252921 is a bioactive complex natural product, belongs to family of potent macrocyclic polyene and act as an immunosuppressive agent. Due to its complexity and architect, FR 252921 has sparked great interest in synthetic community. Herein we report the developement and application of ruthenium catalyzed highly stereo- and chemoselective oxidative coupling reaction of vinyl ketones and acrylates for the formal synthesis of FR252921. The key features for the synthesis FR252921 include preparation of the triene moiety followed by two consecutive peptide couplings of the three fragments.

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P-242: Synergistic Antimicrobial treatment by amino acid & peptide conjugated copper oxide nanoparticles.

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Antimicrobial resistance (AMR) is a potential threat and an international danger to human health and development. To attain Sustainable Development Goals, urgent multisectoral action is required. Drug-resistant infections are usually caused by the improper use and overuse of antibiotics. One of the top 10 worldwide public health hazards to humanity, according to WHO, is antimicrobial resistance (AMR)[1]. This could usher in a time when common bacterial infections and minor wounds can cause death. Therefore, finding a new medicine for AMR is of the utmost importance. Due to their high surface-to-volume ratio, metal oxide nanoparticles, notably copper oxide nanoparticles, exhibit significant antibacterial activity and can more effectively enter tissues and cells[2]. According to studies, amino acid & peptide-based antimicrobial agents are used by researchers for the treatment of antimicrobial diseases[3]. In order to take advantage of the complementary antibacterial properties of both moieties, our work intends to conjugate a single amino acid unit and a peptide separately with produced copper oxide nanoparticles. We successfully established the methodology for the synthesis of copper oxide nanoparticles using the electrochemical method utilizing urban waste. The average particle size of 27±2 nm was further confirmed by the XRD and TEM data. Copper oxide nanoparticles were conjugated with amino acids for synergistic activity against microbial colonization as part of the process to establish a new therapy regimen for microbial infections and the conjugation was confirmed by FTIR results. The produced conjugated nanoparticles have extremely effective antimicrobial action. Individually, both copper oxide nanoparticles and the amino acids demonstrate antimicrobial action and can be assessed for efficacy. For the current issue, we were able to successfully synthesize copper oxide nanoparticles with an amino acid coating and comparative studies of naked, amino acid-coated & peptide-coated nanoparticles are going on.

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P-243: Tetrel-bonding Interaction in Action: C-N Activation Approach Towards the Synthesis of Unsymmetric Tertiary Amines and α-Amino Carbonyl Derivatives

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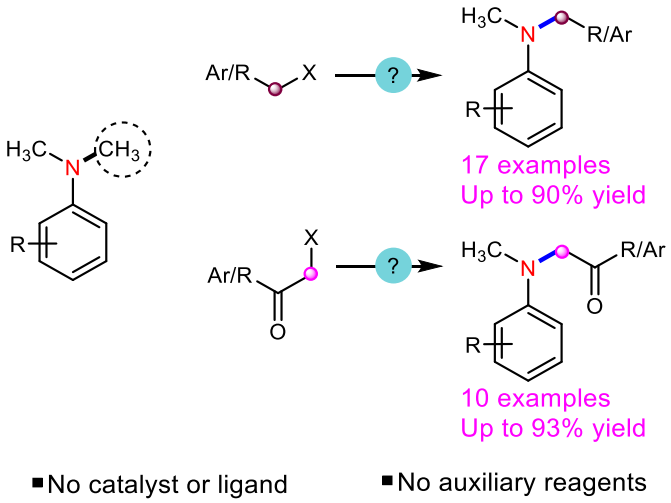

In the absence of a catalyst, ligand, oxidant, or any additives, an operationally easy approach for the synthesis of unsymmetrical amines and α-amino carbonyl derivatives has been established. Unlike previous reductive amination techniques, this protocol can be utilized for substrates containing other reducible groups. The process essentially results in the consecutive cleavage and the formation of C-N bonds. DFT studies and Hammett analysis have been carried out to shed light on the mechanism. The role of noncovalent interactions as a stabilizing element have been examined in the procedure. A wide range of alkyl-bromides have been efficiently linked with a variety of dimethyl anilines to obtain unsymmetric tertiary amines with up to 90% yield. This approach was then applied to the synthesis of α-amino carbonyl derivatives, with yields reaching 93%.

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P-244: Unveiling Phenalenyl as a Potent Photoreductant: Enabling Access to the Reductive Functionalization of Aryl Halides through Visible Light-Induced Electron Transfer Processes

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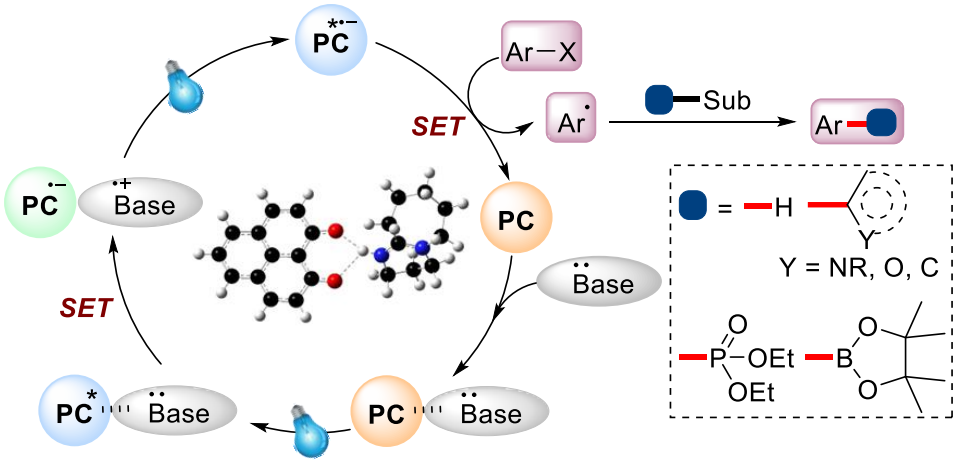

We have recognized a phenalenyl based molecular scaffold as a potent photoreductant, which utilizes the empty NBMO in the presence of a base to form a radical anion undergoes photoexcitation thereby behaving as a stronger reductant and accomplishes the cleavage of strong C-X (X = Cl, Br, I) bonds under milder reaction conditions. Base was involved in a dual role of electron donor as well as hydrogen atom donor. Further, the aryl radical formed by the homolysis of C-X bonds in this technique was captured for the C_{sp2}-C_{sp2} coupling with unactivated arenes. The photoreductant potency of the phenalenyl based catalytic system was further extended to C-P as well as C-B bond formation reactions. EPR and lifetime studies reveal the formation of a persistent radical having sufficient lifetime to take part in the reaction by the PET mechanism. Different spectroscopic techniques combined with DFT calculations were utilized for the characterization of active catalytic species and for the elucidation of plausible mechanistic pathway. Based on the best of our knowledge, this is the initial report of application of phenalenyl as a photoreductant which also provide a completely metal-free approach for the functionalization of aryl halides at room temperature.

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P-245: Palladium Catalyzed Desymmetrization of Diazabicylic Olefins with 4-Halo-1,3-dicarbonyl compounds: Accessing 3(2H)-Furanone Appended Cyclopentenes

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The 3-(2*H*)-furanone moiety is found as a core structure in many natural products that exhibits wide range of biological properties which makes them interesting targets for organic and medicinal chemists. The known synthetic routes towards this heterocyclic motif include transformations of substituted furans, cyclizations of α-hydroxy-1,3-diketones and allenichydroxy ketones, transition-metal and organo-catalyzed protocols. Recently, we have also reported on the synthesis of 4-substituted-3-(2*H*)-furanones by the Pd-catalyzed reaction of 4-haloacetoacetates with activated alkenes, imines and diazocompounds. Desymmetrization of diazabicyclic olefins is an interesting and well explored area, while the reactivity of soft nucleophiles with the same is the least studied one. Inspired by the reports on the reactions of 1,3-diactivated methylene species and desymmetrization of diazabicyclic olefins we have developed synthetic protocols towards 4-substituted 3-(2*H*)-furanones. Since 4-halo-1,3-dicarbonyl compounds are soft nucleophiles, by employing carefully designed active methylene species, the ring-opening of diazabicyclic olefins could lead to the generation of 3(2*H*)-furanone substituted *cis*-disubstituted cyclopentenes.

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P-246: GO Driven Fluorescence Modulation of Rhodamine B in Aquoline: A Water-Based Deep Eutectic Solvent

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The fluorescence behaviour of rhodamine B (RB) in water-based, deep eutectic solvents (*aquoline*) with or without graphene oxide (GO) is less known. Aquoline is an eutectic mixture formed by the mixing of cholinium chloride (ChCl, a quaternary salt) and a judicious amount of water (ChCl : nH_2O, n = 2,3 and 4) followed by 30 minutes of stirring [1]. RB and its derivatives are used in fluorescence levelling and DNA sequencing [2]. The application depends on [RB] and the choice of solvent. The present study embodied photophysical data in various conventional and designer solvents (*aquoline*) λ_{em} values were red shifted with the polarity of the solvent. Further effects of the addition of GO on the fluorescence intensity of RB have been investigated. The emission intensity of RB was gradually enhanced up to the addition of 5 µg/ml GO without shifting the emission maximum. Further, the gradual addition of GO led to a decrease in the emission intensity of RB. The switching of the role of GO from an enhancer to a quencher of fluorescence depending on the [GO] in aquolines has been observed. Proton transfer from GO surfaces to aquoline appears to be responsible for GO switching roles [3].

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P-247: Unfolding the Impact of Diverse Morphology of Ionic Porous Organic Polymer with Mechanistic Investigation on the Rapid and Selective Sequestration of Toxic Pollutants from Water

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Nowadays, there is a lot of interest in the detoxification of tainted water using various materials. However, their usefulness is constrained by a lack of an in-depth understanding of the contribution of different physical features of such materials to increased sorption efficacy. In general, due to a lack of appropriate synthetic techniques, the purification of oxoanions-polluted water by porous material with diverse morphologies is unexplored. By adjusting the morphologies of an imidazolium-based cationic polymeric network, systematic adjustment of sequestration performance towards effective decontamination of harmful oxoanions-polluted water has been achieved here (iPOP-5). The chemically stable ionic polymer displayed many morphologies, including spherical, nanotube, and flakes, according to a detailed analysis of morphological progression. With regard to chromate [Cr(VI)] and perrhenate [Re(VII)] in water, the flake-like material [iPOP-5(F)] demonstrated ultrafast capture efficiency (up to 99% in 1 min). The removal kinetics of the two oxoanions from the spherical-shaped polymer [iPOP-5(S)] were somewhat slow (99% in >5 min). Notably, iPOP-5(F) removed Cr(VI) and Re(VII) preferentially from both high and low concentrations of polluted water, even in the presence of significant competing anions. Additionally, the substance showed remarkable regeneration ability while efficiently capturing those oxoanions across a wide pH range and in different water systems. Additionally, experiment by iPOP-5(F) has been conducted a column exchange-based water treatment experiment to lower the content of Cr(VI) and Re(VII) below the WHO-permitted standard as a proof of concept. Mechanistic analysis revealed that flakes' infrequent in situ exfoliation into thin nanosheets aids in achieving rapid capture efficiency.

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P-248: Redox Non-Innocence Behavior of Hinge-like Deprotonated Bis-lawsone on Ruthenium and Osmium Platforms

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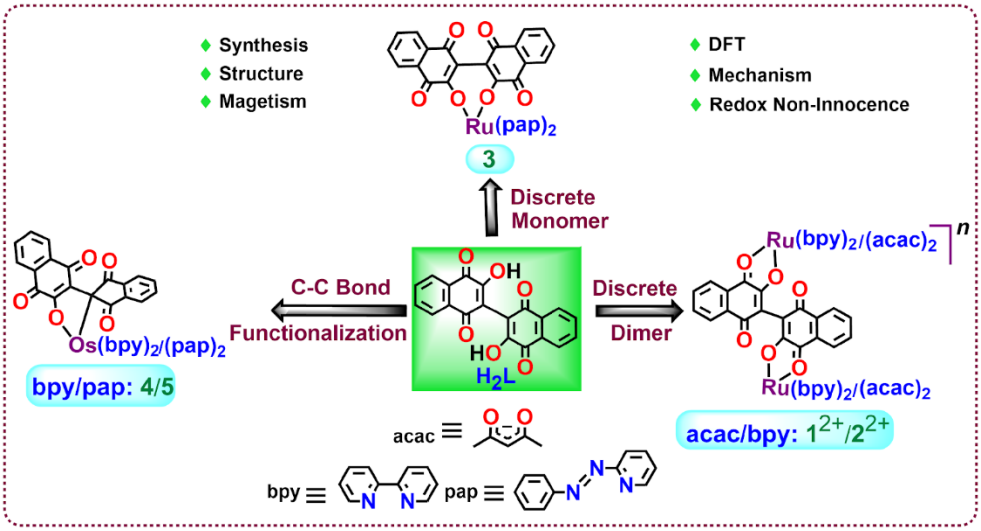

The conformational flexibility of the hinge-like H_2L (2,2'-bislawsone or 3-hydroxy-1,4-napthoquinone) due to its free rotation about the central C-C single bond involving two hydroxynaphthoquinone units provides structural diversities including supramolecular assemblies, zig-zag, helix, square, and Cu, Co based coordination polymers.[1] On the similar note, the present deliberation is intended to highlight our recent contribution in the direction of developing L^{2-} derived discrete diruthenium frameworks $[(bpy)_2Ru^{II}(\mu\text{-}L^{2-})Ru^{II}(bpy)_2](ClO_4)_2$ [**1**]$(ClO_4)_2$ (S=0), $(acac)_2Ru^{III}(\mu\text{-}L^{2-})Ru^{III}(acac)_2$ **2** (S=1) and monoruthenium framework $(pap)_2Ru(L^{2-})$ **3** (S=0).[2] In addition, it also highlights the transformation of bis-lawsone (H_2L) to deprotonated 3-(1.3-Dioxoindan-2-yl)-2-hydroxy-1,4-naphthoquinone ($L1^{2-}$) on the selective osmium platform to give monomeric frameworks $[(bpy)_2Os^{II}(L1^{2-})]$ **4** (S=0) and $[(pap)_2Os^{II}(L1^{2-})]$ **5** (S=0) where one of the hydroxynaphthoquinone units of H_2L has been transformed to 1,3-dioxoindan via C-C bond activation step.[3] Besides structural authentication of $\mathbf{1}^n$-$\mathbf{5}^n$, magnetic study, mechanistic aspects and electronic structural aspects in accessible redox states of the complexes including mixed valent features have been investigated via UV-Vis-NIR-EPR spectroelectrochemistry in combination with DFT/TD-DFT calculations and these studies have revealed bidirectional non-innocence of L^{2-} under the stated selective coordination situations.

P-249: Intranasal delivery using Acetylcholinesterase Targeted Micellar nanocarrier for C-site Directed Designer Oximes for Reversible Reactivation

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Organophosphorus nerve agents (NAs) are the potent inhibitors of acetylcholinesterase (AChE), an enzyme responsible for degradation of an important neurotransmitter acetylcholine responsible for neurotransmission. Organophosphates are lethal in nature, they inactive the cholinestaerase by blocking the enzyme's active site by phosphorylation of serine residue. For the reactivation of AChE, a compound is required which can compete the phosphorylated enzyme and can prevent the enzyme inactivation and thus help in restoring the activity of the enzyme. To achieve this, a new re-activator with an optimal reactivation potency and liphophilicity is designed to decrease lethality of NAs and to increase the blood brain barrier BBB penetration. A novel ligand has been designed and molecular docking has been performed using 2ckm (Torpedo California acetylcholineasterse). Based on docking score as -14.2, this ligand has been synthesized using chalcone oxime with 9-Amino-1,2,3,4-tetrahydroacridine in order to reactive the AChE by the oximes which have the competitive binding affinity to serine residue of enzyme. Chalcone oxime ethers were evaluated for inhibitory activities against monoamine oxidases (MAOs) and acetylcholinesterase (AChE). Micellar nanoparticles are made up of this ligand by solvent injection method and administered through intra-nasal route. Efficiency of the drug/ligand can be checked in vivo by labelling of the drug with ^{99m}Tc in micellar and solution form by intranasal route. Applying the average-sized rat brain blood volume of ~ 30-35 µL/g of tissue for the blood and brain % injected dose (ID) per gram profiles over time indicates that 70-80 % of the brain radioactivity detected over the 2-60 minutes is contributed from the cerebral blood pool radioactivity within brain tissue.

Thus, "Nose-to-brain" intranasal oxime administration provides an advantage as it is rapid, non-invasive delivery to the brain and effective at reducing central AChE inactivation and protecting the neurons from damage caused by organophosphate poisoning in short period of time.

P-250: Binding enabled catalytic activation of SO_2 by copper koneramine complexes under ambient conditions

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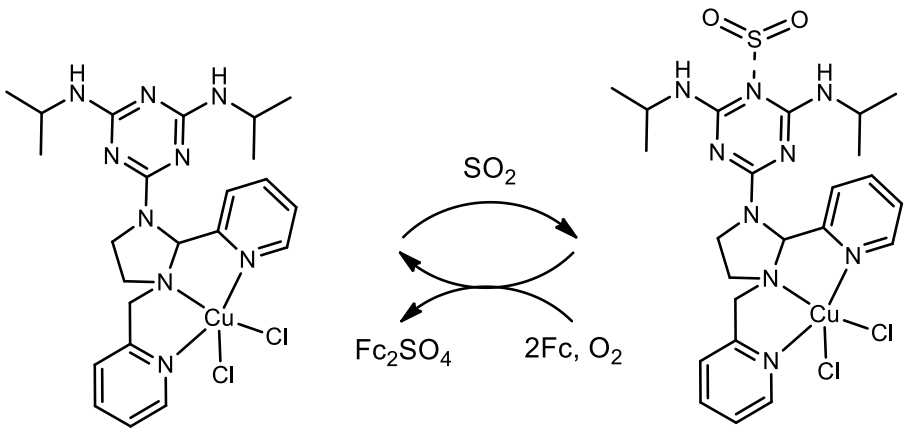

Figure 1. SO_2 binding induced formation of sulfate.

Reported is an unprecedented, simple and sustainable strategy to catalytically convert SO_2 gas into sulfate dianions under ambient conditions utilizing ferrocene (SO_2 + 2Fc + aerial $O_2 \rightarrow Fc_2SO_4$) and aerial oxygen, whereby ferrocenium sulfate was formed without any unwanted byproducts. The frequent urban haze and increase in respiratory health issues connected to the atmospheric SO_2 concentration attracted interest in the sequestration and valorization of SO_2. Even though a number of methods have been reported in the past decade for the stoichiometric sequestration and activation of SO_2, effective catalytic activation of SO_2 through homogeneous catalysis has not been realized before. The copper(II) koneramine complex [Cu(L-H)Cl_2] was designed to have exclusive basic sites for SO_2 binding, which complemented efficient electron transfer from ferrocene to SO_2 that underwent S-oxygenation to yield sulfate dianions. In this proof of concept study, SO_2 binding coupled electron transfer (SOCET) from ferrocene was established with the assistance of control experiments, electronic absorption spectroscopy, cyclic voltammetry and electrospray ionization mass spectrometry.

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P-251: Synthesis, Characterization, and Applications of Nanoglass

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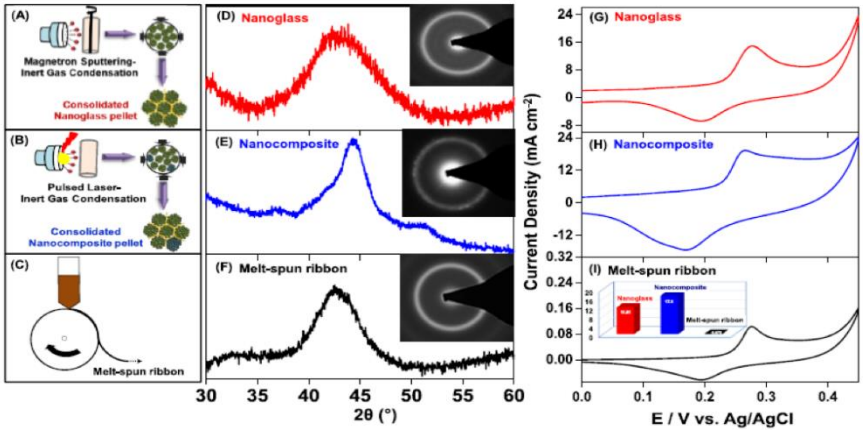

Figure 1: Schematics in A to C show preparation methods of nanoglass, nanocomposite, and melt-spun ribbon, respectively. Amorphous phase in D & F is indicated through XRD and TEM SAED analysis. Cyclic voltammograms of 0.10 mM glucose in alkaline solution are shown in G - I. Variation of anodic peak current density of all the materials is shown in the inset of I.

Control in the microstructure of the nanocrystalline and glassy materials is manifested through their property and reactivity. Synthesis through different routes, detailed microstructural characterization and applications (e.g., glucose sensing) of a nanoglass ($Ni_{60}Nb_{40}$) starting from amorphous nanoparticles is demonstrated and compared the results with a melt-spun ribbon (MSR) and nanocomposite of identical atomic composition (Figure 1).[1] Three different $Ni_{60}Nb_{40}$ systems with the same elemental composition, but varying microstructures are created following different synthetic routes and tested for their glucose-sensing performance. Among melt-spun ribbon, nanoglass, and amorphous−crystalline nanocomposite materials, nanoglass showed the best performance in terms of high anodic current density, sensitivity, limit of detection. The effect on the magnetic property during the consolidation of glassy nanoparticles at different uniaxial pressures to create such nanoglass is studied. While nanoglass showed ferromagnetic behaviour at every compaction pressure, the MSR always remained paramagnetic although its density was comparable. Presence of glass-glass interface in the nanoglass is responsible for such distinct behaviour. Some of these exciting results will be demonstrated in the presentation.

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P-252: Development of Novel Triazine-based Chemosensor for Cu(II) detection and DNA binding Studies.

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Novel ligand 2,4-bis(4-imino)-1,2,4-triazolyl-6-phenylamino-1,3,5-triazine(BITPAT) and its copper complex{Cu (BITPAT)CI_2} was synthesized and characterized through physicochemical studies such as elemental analyses, molar conductivity, cyclic voltammetry and spectroscopic techniques in the solid state (IR) and in solution (^{1}H NMR and UV-visible). Further, X-ray powder diffraction (XRD) analysis of {Cu(BITPAT)CI_2}was carried out to point out the complex formation. The selective and sensitive determination of Cu^{2+} was done by both colorimetry and electrochemical sensing. The stoichiometric composition of {Cu (BITPAT)CI_2} has been authenticated by Jobs plot and the stability constants were determined. IR spectral studies suggested the tridentate nature of ligands involving bonding through two triazolyl nitrogen and triazine ring nitrogen. The mass spectral data have indicated the Cu(II) complex to be mononuclear. The optimized geometry of the BITPAT and Cu (BITPAT)CI_2 complex was arrived at by DFT calculation methods. The binding affinities of Cu (II) complex with calf thymus DNA (CT-DNA) have been studied by using absorption titration techniques. The binding of the synthesized complex to bovine serum albumin (BSA) and human serum albumin (HSA) was studied using computational tools. The copper complex shows high values of binding constants for the interactions with bovine serum albumin (BSA) and human serum albumin (HSA)**.** In order to infer the biological relevance of newly synthesized complex, the *in vitro* antimicrobial activity assay against pathogenic gram-negative bacteria, viz. *Escherichia coli*; gram-positive bacteria *Staphylococcus aureus* and fungi *candida albicans* were studied by the MIC method. The results were compared with standard Amikacin and Ketoconazole and found that the metal complex possesses appreciable antimicrobial potential

Keywords: Triazines, Schiff base complexes, Colorimetric and Electrochemical, sensor Molecular docking.

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P-253: Design, Synthesis, and *in silico* Study of New Coumarin-Piperazine Hybrids as Potential Antibacterial and Anticancer Agents

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The versatile and significant therapeutic property of coumarin and piperazine; and further recent year reports of potent hydroxycoumarin and piperazine scaffolds, motivated us to design coumarin-piperazine hybrid derivatives. 4-Hydroxy-7-methylcoumarin was synthesized from *m*-cresol and malonic acid. The 4-hydroxy group of coumarin is replaced by the bromopropoxy group in basic media. Further, the bromine is substituted by various piperazine scaffolds to have a series of new coumarin-piperazine hybrid derivatives. In addition, these analogs were evaluated for their antibacterial and anticancer activity. A lot of structurally diverse coumarin analogs were found to display a remarkable array of affinity with the different molecular targets. Compound 3 (MIC= 12.5 µg/ml, E. coli) and compound 6 (MIC=12.5 µg/ml, E. coli and 25 µg/ml, S. aureus) showed potent activity against bacterial pathogens. Compound **3** showed excellent antibacterial activity against *S. aureus* with MIC=6.25 µg/ml. Compound **6** showed marvelous activity against the MCF-7 cell line. This is also proclaimed by a docking study too.

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P-254: Robust and promising hydrogen and oxygen evolution reaction by nanostructured bifunctional FeCoPd alloy electrocatalyst

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The electrochemical routes to energy storage and electrochemical/photocatalytic routes energy conversion processes have attracted a great deal of research attention in recent years to find sustainable and highly efficient alternative energy as a substitute for exhaustible fossil fuels.[1-4] Herein, we developed trimetallic FeCoPd polyhedral alloy nanoparticles (NPs) as a new highly efficient and promising bifunctional electrocatalyst for hydrogen and oxygen evolution reaction (HER, OER).[5] The as-synthesized polyhedral NPs possess mainly octahedral and cuboctahedral particles with exposed highly active {100} and less active {111} facets. The partial atmospheric surface oxidation of FeCoPd NPs led to the formation of oxidized metal ion sites for the adsorption of *OH and *OOH reactive species, and the catalyst on graphite sheet substrate in a 1.0 M KOH electrolyte can afford 10 mA cm^{-2} current density at 197 mV overpotential in the OER. The surface metal sites of the catalyst act as the active site for the adsorption of H_{ads} reactive species for the HER, exhibiting 52 mV overpotential at 10 mA cm^{-2} in 0.5 M H_2SO_4. The FeCoPd electrocatalyst offered high current density of 1000 and 550 mA cm^{-2} in acidic (at 0.144 V, HER) and basic (0.677 V, OER) mediums, respectively. With high mass activity of 4.67 A g^{-1}, it also showed long cycling stability of 10000 cycles and 100 h durability at high constant current density (100 mA cm^{-2}) without any degradation of the catalyst. It also demonstrated OER stability in 30 wt.% KOH with 180 mV overpotential at 10 mA cm^{-2}.

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P-255: Design and Synthesis of BODIPY Helicenes as Heavy-Atom-Free Triplet Photosensitizers for Photodynamic Therapy of Cancer

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Photoactive materials which on photo-excitation efficiently converts into its triplet state are very useful as triplet photosensitizers (PSs) in many applications including photodynamic therapy (PDT), a noninvasive treatment modality of cancer cells. For efficient PDT applications, PSs should have high absorption in the visible or NIR region, high triplet conversion efficiency, high photostability etc. Helicenes are the twisted polycyclic aromatic hydrocarbons (PAHs) having efficient ISC and importantly ISC efficiency is proportional to the twisting angle. But difficulties in their syntheses and derivatization, and weak absorption profile in the visible spectral region restricted their use as heavy-atom-free triplet PSs for PDT applications. Boron containing PAHs are highly recognized for their outstanding optical properties. Among these, BODIPY (4,4-difluoro-4-bora-3a,4a-diaza-*s*-indacene) class of dyes has emerged as one of the most versatile fluorophores. But planner BODIPY structure causes high S1-T1 energy gap which reduces ISC and eventually results unusually high fluorescence yields. Thus, in general the BODIPY dyes are not very effective as PDT agents but their modular structure, feasible synthesis and controlled structure–property tunability are attractive for application as PSs. Thus, efforts were made to enhance their triplet conversion and majority of the reports are based on halogenation of the BODIPY core[1] which adds many drawbacks as heavy atoms causes environmental pollutions, enhances dark toxicity, alters bio-distribution as well as pharmacokinetics important for biological applications. Halogen free BODIPY dyes are also developed mainly based on twisted structures, fullerene-conjugates, thionation etc.[2] In this work, we designed facile synthesis of BODIPY based helicenes. It is anticipated that the designed organo-boron complexes will have highly red shifted absorbance with respect to helicenes and the helical structures will enhance the ISC. In the current design one of the pyrrole units of the BODIPY core is replaced by a thiazole unit to further enhance the triplet conversion. Finally, their potential applications as PDT agents are investigated.

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P-256: Understanding Cyclic(alkyl)(amino)carbene-Copper Complex Catalysed N-H and O-H Bond Addition to Electron Deficient Olefin

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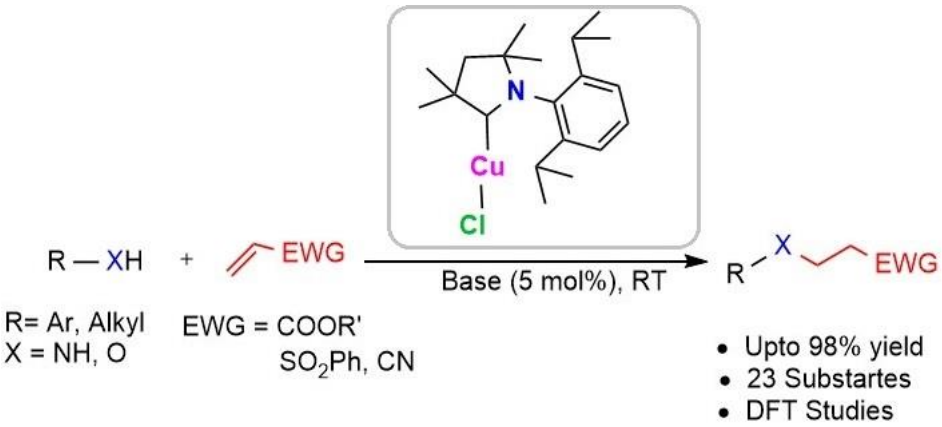

Since their discovery in 2005, cyclic (alkyl)(amino) carbenes (CAACs) have received much attention and are regarded as excellent donor ligands.[1] In comparison to N-heterocyclic carbenes (NHCs), CAACs proved to have stronger nucleophilicity (higher HOMO, more σ-donating) and electrophilicity (lower LUMO, more π-accepting).[2] Inspired by the progressive development in catalytic reactions using CAAC-metal complexes, we investigate the potential application of CAAC-CuCl complex towards hydroamination and hydroalkoxylation reactions. The CAAC-Cu catalyst showed higher efficiency than the corresponding NHC-based catalyst[3] reported previously. For the first time, we did an extensive investigation of the mechanistic pathway for this reaction using *ab initio* DFT calculations. Computational studies reveal that the reaction proceeds *via* either a four-membered or a six-membered cyclic transition state containing the copper ion.

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P-257: In-silico Drug Design and Discovery using MMP (Matrix Metalloproteinases)

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Discovery and Development of new drugs are very much time taking and very expensive processes. Therefore, to overcome this problem, in-silico techniques are used at early stages; which are successful in drug discovery and reduce costs and hard work associated with drug discovery.[1] MMPs (Matrix Metalloproteinases) are a family of zinc-dependententendopeptidases that degrades various proteins in the extracellular matrix.[2] MMP plays role in tissue remodeling during various physiological processes like angiogenesis, embryogenesis, and wound repair as well as pathological conditions like osteoarthritis, cancer, and fibrotic disorder. An increase in MMP level is associated with tumor progression andinvasiveness. MMP can be regulated by endogenesis tissue inhibition of metalloproteinases (TIMPS) and MMP/TIMP ratio determines the extent of ECM protein degradation and tissue remodeling. MMPs are biomarkers of many diseases. The discovery of lead molecules against MMPs using in-silico methods will be presented therein.

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P-258: Theoretical investigation of Donor-Acceptor behaviour of Nitrogen containing Heterocycles

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A number of organic compounds form charge-transfer complexes, which are often synonymously described as electron-donor-acceptor complexes (EDA complexes). Typical organic moieties that act as donors (D) are dibenzotetrathiafulvalene, pentacene, tetrathiafulvalene, 5,10-dimethylphenazine, and tetramethyl-p-phenylenediamine and acceptors (A) are TCNE, DDQ, Chloranilic acid, TCNQ etc. The strength of interaction between D and A in these complexes can be correlated with the ionization potential and electron affinity of the components.

Conjugated heterocycles bearing one or more nitrogen atoms are well known for their use as a CT chromophores and investigated as active components of optoelectronic devices, organic light-emitting diodes (OLED), photovoltaic cells, semiconductors, switches, data-storage devices, etc. The donor-acceptor properties and applications of such compounds are largely determined by the π-electron system in their structure which in turn depend upon the relative position of their frontier molecular orbital energy levels. The molecular topology can estimate the donor/acceptor strength of these compounds.

In the present study, the donor/acceptor ability of nitrogen containing simple and benzofused five membered heterocycles has been investigated theoretically on the basis of topological index and ionisation energies using Gaussian 16 suite of program at DFT level using 6-31+g* basis set.

The study will assist in tailoring heterocyclic systems to specific applications by altering their electronic properties. The results will be presented in detail.

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P-259: Synthesis of Biologically Important sulphonamide Linked Trifluoromethylated Pyrazoles

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Chemistry of fluorinated heterocycles has gained a lot of attention due to the widespread application of their derivatives in pharmaceutical and drug discovery as they can be of high utility for designing of biologically active compounds. Among heterocycles the pyrazole core is a privileged structural motif which is a part of modern drugs. Many fluorinated pyrazoles show diverse types of biological activity and are of immense applications as medicines. Encouraged by the versatility of these heterocyclic units we have synthesized diversely substituted trifluoromethylated pyrazoles containing sulfonamide derivatives. Trifluoromethylated α-oxoketene dithioacetals were utilized as synthons and coupled with sulfonamide substituted hydrazine moieties to synthesize the desired compounds. All the compounds were analysed by ^{1}HNMR, ^{13}CNMR, and Mass data.

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P-260: Reaction of imidazo[1,2-a]pyridines with acetylenic esters: Formation of new cross-conjugated mesomeric betaines

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Cross-conjugated mesomeric betaines (CCMB) are the dipolar species in which positive and negative charges are *exclusively* restricted to different parts of the molecule. Imidazo pyridines having two nitrogen lone pairs in conjugation are expected to be good donors and acetylenic esters are good acceptors. In view of this, we carried out the reactions of imidazo[1,2-*a*] pyridine with acetylenic esters namely, DMAD and methyl propionate which reacted in 1:2 molar ratio to give brown colour solids. The structure of these compounds was established on the basis of extensive spectral studies namely, ^{1}H, ^{13}CNMR and HRMS. As new CCMBs, the most interesting part of these molecules is revealed by theoretical calculations which indicate that the two parts of the molecule having opposite charges face each other which result in intramolecular charge transfer. This phenomenon was confirmed by UV-vis spectroscopy.

The whole sequence of reactions initiated by the attack of imidazo[1,2-a]pyridine on DMAD could be rationalized on the basis of the computational study of a model reaction sequence at the DFT (B3LYP/6-31+G(d)) level. The electronic excited states of the product were investigated by time-dependent density functional theory (TDDFT) calculations at the wB97XD/6-311++G(d,p) level, which indicate low-lying charge transfer that is characteristic of the CCMBs.

P-261: An Atom economical Approach Metal-free C-5 Chalcogenation of 8-Aminoquinolines: under Mild Conditions

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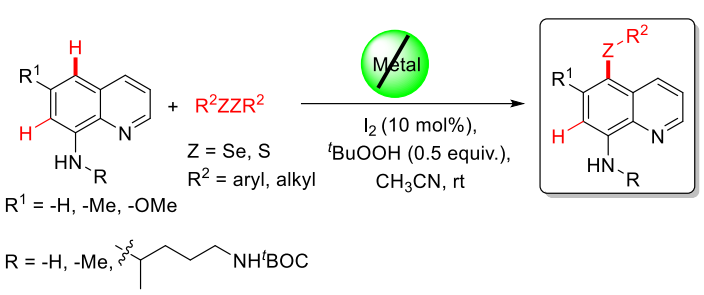

- **Atom Economical**
- **Transition Metal Free**
- **Room Temperature**
- **C-5 Regioselectivity**
- **Unprotected -NH_2 Group**
- **Yield upto 90%**
- **Scalable to Gram Scale**
- **Late-stage diversification of primaquine analogue**

A general and simple metal-free protocol for expedient C-H functionalization leading to regioselective generation of C-5 chalcogenated 8-aminoquinoline analogues up to 90% yield at room temperature (25 oC) has been established. This methodology provides an eco-friendly approach to atom-economical utilization of diaryl /dialkyl chalcogenides toward direct access to chalcogenated quinolines and scalable to gram scale without considerable decrease in the yield of product. It represents a practical alternative to the existing metal-catalyzed functionalization of 8-aminoquinoline derivatives with broad functional group tolerance. The controlled experiments suggest that the reaction possibly proceeds through an ionic pathway at room temperature. Furthermore, the potentiality for functionalization of free amines in chalcogenated-8-aminoquinolines features an attractive perspective to further elaboration of the amine substituent through chemical manipulations. The applicability of standardized method has been augmented through late-stage antimalarial drug diversification of primaquine analogue

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P-262: Electricity Induced Rhodium-Catalyzed Oxidative C–H/N–H Annulation of Alkynes with Dihydrophthalazinediones

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The development of stoichiometric oxidant free regioselective annulation protocol is a challenging aspect in organic synthesis. Herein, we disclosed electricity as greener oxidant for the C-H/N-H annulation to construct cinnolines, using Rhodium (III) catalyst under mild conditions. Detailed mechanistic investigation revealed the possibility of both Rh (III/I) and Rh (III/IV) catalytic cycle for the formation of annulated product. Exclusive regioselectivity, diverse substrate scope, and commercially available cheap graphite electrodes are key features of this protocol.

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