CSIR

National Chemical Laboratory

NCL

Annual Report 2017-18

सीएसआईआर

राष्ट्रीय रासायनिक प्रयोगशाला

वैज्ञानिक तथा औद्योगिक अनुसंधान परिषद

वार्षिक प्रतिवेदन 2017-18

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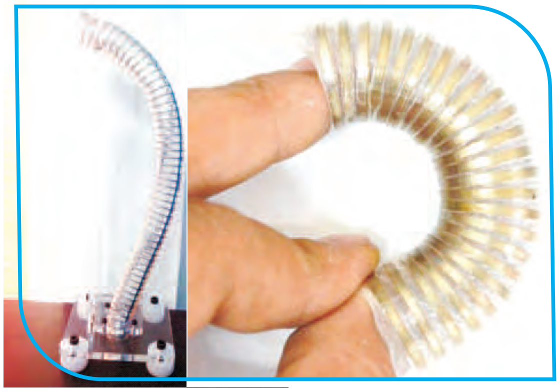

सीएसआईआर-राष्ट्रीय रासायनिक प्रयोगशाला
वैज्ञानिक तथा औद्योगिक अनुसंधान परिषद

With Best Compliments from...

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Director

CSIR-National Chemical Laboratory

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निदेशक की कलम से...

सीएसआईआर–राष्ट्रीय रासायनिक प्रयोगशाला की वर्ष 2017–18 हेतु वार्षिक रिपोर्ट बुनियादी विज्ञान के क्षेत्र के साथ–साथ प्रक्रियाओं और प्रौद्योगिकियों संबंधी हमारी उपलब्धियों का सारांश है, जो इस वर्ष के दौरान विकसित हुई। हमारी प्रयोगशाला ने प्रकाशनों की संख्या और गुणवत्ता में प्रगति की है और साथ ही हमने उद्योगों के साथ हमारे सहयोग को मजबूत किया है।

वर्ष के दौरान बहुत से महत्वपूर्ण कार्यक्रमों का आयोजन हमारे द्वारा किया गया। इंडिया ग्लायकोल्स के अनुसंधान एवं विकास तथा व्यवसाय विकास अध्यक्ष प्रो. आर.के. खंडाल ने दिनांक 29 सितंबर, 2017 को आयोजित सीएसआईआर– स्थापना दिवस समारोह में 'Sustainability of Indian Chemical Industry Role of CSIR' नामक विषय पर व्याख्यान दिया। डॉ. कोटा हरिनारायणा, INAE Satish Dhawan Chair, सीएसआईआर–एनएएल, बंगलौर द्वारा दिनांक 5 जनवरी,2018 को आयोजित एनसीएल –स्थापना दिवस समारोह में “Changing Role of Materials in Aviation” नामक व्याख्यान प्रस्तुत किया गया। राष्ट्रीय विज्ञान दिवस के उपलक्ष्य में दिनांक 28 फरवरी,2018 को प्रो. अनिल के. भौमिक, विशिष्ट प्राध्यापक एवं INAE, अध्यक्ष, भारतीय प्रौद्योगिकी संस्थान, खड़गपुर द्वारा 'Sustainable Materials in the Polymer Industry: Science & Technology' विषय पर व्याख्यान प्रस्तुत किया गया।

वर्ष के दौरान प्रयोगशाला के द्वारा विभिन्न कार्यशालाओं, संगोष्ठियों एवं सम्मेलनों का आयोजन किया गया, जिनमें Sustainable Catalytic Technologies at CSIR-NCL; Crystallography and Society: सैटेलाइट संगोष्ठी ; “Modern Trends in Inorganic Chemistry; इंडो–जापान अंतरराष्ट्रीय संगोष्ठी; Ramanujan Conclave – 2018 इत्यादि के आयोजन सम्मिलित हैं। सीएसआईआर–एनसीएल द्वारा सीएसआईआर प्लेटिनम जुबली प्रदर्शनी का आयोजन भी किया गया।

प्रयोगशाला द्वारा राष्ट्रीय तथा अंतर्राष्ट्रीय स्तर के विशेषज्ञ समीक्षित जर्नल्स में 621 शोधपत्र प्रकाशित किए गए, जो कि वैज्ञानिक प्रकाशन के क्षेत्र में एक बड़ी उपलब्धि है। वर्ष के दौरान प्रयोगशाला ने 59 भारतीय एवं 81 विदेशी पेटेंट/एकस्व दर्ज किए गए। सीएसआईआर–एनसीएल को 14 भारतीय एवं 176 विदेशी पेटेंट प्रदान किए गए। सीएसआईआर–एनसीएल के वैज्ञानिकों के मार्गदर्शन में 63 शोध छात्रों ने पीएच.डी. पूर्ण की ।

इस प्रयोगााला ने प्रौद्योगिकियों/प्रक्रियाओं को प्रायोजित परियोजनाओं के द्वारा विकसित करने के अपने प्रयास को जारी रखा है, जिनमें निम्नांकित का समावेश है– Direct synthesis of dimethyl carbonate (DMC) from CO_2 and Methanol; Development of a new stable fluromodifiers; Microencapsulation of insect pheromones for controlled release in Agriculture; Development of emulsion polymer with good wet adhesion and hydrophobicity and Continuous process for Alpha Nitro Napthalene.

इन अनुसंधान गतिविधियों के दायरे में कार्बनिक एवं अकार्बनिक रसायन, बहुलक एवं यौगिक, प्रक्रिया अभियांत्रिकी एवं प्रतिक्रिया अनुकूलन, उत्प्रेरण डिजाइन एवं संश्लेषण, सिंथेटिक रूपांतरण एवं ड्रग अणु, स्पैक्ट्रोस्कोपिक तकनीक एवं विश्लेषणात्मक लक्षण वर्णन, जैवरासायनिक प्रक्रियाएं, एंजाइम्स इत्यादि क्षेत्र शामिल हैं। सीएसआईआर–एनसीएल ने भारतीय फार्माकोपिया आयोग (IPC), भारतीय विज्ञानशिक्षा और अनुसंधान संस्थान (IISER), पुणे, रॉयल मेलबोर्न इंस्टीट्यूट ऑफ टेक्नोलॉजी (RMIT) आस्ट्रेलिया, एशियन रिसर्च नेटवर्क, कोरिया, राष्ट्रसंत तुकड़ोजी महाराज नागपुर विश्वविद्यालय. (RTMNU), ग्रीनवेन्शन बॉयोटेक प्रा.लि. एंड औरेफेल इनोवेंचर्स इंडिया प्रा.लि, अरिहंत स्कूल ऑफ फार्मेसी एवं बॉयोरिसर्च इंस्टीट्यूट एवं ए.जी. बॉयो सिस्टम्स प्रा.लि. के साथ समझौता ज्ञापन (MoU) पर हस्ताक्षर किए।

मैं सीएसआईआर–एनसीएल के अनुंसधान परिषद और प्रबंधन परिषद के साथ ही महानिदेशक, सीएसआईआर एवं सीएसआईआर मुख्यालय, नई दिल्ली के स्टाफ को उनके निरंतर समर्थन एवं सहयोग के लिए धन्यवाद देना चाहता हूं। अंत में मैं सीएसआईआर–एनसीएल के विभिन्न हितधारकों, वैज्ञानिकों, स्टाफ एवं विद्यार्थियों के प्रति अपनी कृतज्ञता प्रगट करता हूँ, जिनके उत्कृष्ट कार्यनिष्पादन को इस वार्षिक रिपोर्ट में सम्मिलित किया गया है ।

आश्विनी कु. नांगिया

(अश्विनी कुमार नांगिया)

From the Director's Desk...

The Annual Report of CSIR-NCL for the year 2017-18 summarizes the achievements in the areas of basic sciences as well as processes and technologies developed. The laboratory has progressed in the number and quality of publications and strengthened its association with industry partners.

Several important events took place during the year. The CSIR Foundation Day lecture was delivered by Prof. R. K. Khandal, President, R&D and Business Development, India Glycols on the 'Sustainability of Indian Chemical Industry Role of CSIR' on 29 September, 2017. NCL Foundation Day Lecture was presented by Dr. Kota Harinarayanana, INAE Satish Dhawan Chair, CSIR-NAL, Banglore gave away the CSIR-NCL Foundation Day Lecture on the topic "Changing role of materials in Aviation" on January 5, 2018. The National Science Day lecture was given by Prof. Anil K. Bhowmick, Professor of Eminence & INAE Chair Professor IIT, Kharagpur on 'Sustainable Materials in the Polymer Industry: Science & Technology' on February 28, 2018.

The Laboratory hosted different workshops, conferences and symposia including Conference on Sustainable Catalytic Technologies at CSIR-NCL; Crystallography and Society: Satellite Conference in Pune at CSIR-NCL; Symposium on "Modern Trends in Inorganic Chemistry; Indo-Japan International Conference; Ramanujan Conclave – 2018. CSIR-NCL also hosted the CSIR Platinum Jubilee Mega Exhibition as a part of CSIR Platinum Jubilee Celebrations.

The laboratory achieved major milestones in scientific publications having published 621 research papers in national and international peer reviewed journals. CSIR-NCL has filed 59 Indian and 81 foreign patents during the year. 14 Indian and 176 foreign patents were granted for CSIR-NCL. 63 Research students have completed Ph.D. under the guidance of CSIR-NCL scientists.

The laboratory has continued the efforts to develop the technologies / processes through Sponsored projects that included Direct synthesis of dimethyl carbonate (DMC) from CO_2 and Methanol; Development of a new stable fluromodifiers; Microencapsulation of insect pheromones for controlled release in Agriculture; Development of emulsion polymer with good wet adhesion and hydrophobicity and Continuous process for Alpha Nitro Napthalene. The breadth and scope of the research activities cover organic and inorganic chemistry, polymers and composites, process engineering and reaction optimization, catalysis design and synthesis, synthetic transformations and drug molecules, spectroscopic techniques and analytical characterization, biochemical processes, enzymes, etc.

CSIR-NCL signed memorandum of understanding with the Indian Pharmacopoeia Commission (IPC); Indian Institute of Science Education and Research (IISER), Pune; Royal Melbourne Institute of Technology (RMIT), Australia; Asian Research Network, Korea; Rashtrasant Tukadoji Maharaj Nagpur University (RTMNU); Greenvention Biotech Pvt. Ltd. & Auraphyll Innoventures India Pvt. Ltd.; Arihant School of Pharmacy & Bio-Research Institute and A.G. Bio Systems Private Limited.

I thank the Research Council and Management Council of CSIR-NCL as well as DG-CSIR and staff at CSIR HQ, New Delhi for their constant support and cooperation. Lastly, I acknowledge the role of stakeholders, the scientists, staff and students of CSIR-NCL who made possible this outstanding output for inclusion in the Annual Report.

Ashwini Nangia

(Ashwini Kumar Nangia)

Vision
Mission
Guiding principles & Values

Vision

To be a globally recognized and respected R&D organization in the area of chemical sciences and engineering

To become an organization that will contribute significantly towards assisting the Indian chemical and related industries in transforming themselves into globally competitive organizations

To become an organization that will generate opportunities for wealth creation for the nation and, thereby, enhance the quality of life for its people

Mission

To carry out R&D in chemical and related sciences with a view to eventually deliver a product, process, intellectual property, tacit knowledge or service that can create wealth and provide other benefits to CSIR-NCL's stakeholders

To build and maintain a balanced portfolio of scientific activities as well as R&D programs to enable CSIR-NCL to fulfill the demands of its stakeholders, present and future

To create and sustain specialized Knowledge Competencies and Resource Centers within CSIR-NCL which can provide support to all stakeholders of CSIR-NCL

To contribute to the creation of high quality Ph.D. students with competencies in the area of chemical, material, biological and engineering sciences

Guiding Principles & Values

To be deeply committed to the success of our stakeholders

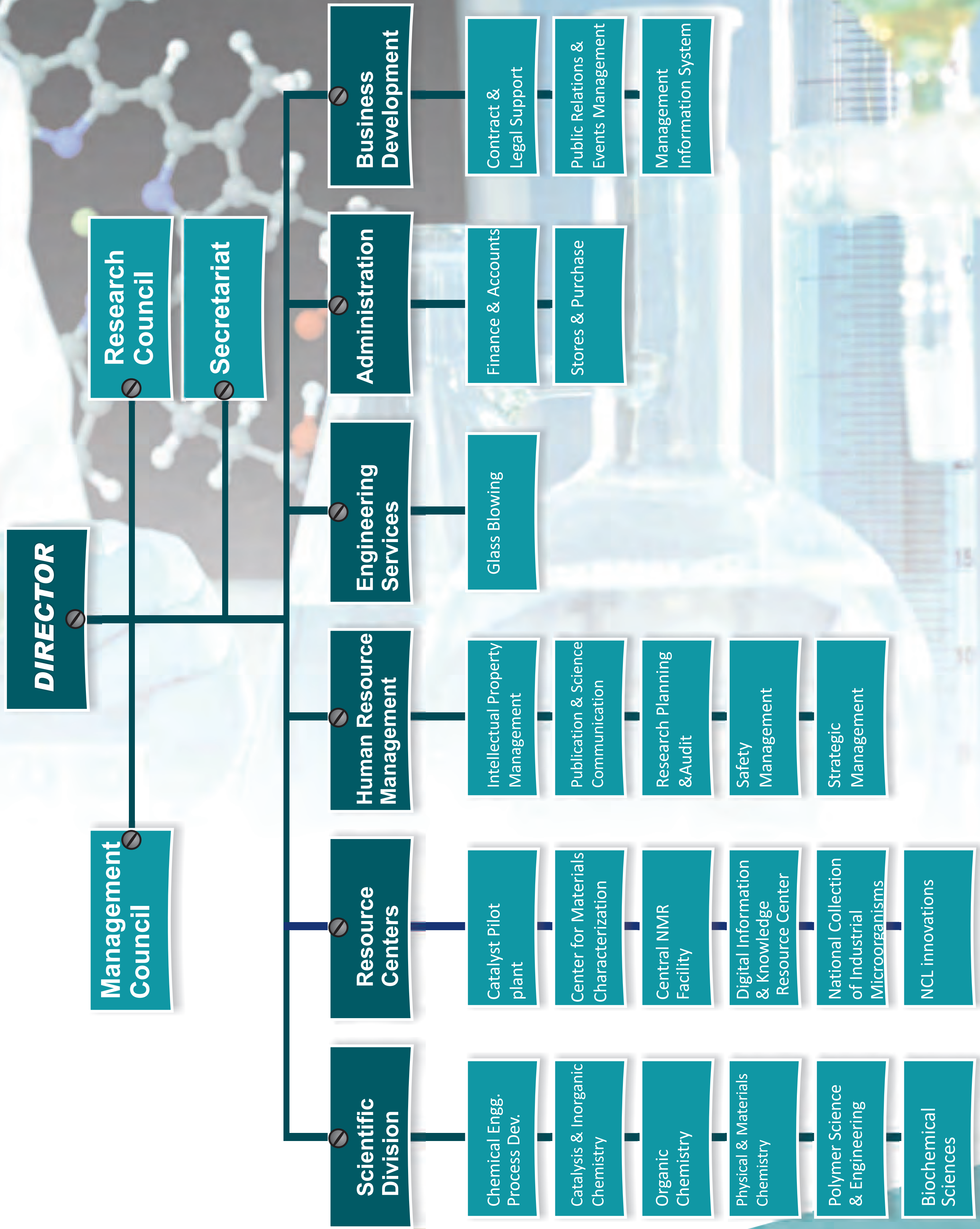
To create and sustain a self - driven and self - managed learning organization with a high degree of internal and external transparency

To encourage a culture of collective and principle-centred leadership

To value the dignity of the individual and deal with people with a sense of fairness and without bias, prejudice or favour

To nurture the highest standards of integrity and ethical conduct

Organization Chart



- **DIRECTOR**
  - Research Council
  - Secretariat
  - Management Council
  - Business Development
    - Contract & Legal Support
    - Public Relations & Events Management
    - Management Information System
  - Administration
    - Finance & Accounts
    - Stores & Purchase
  - Engineering Services
    - Glass Blowing
  - Human Resource Management
    - Intellectual Property Management
    - Publication & Science Communication
    - Research Planning &Audit
    - Safety Management
    - Strategic Management
  - Resource Centers
    - Catalyst Pilot plant
    - Center for Materials Characterization
    - Central NMR Facility
    - Digital Information & Knowledge Resource Center
    - National Collection of Industrial Microorganisms
    - NCL innovations
  - Scientific Division
    - Chemical Engg. Process Dev.
    - Catalysis & Inorganic Chemistry
    - Organic Chemistry
    - Physical & Materials Chemistry
    - Polymer Science & Engineering
    - Biochemical Sciences

Research Areas

Catalysis

- Heterogeneous Catalysis
- Organometallic Chemistry
- Surface Science

Chemical Engineering and Process Development

- Biochemical & Biological Engineering
- Energy and Environmental Engineering
- Industrial Catalysis and Catalytic Processes
- Industrial Flow Processes
- Mathematical & Computational Modeling
- Process Development and Scale-up
- Process Intensification and Engineering

Organic Chemistry

- Catalysis and new methods
- Chemical Biology
- Industrial Organic Chemistry
- Natural Product Chemistry
- Medicinal Chemistry
- Total Synthesis

Biochemical Sciences

- Enzymology and Microbiology
- Plant Molecular Biology
- Plant Tissue Culture
- Proteomics and Metabolomics
- Structure Biology

Polymer Science and Engineering

- Advanced Polymeric Materials for Energy
- Healthcare, Water, Security and Strategic areas
- Biomass Chemistry and Technology
- Polymer Chemistry
- Polymer Engineering
- Polymer Physics
- Membrane Science and Technology
- Colloids, soft solids and metastable materials

Physical and Materials Chemistry

- Biomimetic Materials
- Materials for optoelectronics
- Magnetic and Gas storage
- Quantum electronic and structure theory
- Soft Matter: Theory and Simulation
- Synthesis of Materials including Nanomaterials

Research Council

Chairperson

Prof. Gautam R. Desiraju
Solid State & Structural Chemistry Unit
& Centre for Condensed Matter Theory,
Indian Institute of Science,
Bangalore

Internal Member

Prof. Ashwini Kumar Nangia
Director,
CSIR-National Chemical Laboratory,
Pune.

DG Nominee

Dr. Anjan Ray
Director,
CSIR-Indian Institute of Petroleum
P.O. IIP, Mohkampur
Dehradun – 248 005

Member Secretary

Mr. G. Prabhakaran

External Members

Dr. R. K. Khandal
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R&D and Business Development
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USA

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Department of Science & Technology,
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Shaheed Jeet Singh Marg,
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Dr. Mukund K. Gurjar
Executive Director and Chief Scientific Officer (R&D),
Emcure Pharmaceuticals Limited,
Phase-2, ITBT Park, MIDC Hinjewadi,
Pune – 411 057

Dr. A. Ajayaghosh
Director,
CSIR-National Institute of
Interdisciplinary Science & Technology,
Industrial Estate, P.O. Pappanamcode
Thiruvananthapuram - 695019

Dr. S. Chandrasekhar
Director,
CSIR-Indian Institute of Chemical
Technology, Uppal Road, Tarnaka
Hyderabad - 500 007

Management council

Chairperson

Prof. Ashwini Kumar Nangia
Director,
CSIR-NCL, Pune

Members: CSIR-NCL

- **Dr. Utpal Das**
- **Dr. (Mrs.) Nandini Devi**
- **Dr. C. S. Gopinath**
- **Dr. S. P. Chavan**
- **Dr. (Mrs.) V. A. Parshurami**
- **Shri G. Prabhakaran**
- **Shri M. Sekar**

Special Invitee

- **Dr. R. K. Sinha**
  PPD, CSIR Hqrs

Sister Lab Director

- **Dr. Amitava Das**
  CSIR-CSMCRI,
  Bhavnagar

Member Secretary

- **Prema Balakrishnan**
  Controller of Administration,

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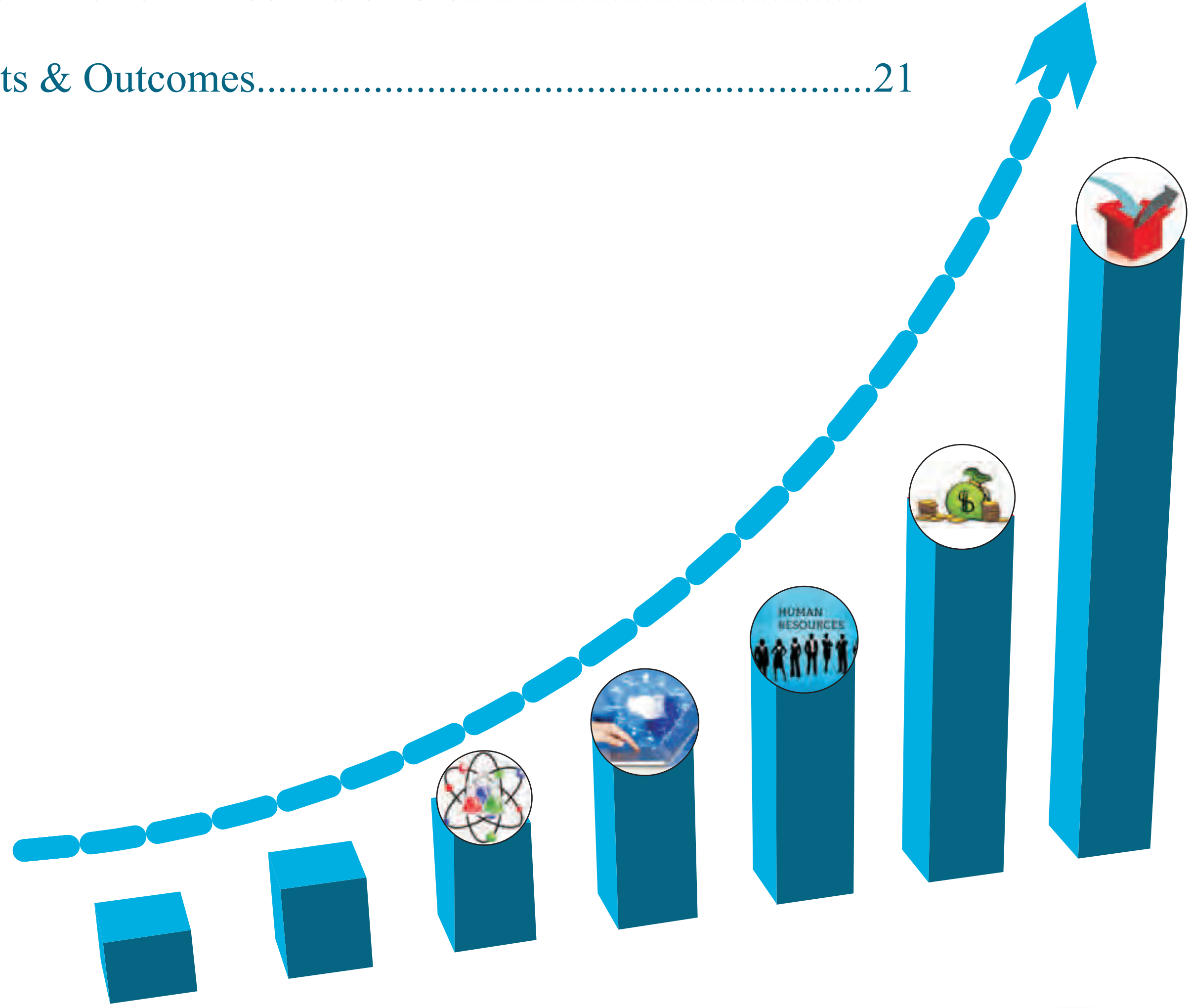
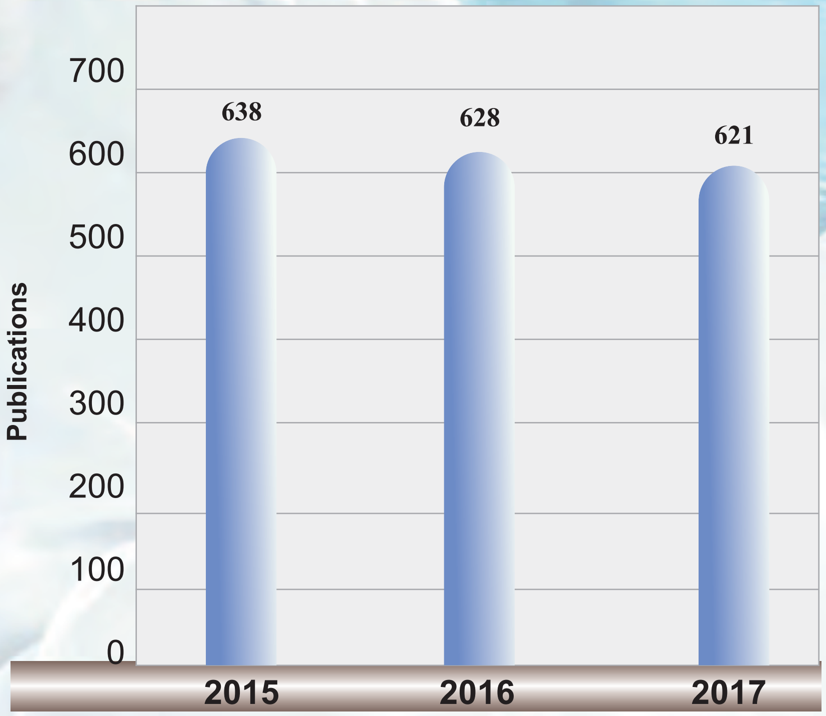
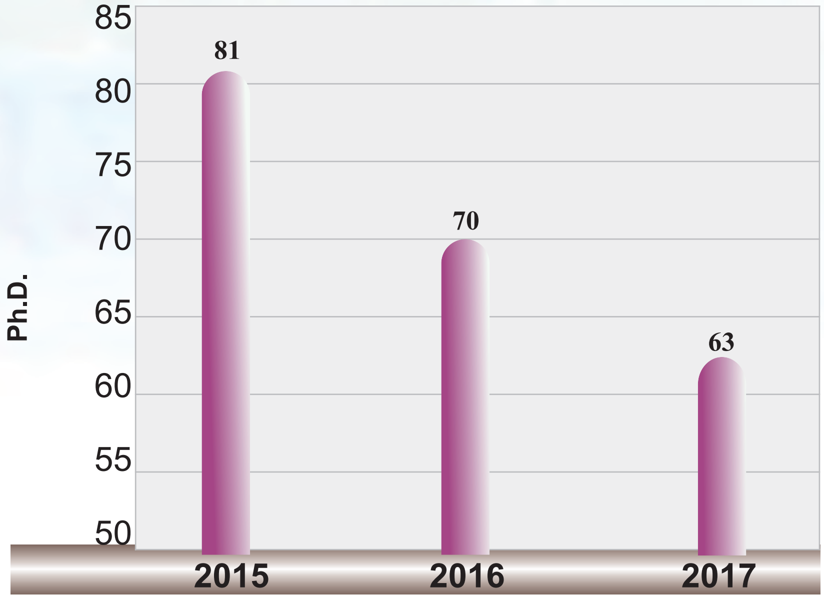


Research Output

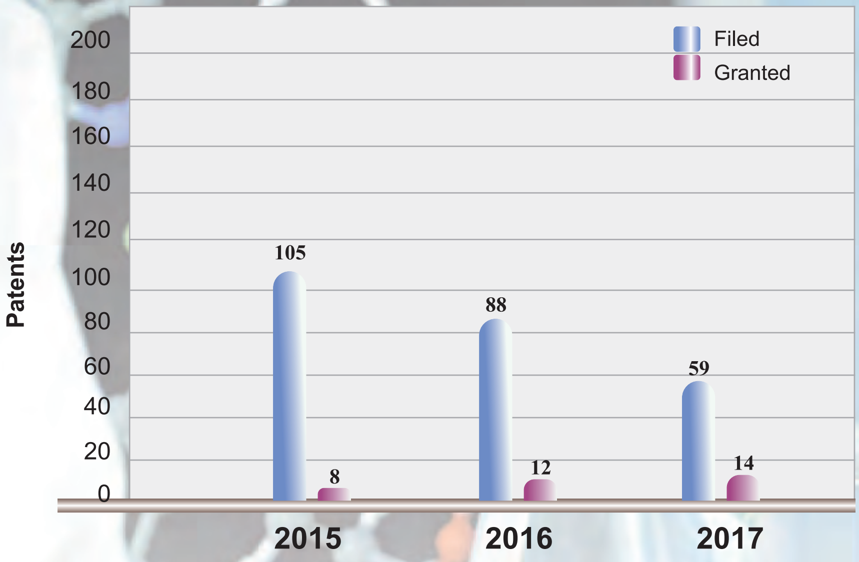
Publications



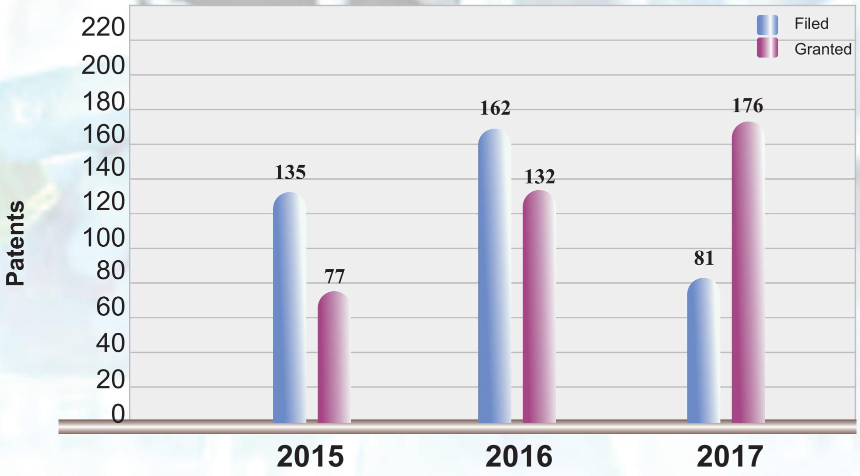
Ph.D. Theses



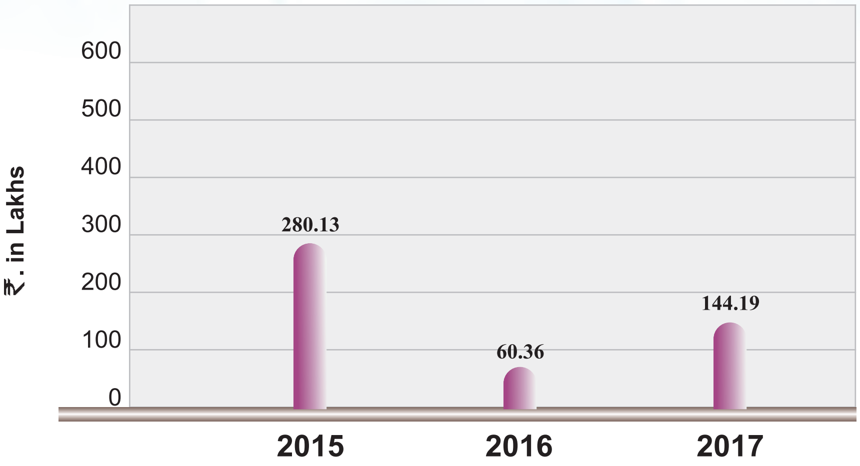
Indian Patents



Foreign Patents



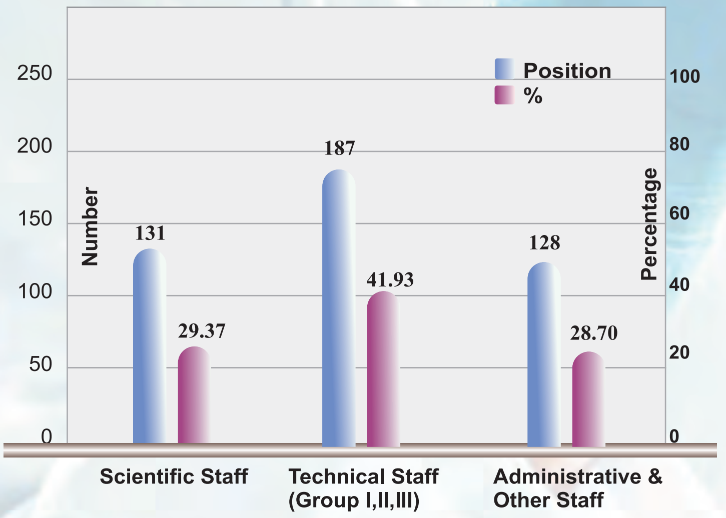
Premia / Royalty Earnings



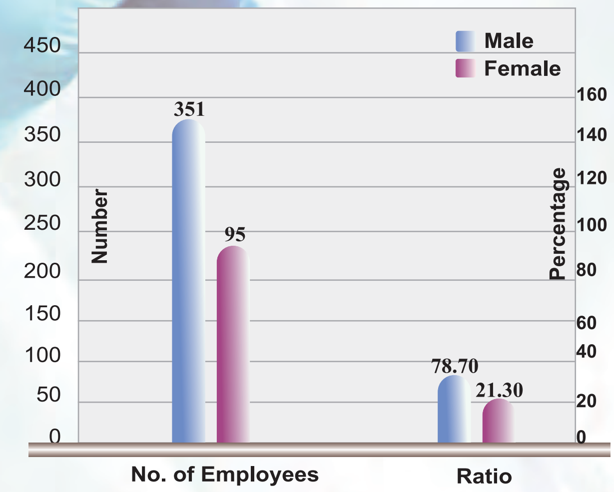
Performance Indicators

HUMAN RESOURCE INDICATORS

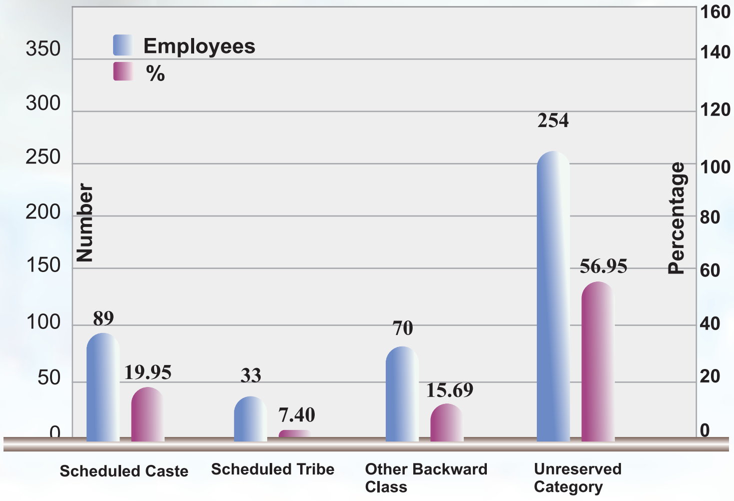
Total Staff: 446



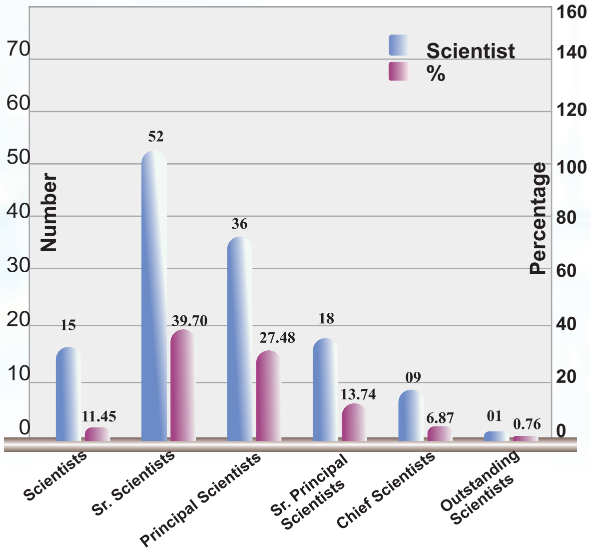
Male / Female Ratio



SC,ST, OBC & Others



Scientific Staff Distribution



Performance Indicators

We Welcome...

Computational Design of Molecules and Materials

Dr. Sailaja Krishnamurty
(08-12-2017)

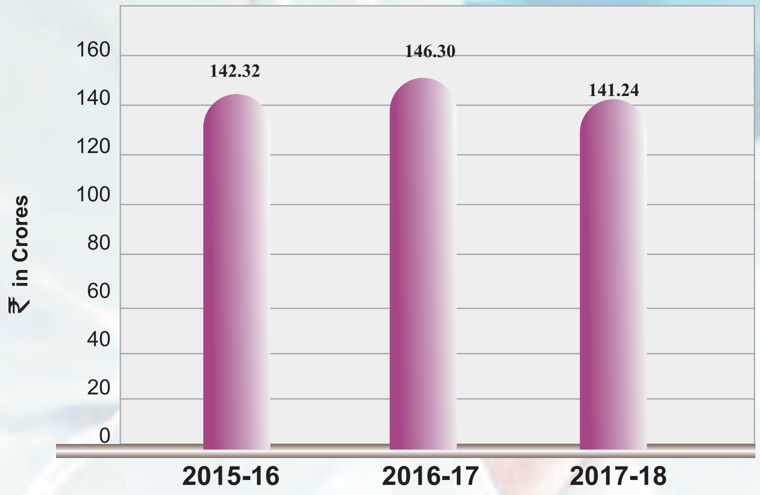
Scientist, CSIR-CECRI (2008-17)

Post-Doctoral Researcher, University of Pune (2005-07)

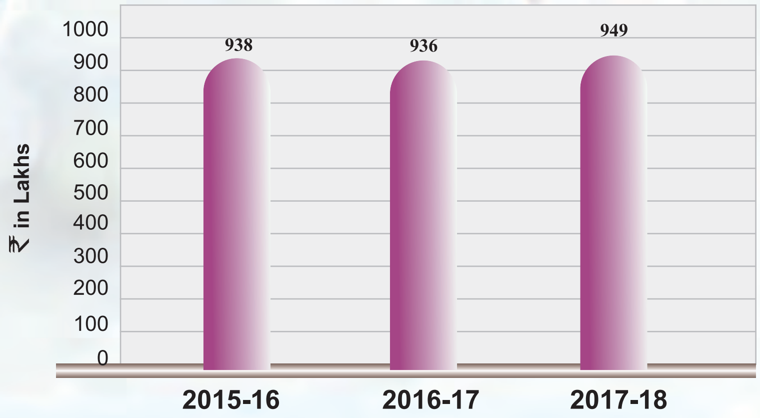
Post Doctoral Researcher, ENSCM, Montpellier, France (2001-05)

Ph. D. CSIR-NCL, University of Pune (2001)

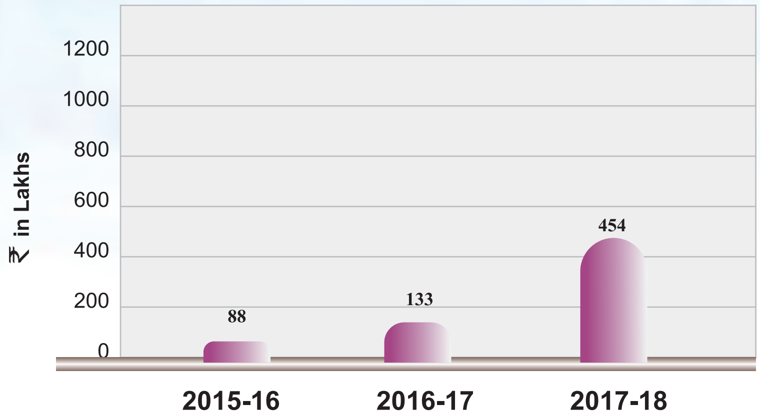
CSIR Budget



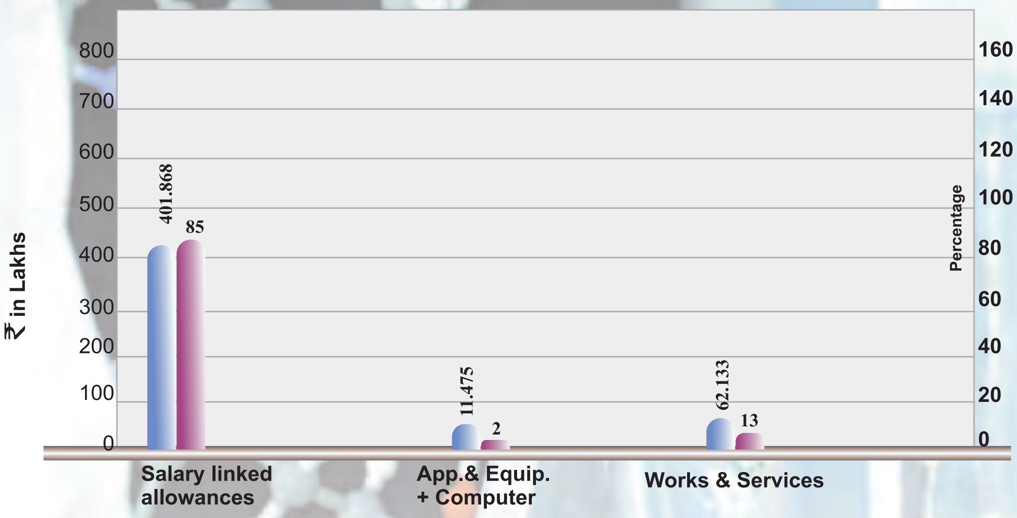
Laboratory reserve: Receipts



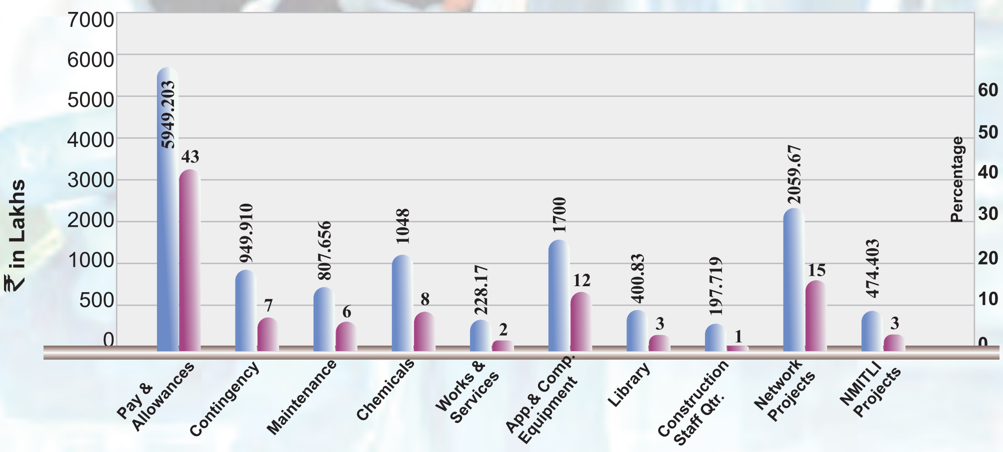
Laboratory reserve: Expenditure



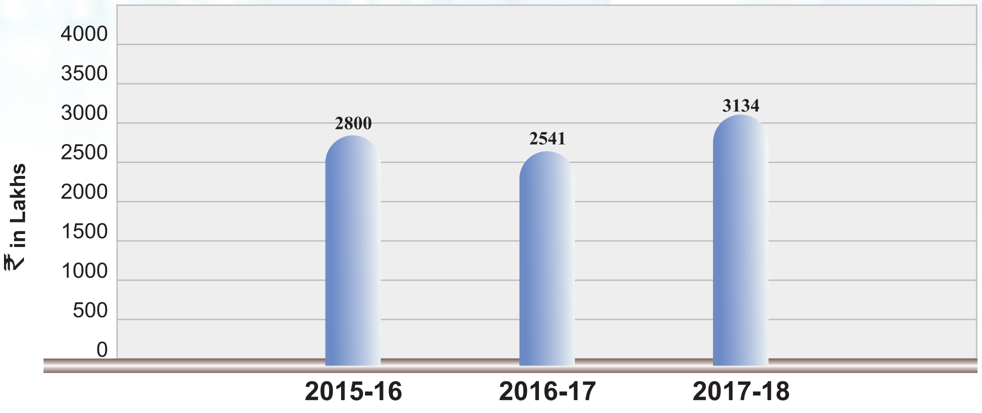
FINANCIAL PERFORMANCE INDICATORS



Laboratory reserve



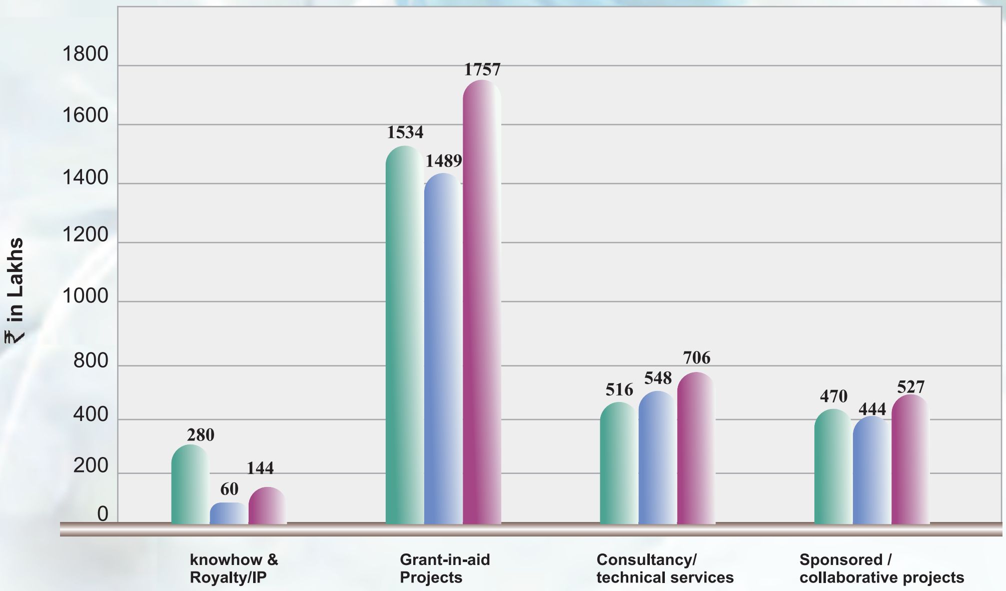
CSIR & Network Projects



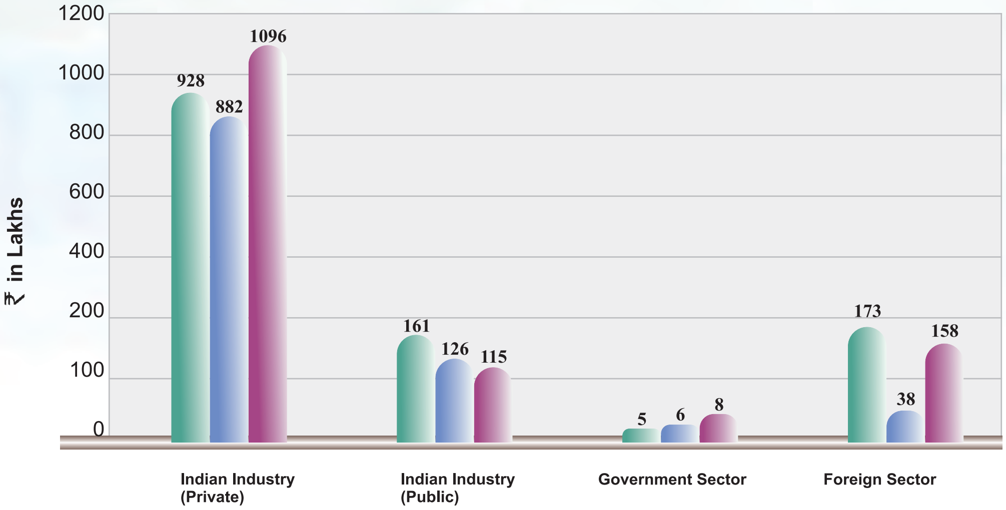
External Income

🟩 2015-16
🟦 2016-17
🟪 2017-18

Research Output



ECF by Source



ECF from Industry

OUTPUTS & OUTCOMES

Category of Benefits	Benefit	Indicators	2015-16	2016-17	2017-18
Public and social goods	Generation of and dissemination of generic knowledge	Number of papers published (Calendar year)	638	628	621
		Number of invention disclosure (Calendar year)	132	107	102
		Number of patents filed in India (Calendar year)	105	88	59
		No of foreign patents filed ** (Calendar year)	135	162	81
		Number of PCT applications filed (Calendar year)	64	49	30
		No of US applications filed	59	67	51
	Highly trained man-power	Number of PhD students as on 31 March, 2017	-	475	404
		Number of PhDs produced (Calendar year)	81	69	63
		Number of NET/GATE qualified students joined (including DBT JRF)	57	71	127
	Science awareness, popularization etc.	Number of popular S&T articles published (in all languages)	-	-	-
		Number of national and regional workshops, seminars organized	2	7	5
	Pride and standing among nations; National image	Number of international awards won -	-	-	-
		Memberships of major international academies and learned societies	12	12	12
		Number of foreign patents granted** (Calendar year)	77	132	176
	Representation in global affairs	Official(s) in global/ trans-national organizations like the UN, WHO etc - IUPAC(Cumulative years of office held) (Data given in no. of years)	8	8	8

1 Crore = 10 Million

Category of Benefits	Benefit	Indicators	2015-16	2016-17	2017-18
Private goods	Research, consulting, teaching And analytical services	Total earnings from projects done for Indian & Foreign businesses/ industry (in Crore) (Industrial ECF, excluding Grant-in-Aid)	12.67	10.52	31.34
	Continuing education	Total earnings from continuing education/ training programs (in Crore)	NA	NA	NA
	Licensing and technology transfer	Total earnings in the form of royalty, knowhow fees etc from Indian clients & contexts (in Crore)	2.80	0.80	1.44
	Other tactical and strategic developments	Total earnings from patent related transaction (in crore)	-	-	-
		No. of patents in new Licensing /assignment/ option arrangements	18	0	3
		No. of unique Licensing /assignment/ option cases	4	0	2
		No. of Indian patents granted (Calendar year)	8	12	14
		No of foreign patents granted** (Calendar year)	77	132	176
	Contributions to projects involving valuable opportunities in the form of technology options	Money inflow from NMITLI projects and other similar strategic projects (in Crore)	0.13	10.05	-
		Money inflow from Technology Mission & GIA projects (other than NMITLI) projects (in Crore)	15.34	14.89	-
Intellectual assets and reputation	Quality, reputation and standing of scientific manpower	No. of Indian patents granted (Calendar year)	8	12	14
		No. of foreign patents granted** (Calendar year)	77	132	176
		Number of scientists who are members of editorial boards of international peer-reviewed journals, covered by SCI	NA	NA	NA
		Number of PhDs granted where lab scientists were research guides	81	69	63
		Number of staff who are members of National academies (Cumulative)	32	32	32
		Number of Bhatnagar awardees (Cumulative)	16	16	16
		Number of Padma awardees (Cumulative)	5	5	5
	Lab’s standing with industry	Total worth of projects with industry (only industry: both Indian & foreign) (excluding Grant-in-Aid) (` in Crore)	12.67	10.52	31.34

*- Individuals who are members of more than one academy have been counted only once

** - Foreign means all filings other than IN & WO

1 Crore = 10 Million

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Energy & Environment...39

Healthcare...41

Sustainable Chemical Industry...62

Agriculture, Food & Nutrition...71

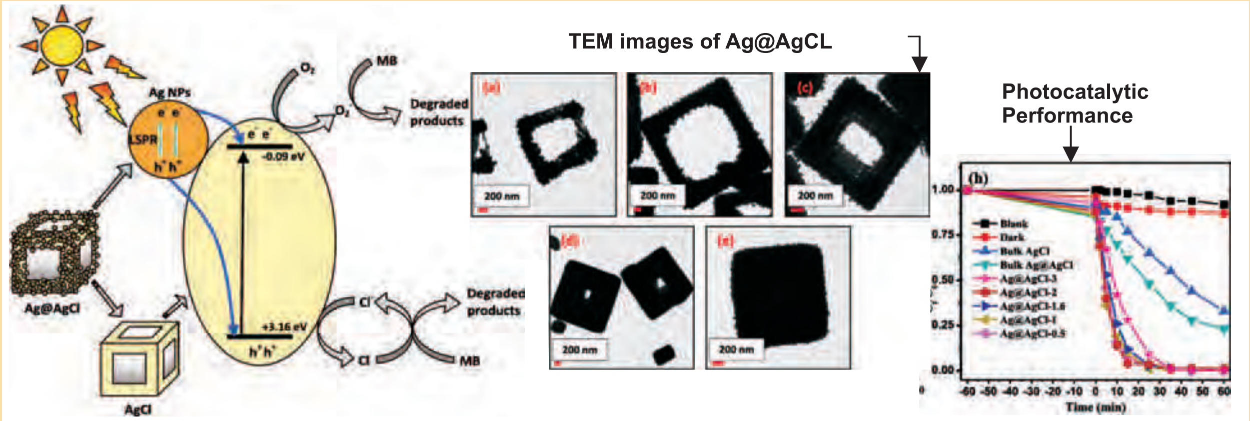
Nanostructured Materials

Meitram Niraj Luwang mn.luwang@ncl.res.in

Detection of explosive materials: This work reports the utilization of water dispersible terbium (Tb3+) doped spherical LaF3 nanoparticles (~5 nm) surface functionalised with p-aminobenzoic acid (pABA) for the detection of aromatic nitro explosives. The functionalised nanoparticles show remarkable sensitivity to a number of highly electron deficient aromatic nitro compounds like picric acid (PA), 2,4,6-trinitrotoluene (TNT), 2,4-dinitrotoluene (2,4-DNT), 2,4-dinitrophenol (2,4-DNP) etc. All of these nitro compounds can be detected easily at ppm level using this luminescence quenching technique whereas in the case of TNT it can detect concentrations as low as 50 ppb. This novel approach of utilising the Tb3+ doped NPs sensitised by pABA has potential application in the detection of explosive materials (US **2017**/0225963A1).

S. P. Mukherjee sp.mukherjee@ncl.res.in

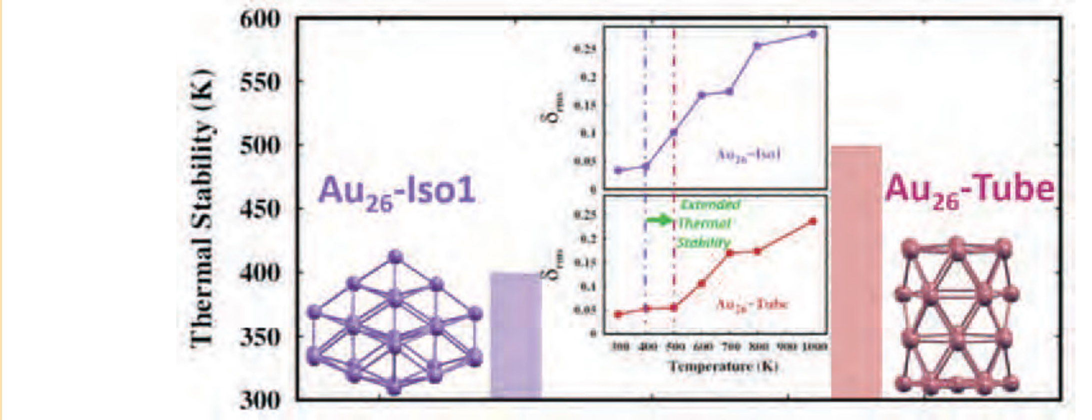
Facile tuning of Ag@AgCl cubical hollow nanoframes with efficient sunlight-driven photocatalytic activity: In this work, a facile controlled synthesis of plasmonic photocatalyst, Ag@AgCl hollow cubic cage with the tuning of nanoframe structures was reported. AgCl cubical hollow nanoframes were primarily prepared using sacrificial NaCl template protocol. Ion exchange reaction between Ag^+ in the solution and NaCl, in presence of poly(vinylpyrrolidone) (PVP) led to continuous nucleation followed by growth of AgCl on the surface of sacrificial NaCl template. The tuning of AgCl nanoframe structures was obtained by changing the $AgNO_3$ concentration in the reactions. Afterwards, ethylene glycol assisted reduction of AgCl, produced Ag@AgCl, the metal@semiconductor composite with the homogeneous distribution of Ag nanoparticles on the surface of the AgCl hollow nanoframes. Efficient sunlight-driven photocatalytic activity to degrade Methylene blue (MB) (50 mL; 10mg/L) with these Ag@AgCl hollow frames was also demonstrated. The plasmonic photo catalysts exhibited photo- degradation rates about 0.098-0.184 min^{-1} with high catalytic activity and recyclability for five cycles. Additionally, active species entrapping experiments were performed and a possible mechanism for the enhanced photocatalytic performance of the synthesized plasmonic photocatalyst was also proposed (*Appl. Surf. Sci.* **2019**, 465, 413).



Nanostructured Materials

Sailaja Krishanamurty k.sailaja@ncl.res.in

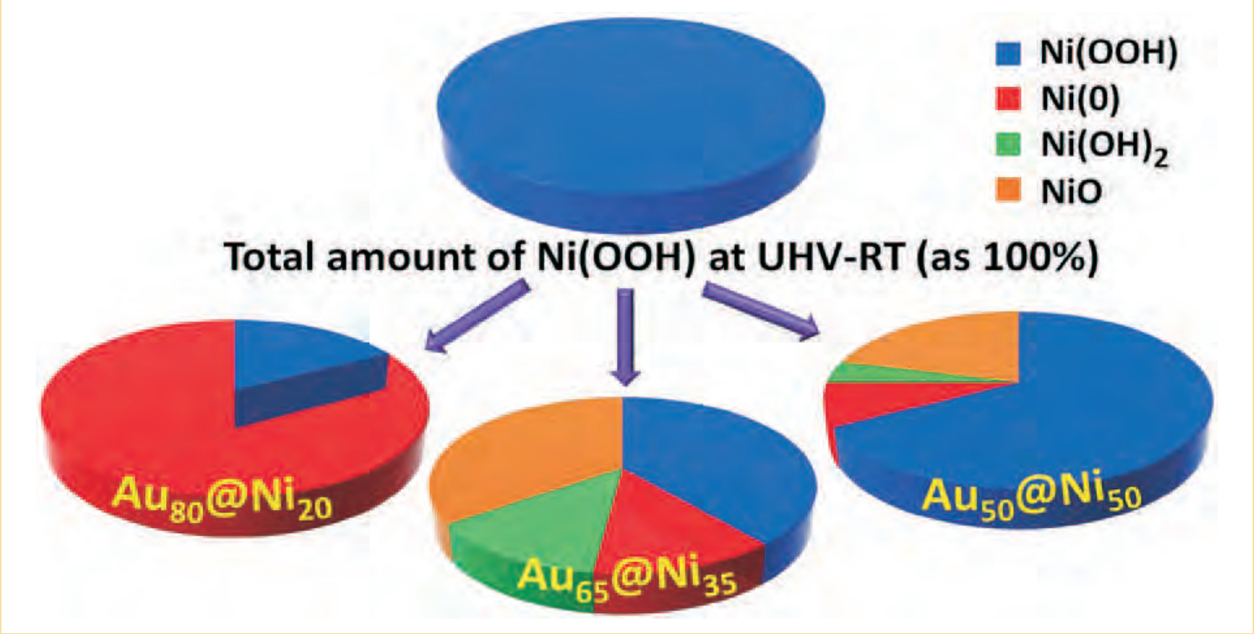
Impact of the position of a nano-structure in the potential energy surface on its physical properties: This study highlights the irrelevance of so called "ground-state" or a low lying conformational structure in nano-particles and their potential existence at room temperatures. Using *ab-initio* molecular dynamical simulations, the case study on a 26 atom nano-particle highlights the possible co-existence of several conformations at working temperatures, thus making the position of a nano-structure in the potential energy surface redundant to its potential existence during a synthesis process (*Phys. Chem. Chem. Phys.* **2018**, *20*, 8616).



C. P. Vinod cp.vinod@ncl.res.in

Application of near ambient pressure X-ray photo-electron spectroscopy to study surface chemical dynamics of bimetallic core-shell nanoparticles: The group has *insitu* probed the dynamic nature of Au@Ni core-shell nanoparticles under oxygen atmosphere using state-of-the-art lab based Near Ambient Pressure X-ray Photoelectron Spectroscopy (NAPXPS) Bimetallic Au@Ni core-shell nanoparticles, where the size of the Ni shell could be tuned from 2 nm up to 8 nm by changing the nickel precursor concentration were used for this study. The landscapes of metastable Ni(OOH) decomposition and theoxidation behavior of Au@Ni has been probed by NAPXPS. The NAPXPS studies show that the decomposition pathways of metastable Ni(OOH) species is vastly different on electronically or geometrically modified $Au_{80}@Ni_{20}$ with extremely thin Ni shell (~ 2 nm) which mainly converts to metallic nickel and is found to be stable in oxygen atmosphere even at 100°C. On the other surfaces, Ni(OOH) surface species predominantly gets converted to more stable oxidic (Ni^{2+}) species. The modified $Au_{80}@Ni_{20}$ surface showed improved catalytic activity in hydrogenation reactions further demonstrating structure vs activity correlations (*Catal. Sci. Technol.* **2017**, *7*, 4489).

Nanostructured Materials



Pie chart demonstrating the percentage composition of various surface species of nickel formed from the decomposition of Ni(OOH) at 0.1 mbar O_2 and 100°C as compared with the initial amount of Ni(OOH) at UHV-RT

Guruswamy Kumaraswamy g.kumaraswamy@ncl.res.in

Fused deposition modeling for 3D printing: Fused Deposition Modeling (FDM) is among the most widely practised 3D printing technologies. This uses a “filament” of thermoplastic polymer and extrudes it in the molten state, depositing it layer by layer, so as to build up a 3D object. Today, by far the most predominant FDM printed polymers are PLA and ABS. FDM printing of semi-crystalline plastics, such as PE and PP remains challenging due to difficulties inherent in printing such polymers. However, PE and PP represent about 70% of all synthetic polymers, and therefore also represent a very large fraction of the plastic waste stream. There are two technical challenges to the 3D printing of HDPE. (i) HDPE does not adhere to the bed of the 3D printer making it difficult to maintain registry while printing. (ii) More importantly, HDPE experiences volume shrinkage as it crystallizes on cooling from the melt. This shrinkage results in the generation of large stresses, which are relieved by the part warping out of the plane of printing. We have demonstrated a novel approach that uses additivation to render high density polyethylene 3D printable. We hypothesized that the difference in polymer modulus between the melt and solid states is the main reason for warpage. Therefore, we used additives that dissolve into the polymer (without affecting its flow ability at melt temperatures) and yet dramatically increase their creep viscosity during printing at lower temperatures. This approach minimized the driving force for polymer part warpage, allowing us to 3D print high density polyethylene. A patent application has been filed to protect this novel 3D printable formulation (Application number: **2017**, 11040358).

Functional Materials

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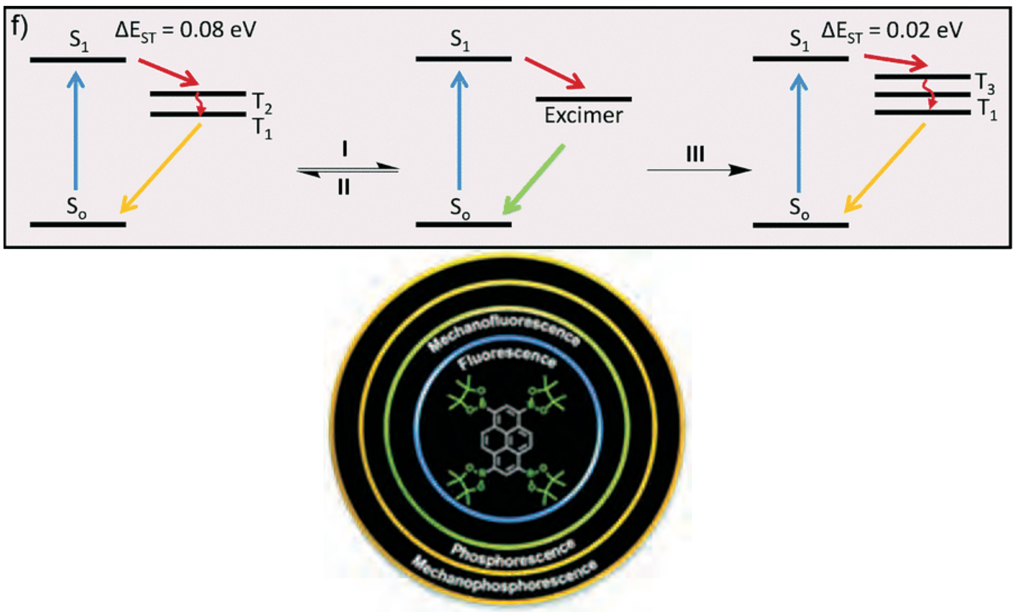
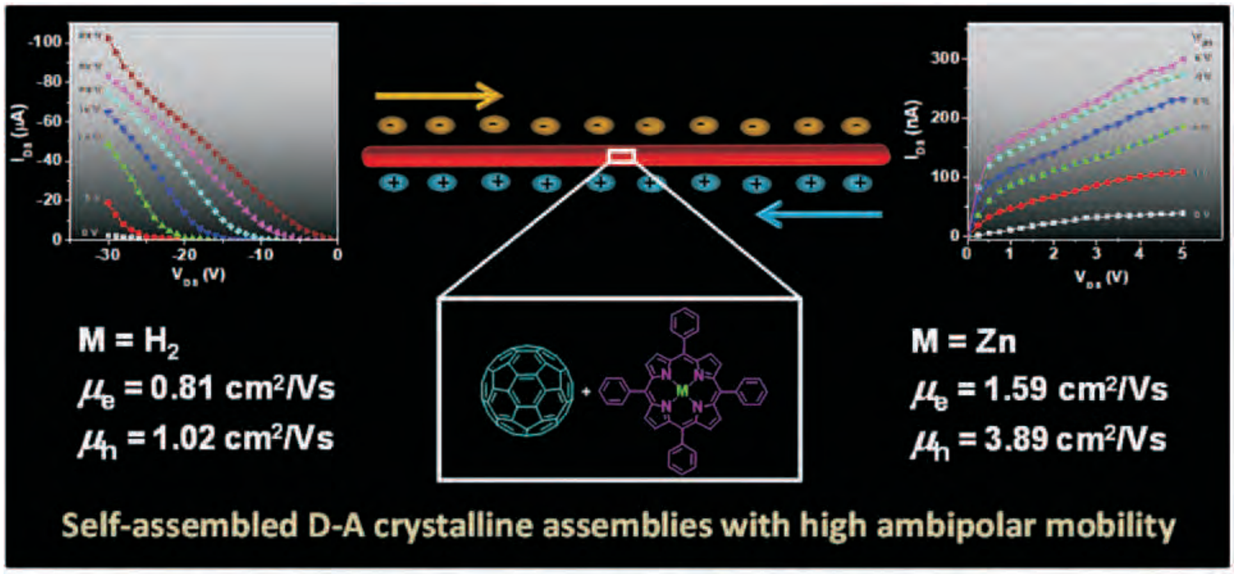
Lighting and light harvesting application materials

Mechano-responsive room temperature luminescence variations of boron conjugated pyrene in air: Stimuli responsive tunable luminescence is a promising field of research. Even though mechano-fluoroscence is widely studied, mechano-phosphorescence stays unexplored. Here, we report the mechanodriven fluorescence and phosphorescence variations of a pyrene tetraboronic ester derivative. The fluoro-chromic and room temperature phosphorescence features are supported by theoretical studies and single crystal analysis. The mechanically ground fluorescence active but phosphorescence inactive pyrene tetraboronic ester exhibits room temperature phosphorescence in air with mechanical force. The efficient intermolecular-electronic coupling in the dimer formed upon scratching enables a good communication between singlet and triplet states, hence results in room temperature mechanophosphorescence (*Chem. Commun.* **2018**, 54, 6028).



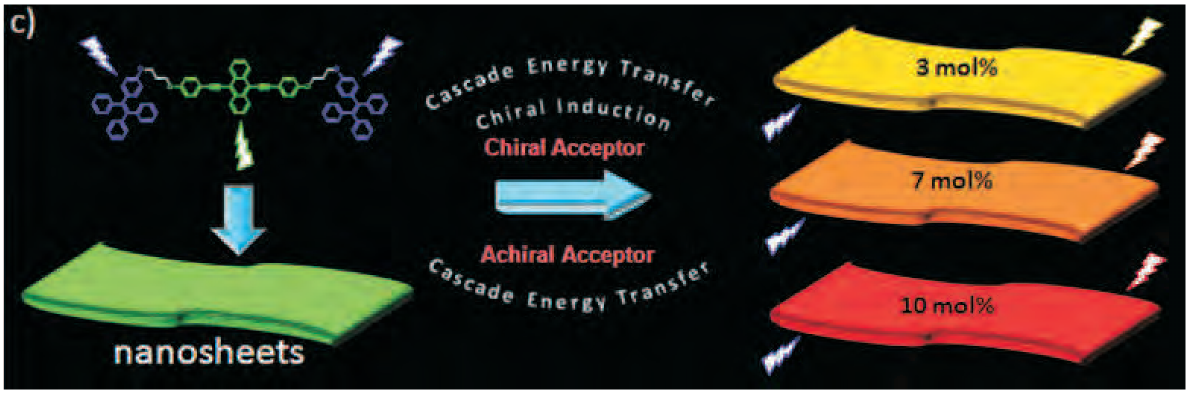
One-dimensional porphyrin-fullerene (C_{60}) assemblies Role of central metal ion in enhancing ambipolar mobility: One-dimensional (1D) nanostructures of π conjugated molecules exhibiting excellent charge carrier mobilities have found much interest in organic electronic devices. Even though it is tedious to form such structures, the availability of highly delocalized electron and hole carriers in these donor (D)-acceptor (A) co-assemblies realize ambipolar charge transport. Here we report the successful demonstration of a simple solution casting method to create ambipolar donor-acceptor single crystalline assembly. 1D assemblies of 5,10,15,20-tetraphenylporphyrins (H_2TPP, ZnTPP) and fullerene (C_{60}) exhibit high ambipolar mobility in the range of 0.8-3.4 cm^2/Vs for electrons and holes with high ON/OFF ratio and low threshold voltage. A direct experimental proof for the pivotal role of central Zn^{2+} in tetraphenylporphyrin, which enables a strong D-A charge transfer interaction in the cocrystal and thereby induces electron (1.35 cm^2/Vs), hole (3.42 cm^2/Vs) mobilities, the highest reported for two component D-A assemblies using solution casting, is demonstrated (*Chem. Eur. J.* **2018**, 24, 7695).

Functional Materials



Self-assembled D-A crystalline assemblies with high ambipolar mobility

Cascade energy transfer and tunable emission from nanosheet hybrids: Light harvesting donor-acceptor assemblies are indispensable to efficiently tap photons. In an attempt to improve the light harvesting efficiency of an acceptor doped assembly, we design and synthesize a donor-acceptor-donor triad which exhibit an exceptional intramolecular energy transfer with excellent efficiency. Moreover, a facile cascade energy transfer (energy funnelling) is observed in the presence of a series of second acceptors (63-91% efficiency) with tunable emission colours. Self -assembled nanosheets formed by the triad in the presence of acceptors, exhibit cascade energy transfer assisted tunable emission. In addition, use of chiral acceptors induce chirality to the triad and results in the formation of chiral nanosheets along with cascade energy transfer. Here chiral induction, nanosheet formation and cascade energy transfer in the presence of chiral acceptor is used as a tool to probe the intercalation of acceptor molecules in the donor scaffold (*Chem. commun.* **2017**,53, 7072).



Functional Materials

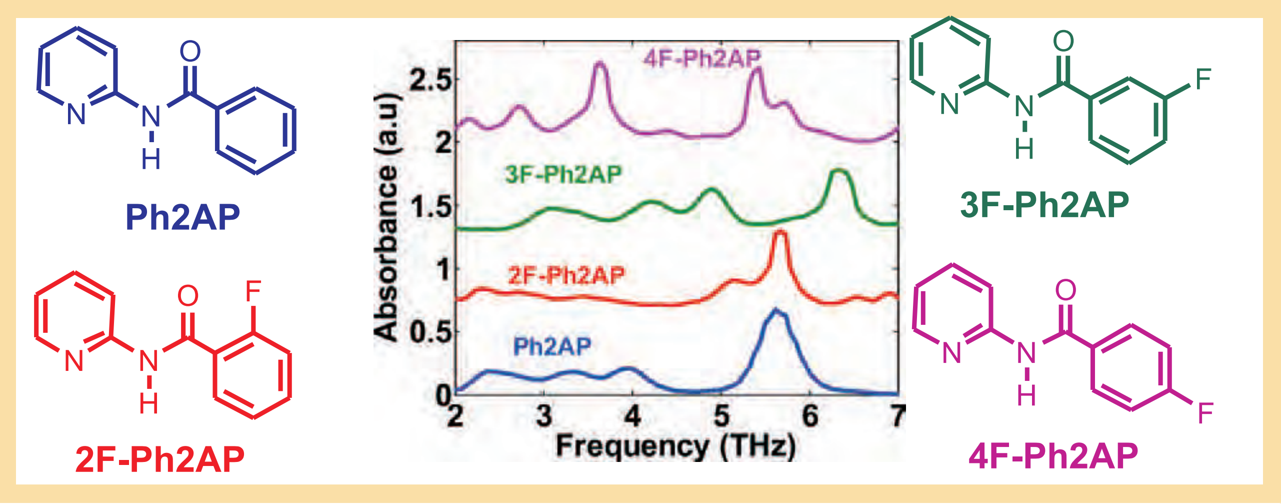
Sapna Ravindranathan s.ravindranathan@ncl.res.in

Unilamellar lipid vesicles based on host-guest interactions: NMR spectroscopy was employed to study the assembling of a naphthyl based long chain lipid derivative and morphological transitions resulting from changes in concentration. The mechanism of the interaction of the assembly with host molecule curcubituril and changes induced was examined in detail by NMR by employing a series of naphthyl derivatives with varying chain lengths. The molecular level information obtained regarding the mechanism of interaction and assembly formation, gives important insights into the basis for the enhanced luminescence response and FRET process observed for the curcubituril capped lipid assemblies on entrapment of luminescent dye molecules. Such studies form the basis for obtaining fundamental knowledge required for the design of new photo-responsive smart or adaptive stimuli responsive functional materials for application in optoelectronics (*Langmuir* **2017**, 33, 10989).

Chiral discrimination by NMR and luminescence: Choice of host molecules with well defined optical activity helps to differentiate guest molecules with different optical activities based on the difference in efficiency of FRET based responses. NMR investigations of the crown ether based hosts and ammonium ion derivative guests reveal that inclusion complexes between hosts and guests of same chirality are more stable relative to those of opposite chirality. However FRET transfer efficiency is higher for complexes between hosts and guests of opposite chirality. It was shown by NMR that the relative orientation of the guest in the host cavity is significantly different when the host binds to a guest of same or opposite chirality; the latter being more favorable for FRET thus enabling efficient discrimination between enantiomers. This idea was shown to be applicable for the design of a solid surface to achieve FRET based chiral discrimination (*Chem. Eur. J.* **2017**, 23, 18303).

Ashootosh V. Ambade av.ambade@ncl.res.in

Tuning of terahertz resonances of organic molecules for application as security tags: Terahertz (THz) radiation is used for detection of drugs, explosives and crystalline polymorphs in pharmaceutical research by incorporating organic molecules possessing characteristic fingerprint in the THz spectrum. For enhanced security, it is important to develop unique



spectral signatures. Here, N-(pyridin-2-yl) benzamide (Ph2AP) derivatives with prominent THz signatures were synthesized. Thz resonances were tuned by introducing fluorine at ortho, meta and para positions in the benzamide. Substitution of fluorine helps in varying the charge distribution of the atoms forming hydrogen bond and consequently strength of the hydrogen bond, which helps in tuning the THz resonances. The meta- and para-derivatives had higher hydrogen bond strength, as shown by calculations and hence higher frequency THz resonances compared to ortho-derivative (*J. Infrared Milli. Terahz. Waves* **2018**, *39*, 636).

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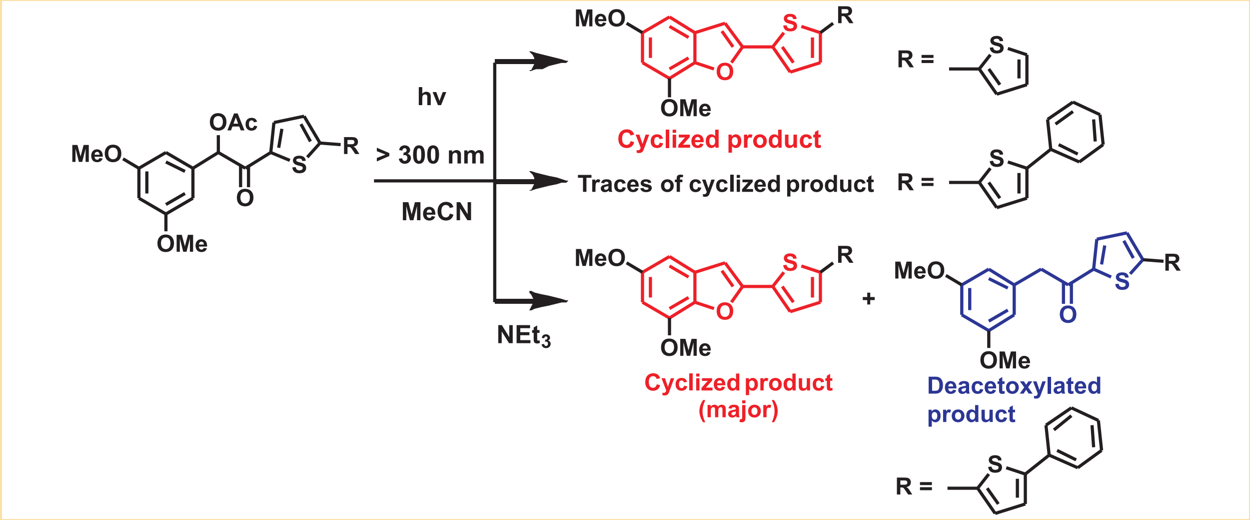
Modulated photochemical reactivities of O-acetylated (3',5'-dimethoxyphenyl) heteroaryl acyloin derivatives: 3',5'-Dimethoxybenzoin esters are imporatnt photoremovable protecting groups which forms 2-phenylbenzofuran derivative upon photo-release. A similar concept was utilized to test a photochemical method of installing benzofuran moiety to the conjugated backbone by subjecting O-acetylated (3',5'-dimethylphenyl)heteroaryl acyloin derivatives through direct photo irradiation and photo-induced electron transfer reaction. These photo-chemical methods were explored for a variety of heteroaromatic substrates appended on the ketone part of the O-acetylated cross-acyloin derivatives. The furan, thiophene and bithiophene derivatives led to the expected cyclized (benzofuran capped) products but the derivatives with extended conjugation decomposed under direct irradiation However, under irradiation in presence of the electron donor such as triethylamine, the extended acyloin derivatives afforded both cyclized and deacetoxylated products. Semiconducting nature of the extended cyclized products was also explored and tested for solution-processed organic field effect transistor which provided maximum hole mobility of 1.3×10^{-6} cm^2 $V^{-1}s^{-1}$ (*Photochem. Photobiol. Sci.* **2018**, *17*, 835).



Benzofuran capped conjugated molecules

Materials for Energy

Arup Kumar Rath ak.rath@ncl.res.in

Solution processed quantum dot solar cell

Surface engineering for quantum dots: Surface chemistry plays a crucial role in determining the electronic properties of quantum dot solids and may well be the key to mitigate loss processes involved in quantum dot solar cells. Surface ligands help to maintain the shape and size of the individual dots in solid films, to preserve clean energy band gap of the individual particles and to control charge carrier conduction across solid films, in turn regulating their performance in photovoltaic applications. We have shown that the changes in size, shape and functional groups of small chain organic ligands enable us to modulate mobility, dielectric constant and carrier doping density of lead sulfide quantum dot solids. Further, we correlate these results with performance, stability and recombination processes in the respective photovoltaic devices. Our results highlight the critical role of surface chemistry on the electronic properties of quantum dots. Our findings, when applied in designing new ligands with higher mobility and improved passivation of quantum dot solids, can have important implications for the development of high-performance quantum dot solar cells (*Nanoscale* **2018**, *10*, 1072).

Doping control in quantum dots: In the development of high performance QD solar cell, the surface ligand chemistry has played the important role in controlling the doping type and doping density of QD solids. For instance, lead sulfide (PbS) QDs which is at the forefront of QD solar cell technology, can be made n-type or p-type respectively by using iodine or thiol as the surfactant. It is shown here, however, that poor Fermi level alignment of thiol passivated p-type PbS QD hole transport layer with the n-type PbS QD light absorbing layer has rendered the photovoltaic devices from realizing their full potential. We developed a control surface oxidation technique using facile ultraviolet ozone treatment to increase the p-doping density in a controlled fashion for the thiol passivated PbS QD layer. This subtle surface modification tunes the Fermi energy level of the hole transport layer to deeper values to facilitate the carrier extraction and voltage generation in photovoltaic devices. In photovoltaic devices, the ultraviolet ozone treatment resulted in the average gain of 18% in the power conversion efficiency with the highest recorded efficiency of 8.98% (*J. Colloid Interf. Sci.* **2018**, 522, 120).

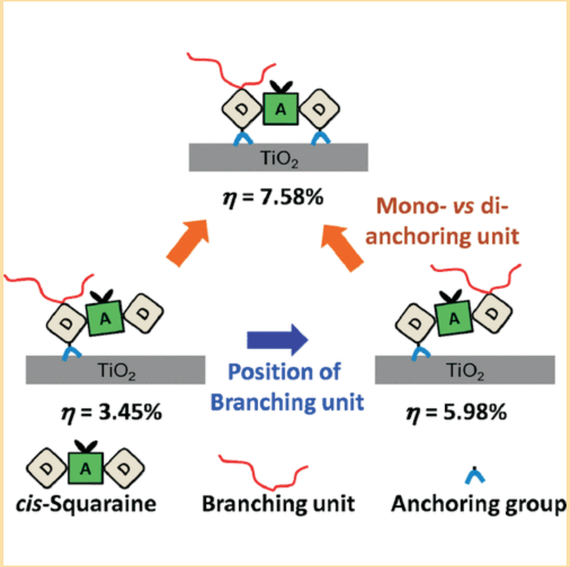
Generic and scalable method for metal sulfide nanocrystals: A rational synthetic method that produces monodisperse and air-stable metal sulfide colloidal quantum dots (CQDs) in organic nonpolar solvents using octyldithiocarbamic acid (C8DTCA) as a sulfur source, is reported. This novel technique is generic and can be applied to prepare diverse CQDs, like CdS, MnS, ZnS, SnS, and In_2S_3, including more useful and in-demand PbS CQDs and plasmonic nanocrystals of Cu_2S. Based on several control reactions, it is postulated that the reaction involves the in situ formation of a metal–C8DTCA complex, which then reacts in situ with oleylamine at slightly elevated temperature to decompose into metal sulfide CQDs at a controlled rate, leading to the formation of the materials with good optical characteristics. Controlled sulfur precursor's reactivity and stoichiometric reaction between C8DTCA and metal salts affords high conversion yield and large-scale production of monodisperse CQDs. Finally, the photovoltaic devices fabricated from PbS CQDs displayed a power conversion efficiency of 4.64% that is comparable with the reported values of devices prepared with PbS CQDs synthesized by the standard methods (*Langmuir* **2018**, *34*, 5788).

J. Nithyanandhan j.nithyanandhan@ncl.res.in

Self-assembly of cis-configured squaraine dyes at TiO_2-dye interface: Far-red active dyes for DSSC: To synergize both steric and electronic factors in designing the dyes for dye-sensitized solar cells (DSSCs), a series of cis-configured unsymmetrical squaraine dyes P11-15 with suitably functionalized alkyl groups and electron withdrawing group containing squaric acid unit were synthesized, respectively. These dyes capture the importance of (i) the effect and position of branched alkyl groups, (ii) mono- and di-anchoring groups containing dyes and (iii) further

Materials for Energy

appending alkyl groups through the cyanoester vinyl unit on the central squaric acid units of D-A-D based *cis*-configured squaraine dyes. All the above factors govern the controlled self-assembly of the dyes on the TiO_2 surface which helps to broaden the absorption profile of the dyes with increased energy harvesting process. With respect to the position of branched alkyl groups, dye P11 with sp^3-C and N- alkyl groups away from the TiO_2 surface, showed the better device efficiency of 5.98% than its positional isomer P12 with 3.45%. However with respect to mono- and di-anchoring groups containing dyes, P13 with two-anchoring units exhibited superior device performance of 7.58% in the presence of optically transparent co-adsorbent CDCA (3a,7a-dihydroxy-5b-cholanic acid) than dyes P11 and P12 (*ACS Appl. Mater. Interfaces* **2018**, *10*, 16541).



Vincent Paul Swamy vp.swamy@ncl.res.in

Ion pairing in 1-butyl-3-methylpyridinium halide ionic liquids studied: A series of DFT calculations were run to predict the features of the NMR spectra of the pure ILs based on a few selected supramolecular ionic aggregates. The effect of temperature, vibrational and conformational motions was tested using the Atom Centered Density Matrix Propagation molecular dynamics model scheme. The aim of our investigation is to test whether a simple DFT based approach of ion-pairing in ionic liquids is capable of providing reliable results and under which conditions the protocol is robust. We obtained a very good agreement between the calculated and experimental spectra for the three halides, where the bulk structure of the ILs is dominated by H-bond interactions between the X– anion (X = Cl, Br and I) and the *ortho* protons of the pyridinium ring (*Phys. Chem. Chem. Phys.* **2018**, 20, 11470).

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Dye Sensitised Solar Cells: We have been working on solar energy conversion with an objective to prepare solar cells that can be indigenously fabricated. Thus, our focus has been on dye sensitized solar cells. Unlike silicon, most of the components of DSSCs are available in India. We were able to fabricate cells with efficiency of over 10%, which is very impressive. These cells are useful in powering small electronic devices. In fact, we fabricated large area DSSCs (5 x 5 cm). These cells could charge power banks under diffused light. This is a significant achievement because Silicon solar cells perform poorly under diffused light. In order to use these cells in wearable electronic devices, we fabricated flexible DSSCs. These cells showed an efficiency of 4.2%. We have developed novel photoanodes, counter electrodes and buffer layers. Our collaborators have developed various dyes. Thus, important components of DSSCs have been developed (*Chem. Commun.* **2017**, 53, 6629; *Electrochim. Acta* **2017**, 246, 1023; ACS Omega **2017**, 2, 6768; *Langmuir* **2017**, 33, 13401; *ACS Appl. Energy Mater.* **2018**, 1, 2793).

Materials for Energy

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Solar hydrogen generation: Photosynthesis principles followed by leaves were taken over to a significant extent to produce hydrogen from water splitting. Hydrogen generation from water and sunlight is totally renewable method and it should reduce the carbon footprint. A solar cell device was fabricated comprising solar light-absorbing semiconductors and they are arranged in energy orderly fashion. This allowed the absorption of different wavelength regime of sunlight and generated charge carriers to produce hydrogen from an aqueous electrolyte solution. Hydrogen evolution (12 ml/h) could be visually observed on shining solar light on 1 cm^2 device (*Sci. Rep.* **2017**, *7*, 6516).

Artificial photosynthesis using Sunlight to generate Fuel

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Solid-state NMR investigation of glasses

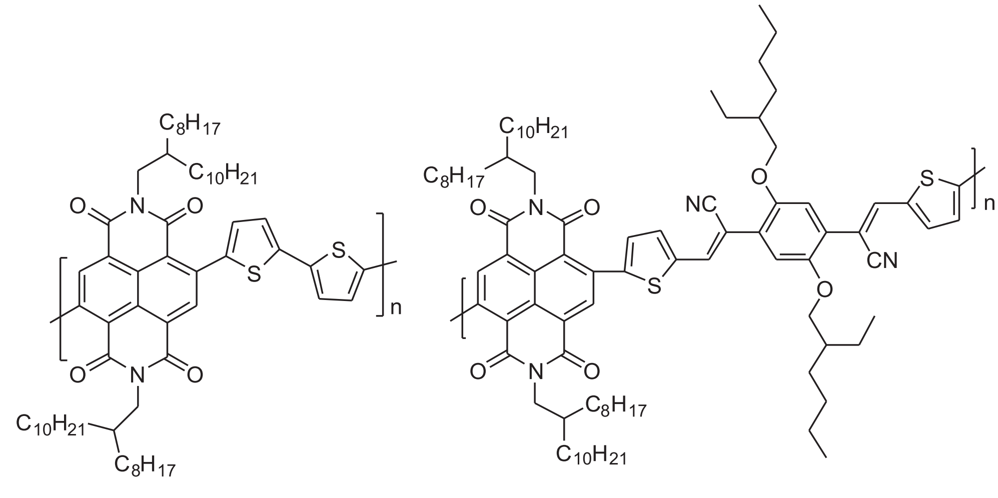
Structural elucidation of NASICON based glass electrolyte materials: Understanding the conductivity variations induced by compositional changes in sodium super ionic conducting (NASICON) (Na3Al2P3O12) glass materials is highly relevant for applications such as solid electrolytes for Na-ion batteries. In this study, NASICON based NCAP glass having the chemical composition $Na_{2.8}Ca_{0.1}Al_2P_3O_{12}$ (NCAP) is selected as a parent glass and the changes in the Na^+ ion conductivity of NCAP bulk glass with the substitution of boron (NCABP) and gallium (NCAGP) for phosphorus is monitored. Detailed structural analysis of NCAP, NCABP and NCAGP glasses using multi nuclear NMR (^{31}P, ^{27}Al, ^{23}Na, ^{11}B and ^{71}Ga nuclei) have been carried out. The variation in the conductivity values have been described based on the structural changes of NCAP glass with the substitution of gallium and boron. This study was carried out in collaboration with CSIR-CGCRI (*RSC Adv.* **2018**, *8*, 14422).

SSNMR study of microwave heated colourless phosphate glasses: Iron impurity in raw material remains a major challenge in producing colourless glass. In this study we report microwave (MW) heating capable of altering Fe-redox ratio (Fe^{2+}/Σ Fe) enabling preparation of colourless phosphate glass. The effect of Sn concentration in retention of Fe[II] in glass melted in MW was compared with conventional glasses. Colour imetric study developing Fe^{2+}- ferrozine colour complex reveals Fe-redox ratio $\geq$0.49 required to obtain colourless phosphate glass. In microwave heating, addition of 1 wt.% Sn metal powder can impart the desired effect whereas addition of 1.9 wt. % Sn metal powder is required in conventional heating. The correlation equation of Fe-redox ratio with concentration of Sn metal is found to be different in microwave and conventional heating. The nature of the P-O network in the glasses and the ^{27}Al coordination were probed using ^{31}P and ^{27}Al MAS NMR. This study was carried out in collaboration with CSIR-CGCRI (*Sci. Rep.* **2018**, *8*, 619).

Materials for Energy

Asha S. K. sk.asha@ncl.res.in

Highly stable supercapacitor electrode materials: Naphthalene diimide based conjugated polymers were developed via the direct (hetero) arylation (DHAP) polymerization route and explored as supercapacitor materials. Their performance was compared against a commercially available N type polymer N2200. A specific capacitance of 124 F/g with excellent stability upto 5000 cycles with almost 100% retention of the initial capacitance was observed for the newly developed NDI based polymer. We are not aware of any other reports of application of donor acceptor conjugated polymer as supercapacitor electrode materials with such exceptional long term cycle life (5000 cycles) with 100% retention of capacitance value (*Macromolecules* **2018**, 51, 954).



N2200

P_2 (P(NDI2OD-OThCNPV))

Synthesis of Polymers

Biomaterials

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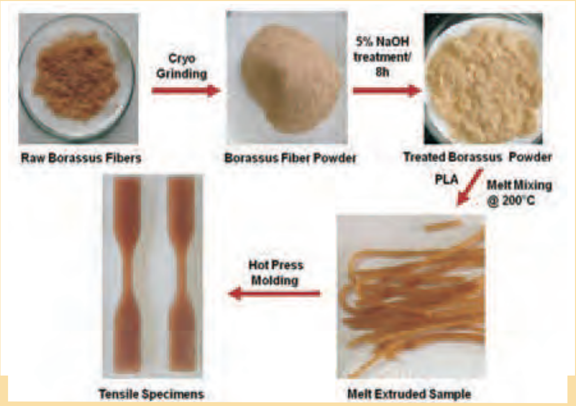
Borassus powder reinforced poly(lactic acid) composites with improved crystallization and mechanical properties: We have prepared a new biocomposite based on PLA and borassus powder with good mechanical strength and crystallization characteristics. It was observed that alkali treated powder-PLA composites have good interfacial interaction between borassus powder and PLA matrix which lead to the superior mechanical properties of the composites than untreated-PLA composites. The degree of crystallization (X_c) of neat PLA increased by ~61% upon loading of 15% treated borassus powder into PLA matrix. Natural fiber reinforced bio-plastics are attracting increasing attention these days due to the environmental issues of synthetic ones. *Borrassus* fiber has become an important natural fiber with good properties for making nanocomposites. This work reports on the development of biocomposites based on PLA and borassus powder (Scheme1). Borassus powder was treated with 5% alkali to remove amorphous hemicelluloses and lignin. PLA/borassus composites were prepared by melt mixing of PLA with 5, 10 and 15-wt% treated/ untreated borassus. Dispersibility of the borassus was studied by SEM and

Biomaterials

X-ray MicroCT. The treated borassus improved the homogeneous mixing with PLA (*J. Appl. Pol. Sci.* **2019** DOI: 10.1002/app.47440).



Scheme 1: Preparation of PLA/Borassus Bio-composites (Tensile Specimens)

The alkali treatment improved the interfacial interaction between the powder and the PLA matrix and improved the tensile strength of the composites.

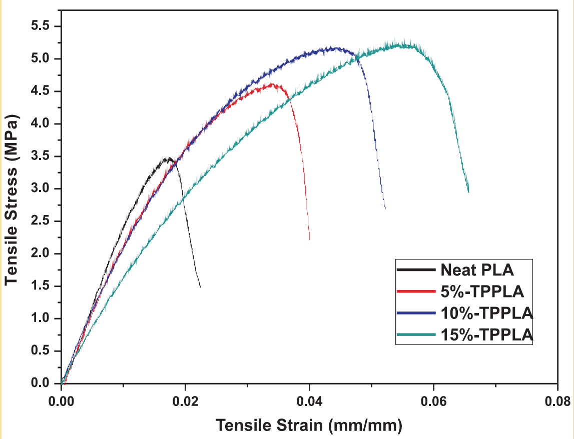


Fig. 1: Typical stress-strain curve of neat PLA and alkali treated-composites

Interestingly, the treated borassus powder also increased the crystallinity of the composites which was attributed to the enhanced interaction between the powder and the polymer and provided more sites for crystallization of PLA. Isothermal cold crystallization also showed highest crystallization rate with 15 wt-% loading of the treated borassus powder (**Fig. 2a**).

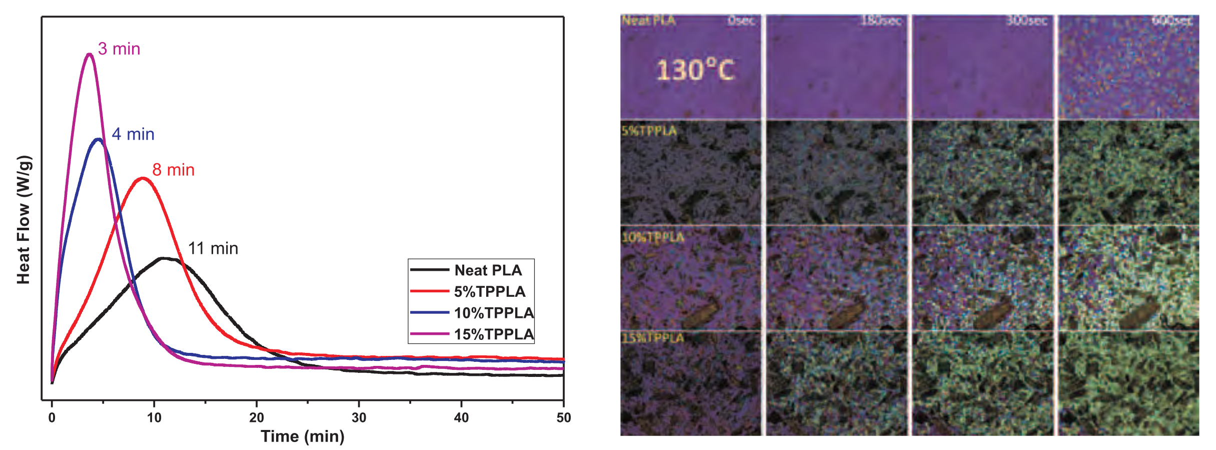


Fig. 2: a) DSC isotherm obtained during cold crystallization and **b)** Polarized micrographs of neat PLA and alkali treated-composites

G. V. N. Rathna rv.gundloori@ncl.res.in

Bioactive oil based polyesteramide nanofibers for wound healing applications: Biodegradable and biocompatible nanofibers were developed using oil based polyesteramides by blending with proteins and or polysaccharides with bioactive agent (pharmaceutical drug) for wound healing and biomedical application. The oils can be either of castor, linseed, neem, etc. The developed blends were prepared in various compositions and fabricated in the form of

Biomaterials

nanofibers. The suitable composition of the individual oil based polyesteramide was immobilized with drug and fabricated nanofibers. The nanofiber mats were non-toxic, showed antibacterial and sustainable drug release and proved to be suitable for biomedical applications (Patent: US20170135963).

B. L. V. Prasad pl.bhagavatula@ncl.res.in

Non-vascular self expandable stents

Background of the need, the development, and targeted outcome: Stents are used in the treatment of numerous GI tract diseases, ranging from benign diseases to malignant strictures. Two types of stents find extensive use: plastic stents and self-expanding metallic stents. Amongst these while the self-expandable metal stents offer longer patency their prohibitive cost makes them unaffordable. On the other hand plastic stents get clogged very often causing great inconvenience to the patient. CSIR-NCL in collaboration with a start-up has developed a new class of self-expandable stents based on a novel scroll design. Because of the novel design these stents could be made a much lower costs than the currently available ones.

Important parameters unique to the development: It is a new class of self-expandable stents based on a novel scroll design. These stents can be made with simple polymer-metal composites unlike the shape memory alloy based stents. The novel design allows these stents to meet the characteristics of shape memory alloy based stents. These stents could be made a much lower costs than the currently available ones (Patent: IN 2463/DEL/2015).

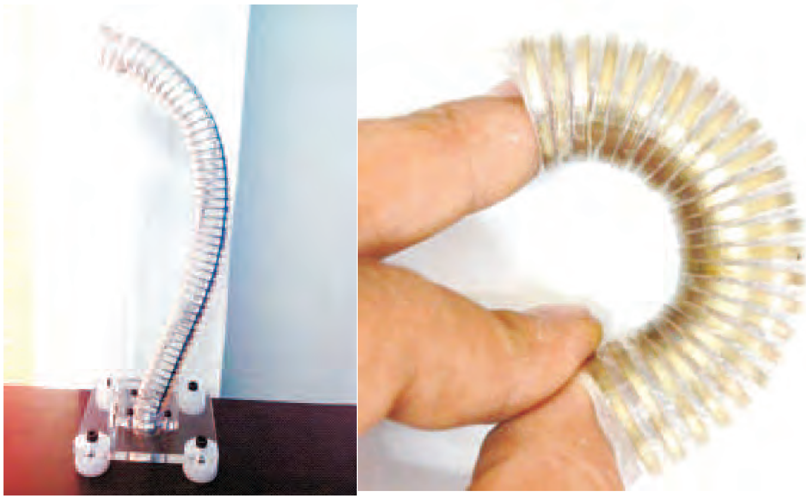


Fig: Prototype of the esoph-ageal stents made by CSIR-NCL and M/s Embryyo Technologies

Polymers

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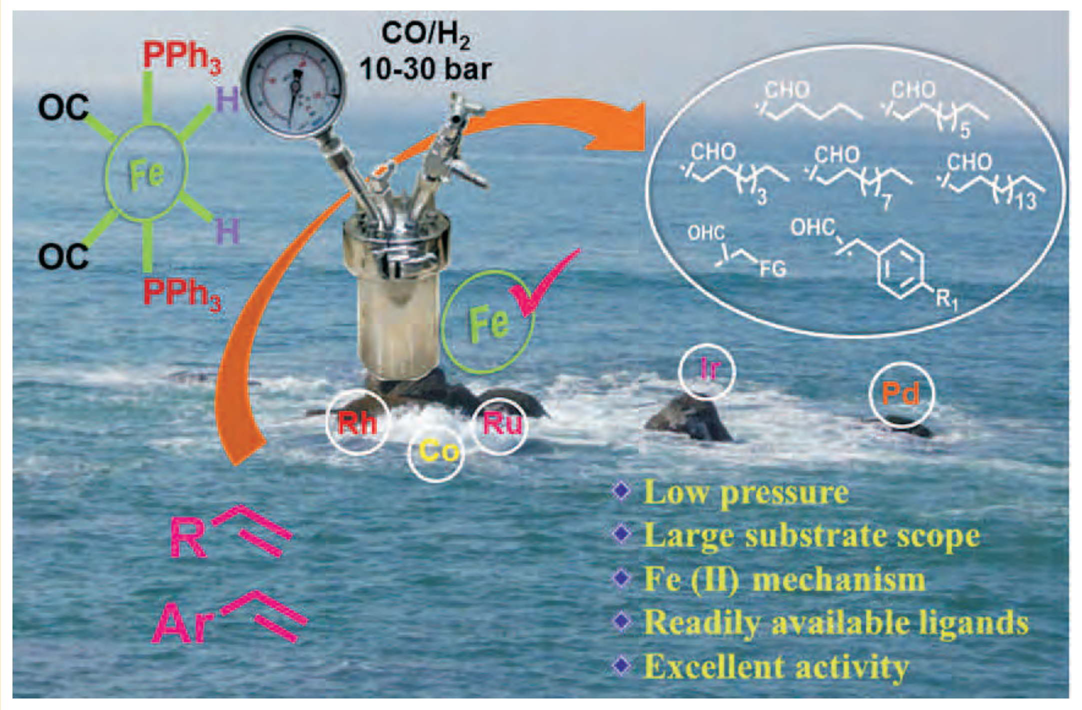
Organometallic chemistry of small and macro-molecules

Iron catalyzed hydroformylation of alkenes under mild conditions: A highly efficient iron catalyzed hydroformylation of alkenes under mild conditions was reported. This protocol operates at 10–30 bar syngas pressure below 100 °C, utilizes readily available ligands, and applies to an array of olefins. We have been able to contribute to industrial sustainability through developing an Iron based catalyst for an industrial process called hydroformylation. This finding was further supported by cyclic voltammetry investigations and intermediacy of an Fe(0)–Fe(II) species was established. Combined experimental and computational investigations support the existence of an iron-dihydride as the catalyst resting state, which then follows a Fe(II) based catalytic cycle to produce aldehyde (*J. Am. Chem. Soc.* **2018**, *140*, 4430).



Cross-metathesis of biorenewable dioxalates and diols to film-forming degradable polyoxalates: Starting from commonly available sugar derivatives, a single step protocol to access a small family of is ohexide-dioxalates (2a–c) has been established. The synthetic competence of 2a–c has been demonstrated by subjecting them to condensation polymerization. The proton NMR of poly (is omannide cohexane) oxalate revealed a 1:2 ratio between is omannide-dioxalate (2a) and 1,6-hexanediol (3a) in the polymer backbone. This intriguing reactivity was found to be an outcome of a cross metathesis reaction between 2a and 3a. The cross metathesis products 3a”[2-(2-methoxya-cetoxy)ethyl 2-(2-hydroxyethoxy)-2-(λ3-oxydanylidene)acetate] and 2a'(3R,6R)-6-hydroxyhexahydrofuro[3,2-b]-furan-3-yl methyl oxalate were isolated in a control experiment. Based on direct and indirect evidence, and control experiments, an alternative polymerization mechanism is proposed (*J. Pol. Sci. A Polym. Chem.* **2018**, 56, 1584).

Polymers

Disentangled ultrahigh molecular weight polyethylene: In a third aspect of sustainability, we have been able to prepare a polymer that is stronger than steel. It is a material called Disentangled Ultrahigh Molecular Weight Polyethylene (dUHMWPE). Heterogeneous Ziegler–Natta and homogeneous metallocene catalysts are known to produce ultrahigh molecular weight polyethylene (UHMWPE) in the entangled state. On the other hand, only (two) homogeneous single-site catalysts are reported to yield disentangled UHMWPE (dis-UHMWPE). This disparity between the two types of catalysts and the two states of polyethylene can be bridged if a heterogeneous single-site catalyst that can yield dis-UHMWPE is made accessible. Here, one-pot two-step synthesis of a MgCl2 supported [Ti(OEt)4] derived catalyst 1 with a two-stage activation strategy is reported to produce dis-UHMWPE (*Macromolecules* **2018**, 51, 4541).

Emission and Effluent Control Including Water and Soil Management

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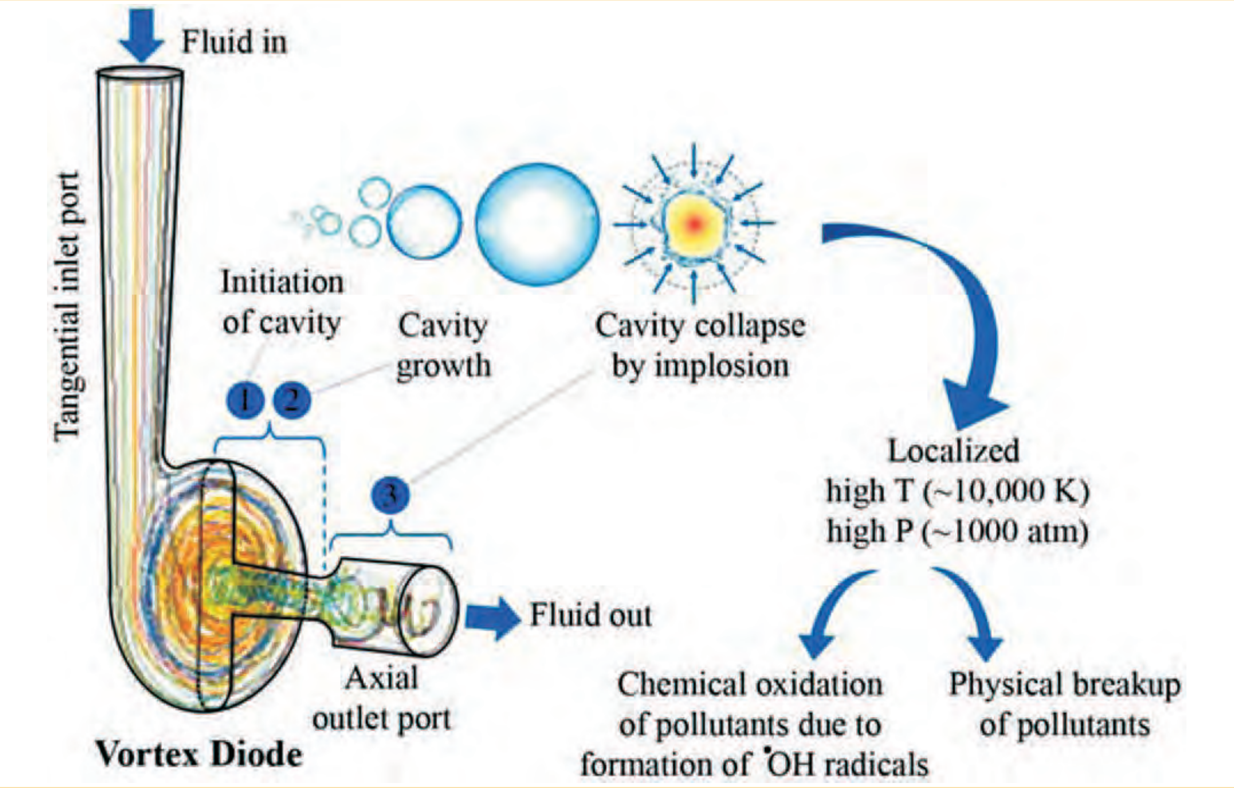
Desulfurization of transportation fuels and organics: A newer technology was developed in the form of hydrodynamic cavitation and newer materials for adsorption to offer an economically viable option to the existing desulfurization processes. The work describes the efficacy of the cavitation process and compares the cavitation yield for two types of cavitation devices-one employing linear flow for the generation of cavities and other employing vortex flow. The process essentially exploits in situ generation of oxidising agents such as hydroxyl radicals for oxidative removal of sulfur. The efficiency of the process is strongly dependent on the nature of device apart from the nature of the organic phase. A very high removal to the extent of 95% was demonstrated. The results were also verified using commercial diesel. The cavitation yield is significantly higher for vortex diode compared to the orifice. The process has potential to provide a green approach for desulfurization of fuels or organics without using any catalyst or external chemicals/reagents apart from newer engineering configurations for effective implementation of hydrodynamic cavitation in industrial practice (*Fuel* **2017**, *210*, 482).

Industrial wastewater treatment

Hydrodynamic cavitation technology was developed using vortex diode for the removal of refractory pollutants. The technology is effective in the treatment of dye wastewaters for removal of variety of dyes, fertilizer industrial wastewaters and has immense potential for other wastewater treatment applications including disinfection. It can also be combined with other conventional processes such as anaerobic biological treatment for increased energy recovery, especially useful for Distillery Industry (*Environ. Prog. Sustain.* **2018**, *37*, 295).



Postulated mechanism of hydrodynamic cavitation in vortex diode

Water Treatment, Disinfection and Purification

Meitram Niraj Luwang mn.luwang@ncl.res.in

Detection of Arsenic in water: This work reports on the novel technique of detection of arsenic in aqueous solution utilizing the luminescence properties of lanthanide doped nanomaterials. Eu3þ (5%) doped YPO4 nanorods were utilized for the said experiment. Co-precipitation method was used fo the synthesis of the materials and characterized them with different instrumental techniques like X-ray diffraction (XRD), Infra-red(IR), UV-absorption, scanning electron microscope (SEM), transmission electron microscope (TEM), X-ray photo electron spectroscopy (XPS) and photo luminescence studies. This nanoparticle can adsorb both arsenic and arsenious acids. We studied the effect of arsenic adsorption on the luminescence behavior of the nanoparticles. Arsenic acid enhanced the luminescence intensity where as arsenious acid quenched the luminescence. This luminescence enhancement or quenching is related with arsenic concentration. This relation of luminescence property with concentration of arsenic can be used to detect arsenic in industrial waste (Patent: US 2017/0241970A1)

Natural Products and Methodology

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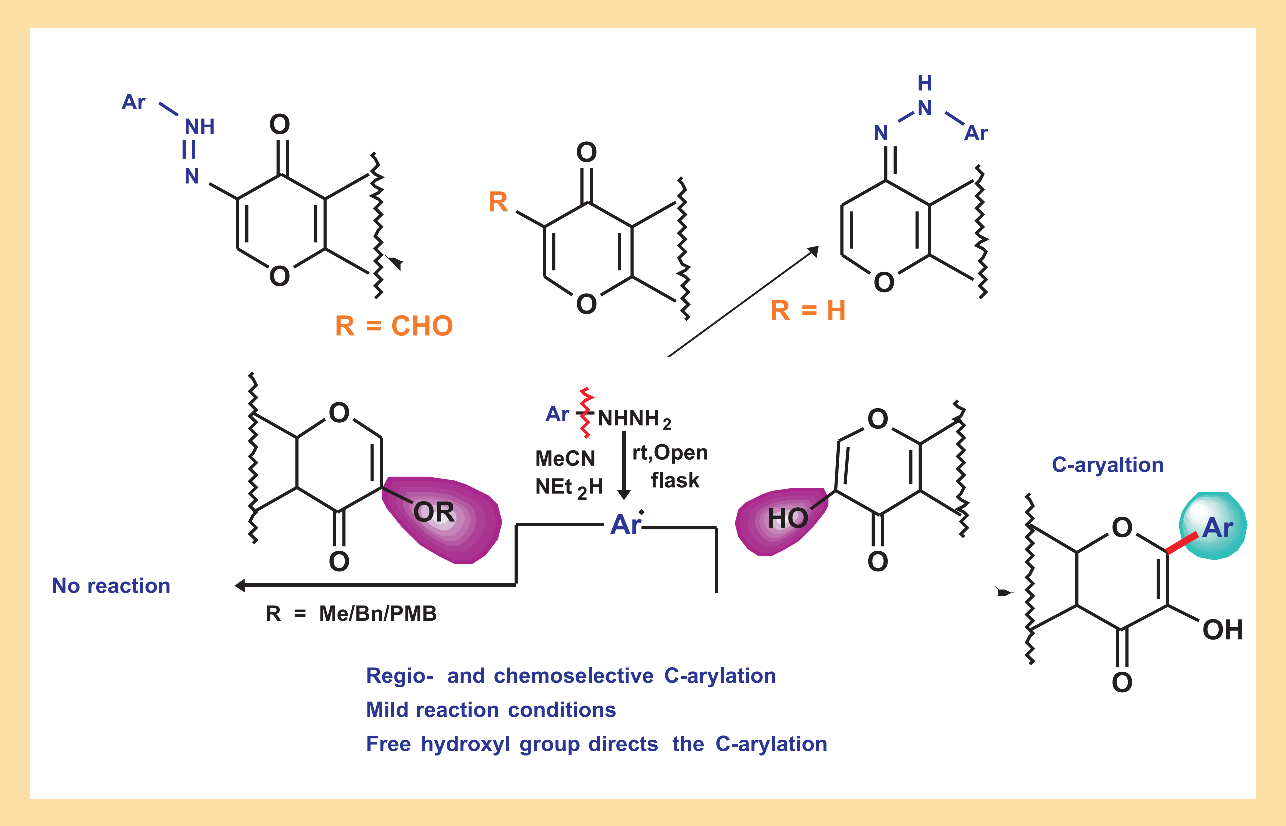
Hydroxyl directed C-arylation: Synthesis of 3 hydroxy flavones and 2-phenyl-3-hydroxy pyran-4-one sunder transition-metal free conditions: Hydroxyl assisted, efficient, transition-metal free and direct C-arylation of 3-hydroxychromone and 5-hydroxy pyran-4-one moieties in presence of base, air as oxidant and arylhydrazines as arylating agent to furnish highly biologically active 3-hydroxyflavones and 2-phenyl-3-hydroxy pyran-4-ones was developed (*Org. Biomol. Chem.* **2018**, *16*, 444).



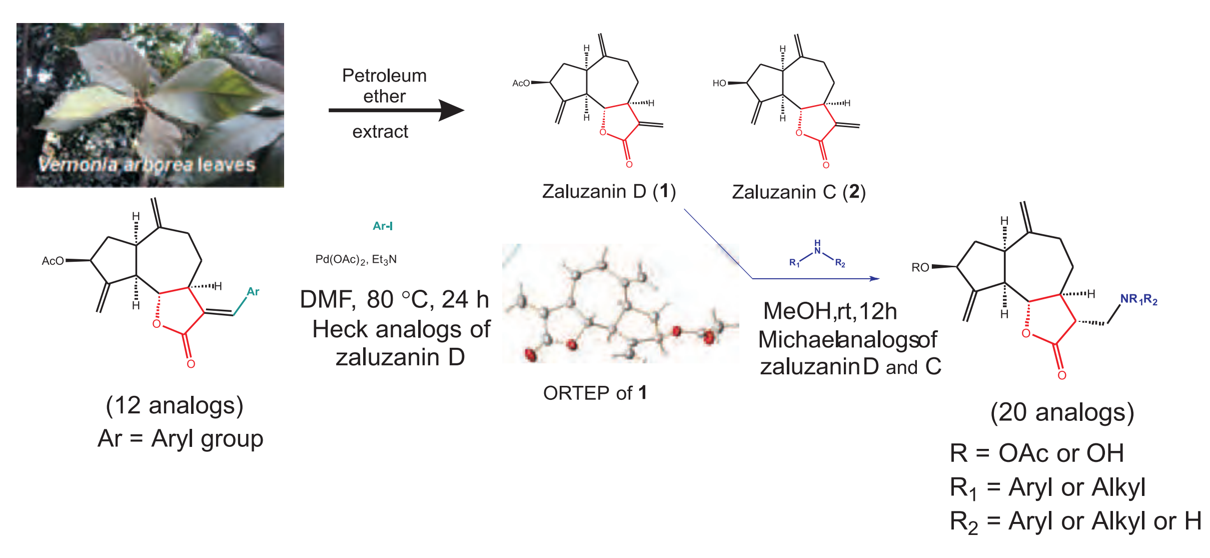
Regio- and chemoselective C-arylation

Mild reaction conditions

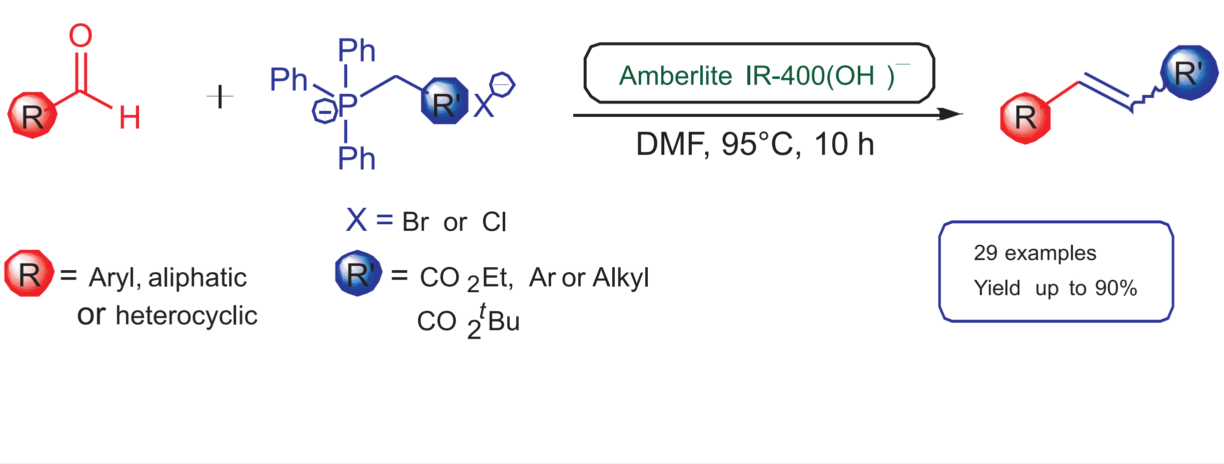
Free hydroxyl group directs the C-arylation

Synthesis and anticancer studies of Michael adducts and Heck arylation products of sesquiterpene lactones, zaluzanin D and zaluzanin C from *Vernonia arborea:* Sesquiterpene lactones containing α-methylene--lactones, zaluzanin D 1 and zaluzanin C 2 were isolated from the leaves of *Vernonia arborea*. Several diverse Michael adducts and Heck arylation analogs of zaluzanin D have been synthesized by reacting with various amines and aryl iodides, respectively and were assayed for their *in vitro* anticancer activities against human breast cancer cell lines MCF7 and MDA-MB-231. Among all the synthesized analogs, two Michael adducts showed better anticancer activities as compared to zaluzanin D. However, among the synthesized compounds, only one compound has minimal cytotoxic effect on normal breast epithelial MCF10A cells. Our detailed mechanistic studies reveal that the two compounds execute their anti proliferative activity through induction of apoptosis and thereby inhibit the cancer cells proliferation and one of the compound could be a lead compound for designing potential anti-cancer compound (*RSC Adv.* **2018**, *8*, 38289).

Natural Products and Methodology



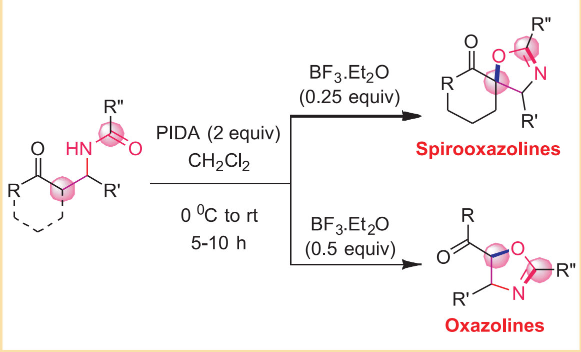
Efficient synthesis of functionalized olefins by Wittig reaction using Amberlite resin as a mild base: A convenient procedure for the synthesis of olefins by the reaction of stabilized, semi-stabilized, and non-stabilized phosphorous ylides with various aldehydes or ketone employing Amberlite resin as a mild base is described. Our developed method offers facile and racemization free synthesis of α β-unsaturated amino esters and chiral allylic amine. The developed methodology offers mild reaction conditions, high efficiency and facile isolation of the final products, a practical alternative to known procedures (*Synth. Commun.* **2017**, 47, 581).



Natural Products and Methodology

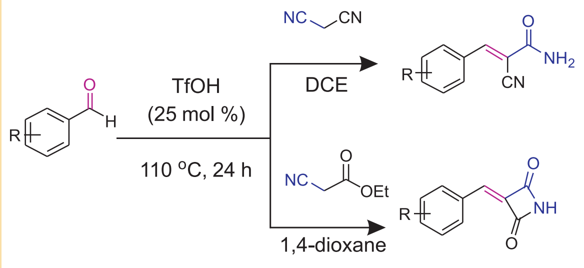
Gurunath Suryavanshi gm.suryavanshi@ncl.res.in

Metal-free annulation of β-acylamino ketones: Facile access to spirooxazo-lines and oxazolines via oxidative C–O bond formation: A metal-free annulation reaction of β-acylamino ketone derivatives has been reported for the synthesis of a group of functionalized spirooxazolines and oxazolines in good to excellent yields under mild reaction conditions, broad substrate scope, simple execution and synthetic potential of the products make this novel protocol very attractive (*Org. Chem. Front.* **2018**, *5*, 544).

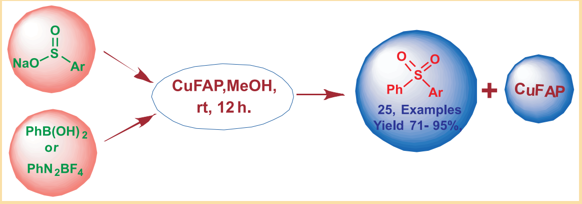


Metal-free hypervalent iodine/TEMPO mediated oxidation of amines and mechanistic insight into the reaction pathways: A highly efficient, metal free rapid protocol studied mechanistically for the oxidation of primary and secondary amines to corresponding carbonyl compounds using $PhI(OAc)_2$ and catalytic TEMPO to provides divers products in excellent yields (*RSC Adv.* **2018**, *8*, 32055).

Triflic acid-catalyzed metal-free synthesis of (E)-2-cyanoacrylamides and 3-substituted azetidine-2,4-diones: A TfOH- catalysed highly efficient synthesis of biologically active (E)-2-cyanoacrylamides and 3-substituted azetidine-2,4-diones has been reported with good yields under metal-free conditions. The attractive features of this tandem process are moderate reaction conditions, high atom economy, broad substrate scope, gram-scale reaction and ease of operation (*New J. Chem.* **2018**, *42*, 6433).

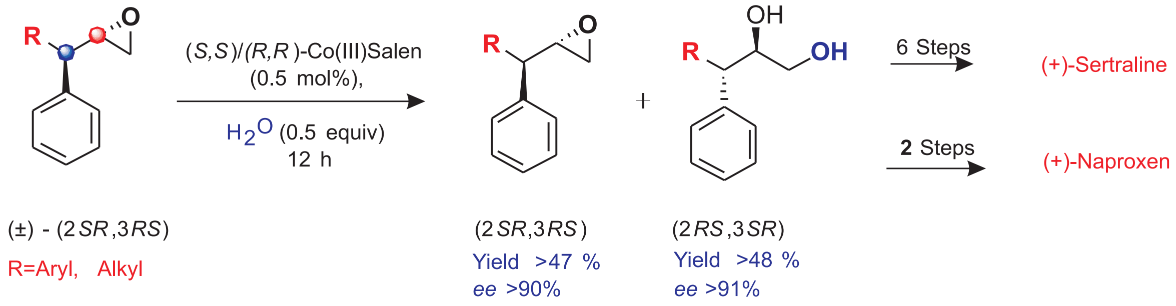


An efficient heterogeneous Copper Fluorapatite (Cu-FAP) catalysed oxidative synthesis of diaryl sulfone under mild ligand-and base free conditions: A simple, eco-friendly and efficient method for the synthesis of unsymmetrical diaryl sulfones using heterogeneous copper fluorapatite (Cu FAP) catalysed coupling of aryl sulfonic acid and phenyl boronic acid has been developed in good to excellent yield without use of any ligand, base or co-catalyst (*New J. Chem.* **2018**, Doi.org/10.1039/C8NJ04845B).

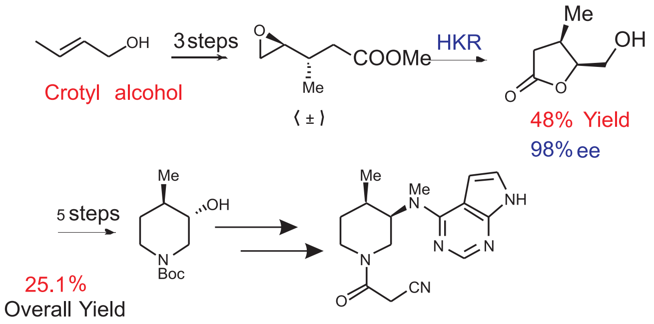


Enantioselective synthesis of (+)-sertraline and (+)-naproxen: The Co(III)(salen)OAc catalyzed two stereocentered HKR of anti-β, β'-diphenylmethyloxirane and anti-3-phenylethyloxiranes affords corresponding anti-1,2-diols and oxiranes in highenantiomeric excess. The synthetic methodology has been used for enantioselective synthesis of (+)-sertraline and (+)-naproxen an anti-inflammatory drug (*New J. Chem.*, **2018**, 42, 10414).

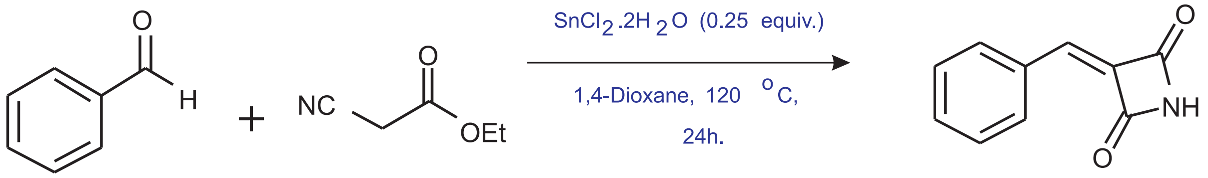
Natural Products and Methodology



Synthesis of key intermediate for (+)-tofacitinib through CoIII (salen)-catalyzed two stereocentered hydrolytic kinetic resolution of (±)-methyl-3-(oxiran-2-yl) butanoate: An enantiopure piperidine, a key intermediate for the synthesis of (+)-tofacitinib has been achieved in high optical purity (98% ee) from readily available crotyl alcohol. The key steps involved is a CoIII(salen)-OAc-catalyzed two stereo centered hydrolytic kinetic resolution of (±)-methyl-3-(oxiran-2-yl) butanoate (*Syn. Comm.* **2018**, *48*, 1045).



An efficient Sn(II)-catalyzed one-pot synthesis of a 3-substituted azetidine-2,4-dione framework: A novel Sn(II)-catalyzed tandem cyclization reaction of aromatic aldehydes with ethyl cyanoacetate has been achieved to afford a series of 3-substituted azetidine-2,4-diones in good to excellent yields (*Org. Biomol. Chem.* **2017**, 15, 2385).



Natural Products and Methodology

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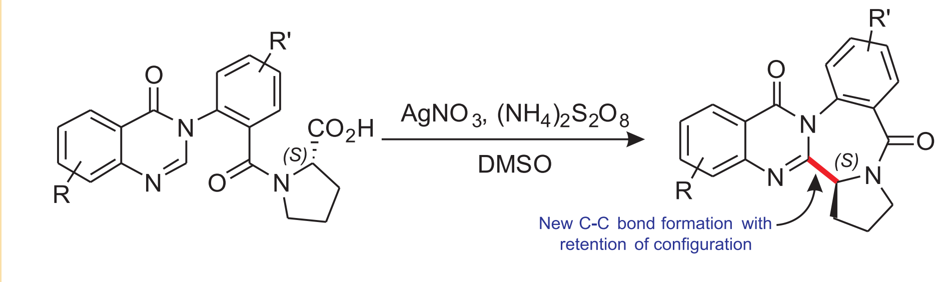
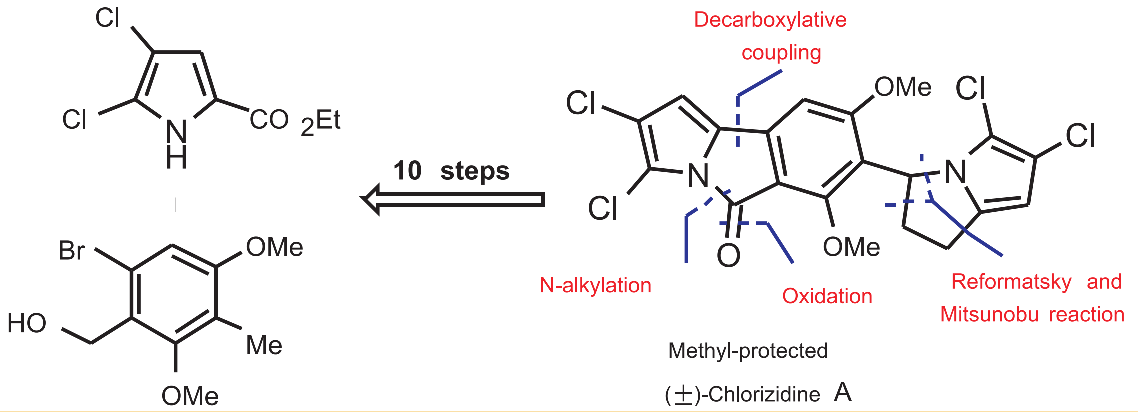
Silver-mediated oxidative decarboxylative intramolecular asymmetric radical cyclization (Csp^3)–Csp^2) via memory of chirality: Access to circumdatin alkaloids



Circumdatin alkaloids

- Memory of chirality
- Retention of configuration
- High er
- Inexpensive catalyst
- Ligand and base free
- Mild reaction conditions
- Applied to natural products

A novel silver-mediated oxidative decarboxylative intramolecular asymmetric radical cyclization has been developed to form a (Csp^3–Csp^2) bond via memory of chirality. The application of the process has been demonstrated for the synthesis of the circumdatin class of alkaloids in high enantiopurity with retention of the configuration. The developed protocol is mild and works with an inexpensive silver catalyst in the absence of ligand, base or additives. The involvement of a monoradical in the reaction has been established by trapping the radical intermediate (*Org. Lett.* **2018**, *20*, 2092).

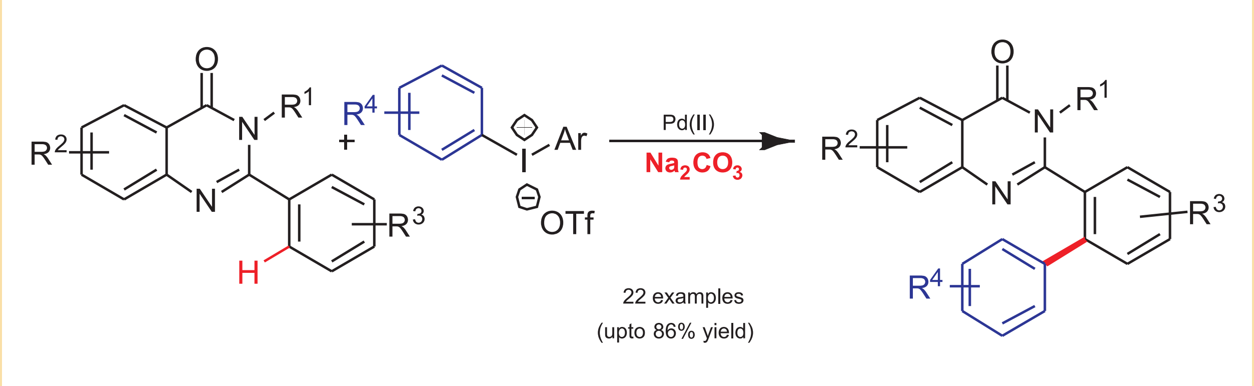


Methyl-protected (±)-Chlorizidine A

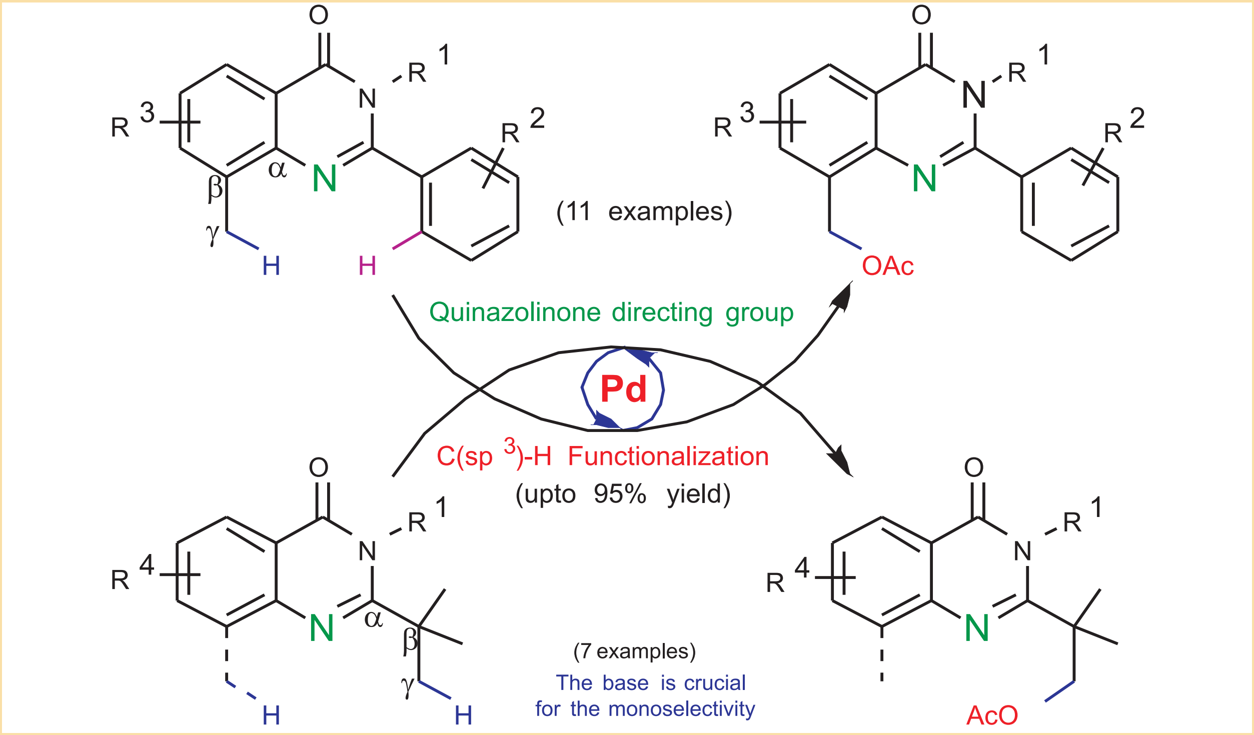
Synthesis of methyl-protected (±)-Chlorizidine A: The first total synthesis of the methyl-protected (±)-Chlorizidine A has been achieved in ten steps. Pd-catalyzed decarboxylative coupling and late-stage oxidation were utilized to construct 5H-pyrrolo [2, 1-a] isoindol-5-one scaffold. Samarium (II) iodide mediated Reformatsky reaction, and intramolecular Mitsunobu reactions were efficiently applied for the synthesis of 2, 3-dihydropyrrolizine ring system. Chlorizidine A is highly prone to degradation, hence methyl-protected (±)-Chlorizidine A was prepared (*Org. Lett.* **2017**, *19*, 2774).

Natural Products and Methodology

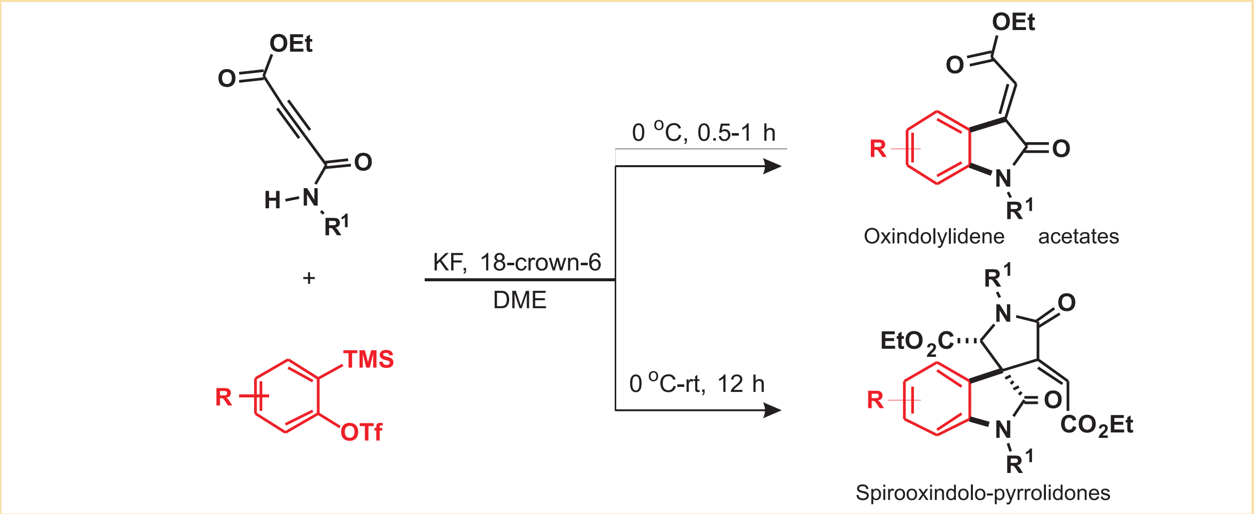
Pd-catalyzed regioselective monoarylation: Quinazolinone as the inherent directing group for C-(sp^2)–H activation: The Pd-catalyzed quinazolinone-directed regioselective mono-arylation of aromatic rings by C-H bond activation is developed. A broad substrate scope is demonstrated for both quinazolinone as well as diaryliodonium triflates. Use of base was found to be crucial for this transformation, unlike the known nitrogen-directed arylations. All the novel quinazolinones of biological interest were synthesized by using operationally simple Pd(II)-catalyzed arylation reaction (*J. Org. Chem.* **2017**, 82, 6366).



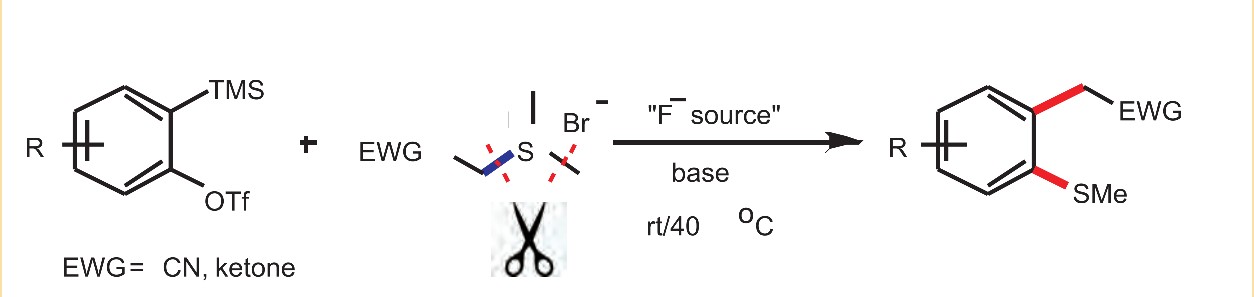
Diversification of quinazolinones by Pd-catalyzed C-(sp^3) acetoxylation: The quinazolinone ring has been exploited as a directing group for C(sp^3)-H functionalization for the first time. The proximal C-(sp^3)-H



bonds have been oxidized by palladium-catalyzed acetoxylation reaction. Various functional groups on the quinazolinone scaffold were tolerated to provide novel quinazolinone derivatives. The use of base was found to be crucial for the monoselective acetoxylations (*J. Org. Chem.* **2017**, *82*, 10470).



Divergent synthesis of oxindolylidene acetates and spirooxindolo-pyrrolidones from arynes: A novel process for the preparation of various (E)-oxindolylidene acetates using arynes and carbamoylpropiolates has been developed. The utility of this protocol is also further extended to the one-potsynthesis of complex spirooxindolo-pyrrolidones. This method provides a milder and transition-metal-free access to both the target scaffolds in moderate to good yields (*Org. Lett.* **2018**, *20*, 1483).



Application of sulfur ylides in 1,2-difunctionalization of arynes via insertion into C–S σ-bond: A novel reactivity of sulfur ylides has been demonstrated in a transition-metal-free protocol to access ortho-substituted thioanisole derivatives by insertion of arynes into C–S σ-bond in moderate to good yields. The reaction involves the formation of C–C and C–S bonds and consecutive breaking of two C–S bonds in an operationally mild reaction condition (*Org. Lett.* **2018**, *20*, 848).

Natural Products and Methodology

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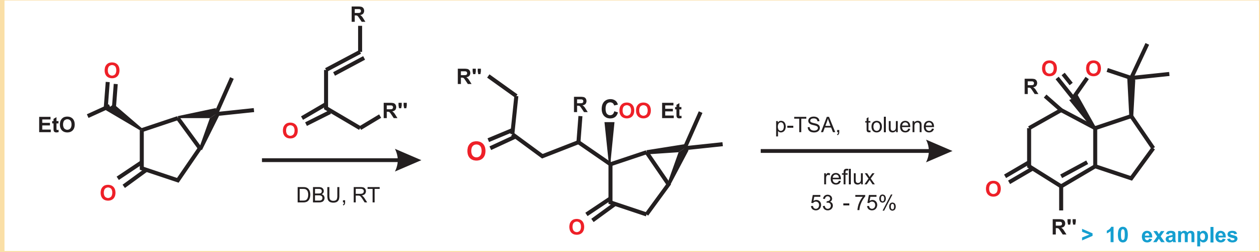
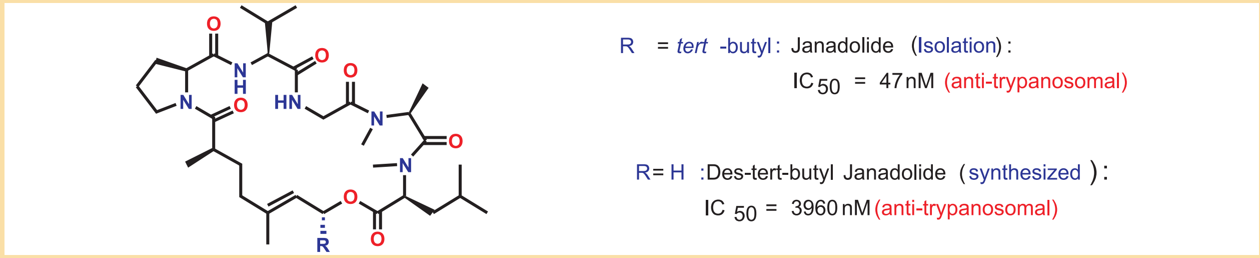
Synthesis of fused tricyclic γ-Butyrolactones, a privileged natural product-like scaffold: Greater than 10% of structurally elucidated natural products bear a γ-butyrolactone core and it is also a common structural constituent of several organic compounds. Monocyclic γ-butyrolactones having mono-, di-, and trisubstitution are well-known in the literature. More complex scaffolds, such as bicyclic and tricyclic ring systems, have also been reported. They exhibit a broad spectrum of biological activities, which includes anti-biotic, anti-helmintic, anti-fungal, anti-tumor, anti-viral, anti-inflammatory, and cytostatic properties. Owing to the diverse biological activities, γ-butyrolactones happen to be interesting lead structures for drug development. In this work, we have described serendipitous findings of an acid mediated skeletal rearrangement of bicyclo-β-ketoester having cyclopropyl ring to access fused tricyclic γ-butyrolactones. This novel transformation has been optimized to 30 mol% *p*-toluenesulfonic acid (*p*-TSA) in toluene using Dean–Stark apparatus, where one pot occurrence of aldol condensation, cyclopropyl ring opening followed by cyclization are the key highlight. The resulting tricyclic compounds thus obtained are interesting chemotype with natural product resemblance and may find useful applications in the future (*J. Org. Chem.* **2017**, *82*, 7614).



Efforts to access potent anti-trypanosomal marine natural product janadolide: Synthesis of des-tert-butyl janadolide and its biological evaluation: Parasitic infectious diseases such as trypanosomiasis and leishmaniasis are a threat to human and animal health, mainly in tropical and subtropical regions. Trypanosomiasis (sleeping sickness), a neglected infectious disease, is caused by protozoan parasite *Trypanosomabrucei*. Though several presentline treatment options are available, none of them are ideal as they often lead to undesired and deadly side effects. Besides, gradual emergence of drug resistance is also a problem to be considered of. In this context, to identify novel anti-trypanosomal agents based on Janadolide, a potent macrocyclic polyketide–peptide hybrid, a macrolactonization strategy was explored. However, our attempts on cyclization in the vicinity of the *tert*-butyl group were unsuccessful, we were able to synthesize des-*tert*-butyl Janadolide and evaluated its anti-trypanosomal activity. Besides, we also demonstrated that the *tert*-butyl group is vital for exhibiting potent anti-trypanosomal activity (*ACS Omega* **2018**, *3*, 2383).



Natural Products and Methodology

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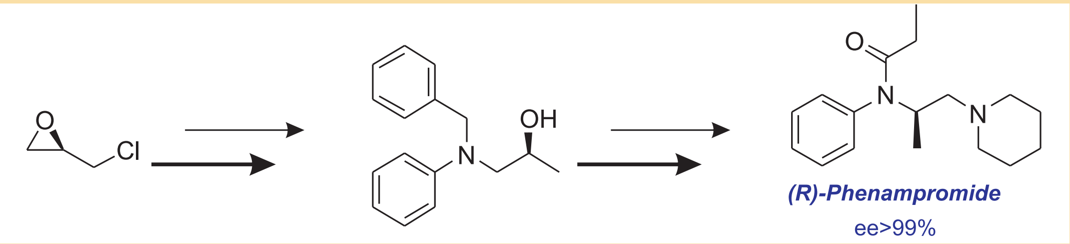
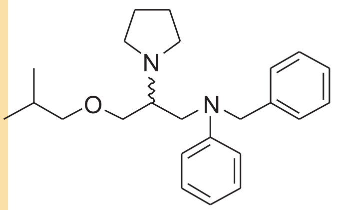
An efficient synthesis of the opioid analgesic (*R*)-phenampromide via an aziridinium ion: Phenampromide is an opioid analgesic, which is considered to be structurally similar to isomethadone. Phenampromide belongs to ampromide family of drugs, which also includes propiram and diampromide. According to the literature, (*R*)-phenampromide has greater analgesic potency than its (*S*)-enantiomer. Studies also revealed that based on the structure of phenampromide, U50,488, a highly selective kappa opioid agonist was discovered. Few reports are currently available for the synthesis of the (*R*)-enantiomer of phenampromide, which mainly involve resolution processes. We have developed an efficient new route for the synthesis of (*R*)-phenampromide via aziridinium ring formation as the key step using simple commercially available starting materials. The final product has been obtained with >99% enantiopurity (*Tetrahedron Asymmetr.* **2017**, *28*, 983).



Asymmetric synthesis of biologically important compounds: Asymmetric syntheses of optically pure compounds are gaining great momentum in recent years mainly because of the increase in number of chiral, non-racemic organic materials in the market place. In particular, the importance of enantiopure drugs are being widely recognized as it is demonstrated that only one enantiomer of the racemic drug is often responsible for the drug activity and the other form is either inactive or may cause unwanted side effects.

Enantioselective synthesis of both enantiomers of the calcium channel blocker bepridil: Calcium channel blockers are an important group of drugs and they have prevalent use in treating hypertension, heart failure, cardiac arrhythmias, *etc*. Bepridil (Trade name: Vascor®) is a long acting calcium-blocking agent with significant antianginal activity. It has antihypertensive and selective anti-arrhythmia activities and acts as a calmodulin antagonist. Although it contains one stereogen iccentre, it is generally administered as a racemate. However, pharmacological studies reveal that there are significant variation in activity amongst bepridil enantiomers and (*R*)-enantiomer of bepridil is more active than (*S*)-enantiomer. In recent years, it has been recognized that bepridil could be important in new therapeutic areas such as alzheimer's, antiviral, atrial fibrillation and in certain neurological disorders. Very recently, bepridil has been identified as a potential lead molecule against Ebola virus disease (EBOV) by inhibiting a late stage of viral entry. Presumably, bepridil being an approved drug, repurposing of this may rapidly move to human testing and have a potential to become a frontline against Ebola virus infection. By understanding the significance of bepridil in many new therapeutic indications, we developed a short and efficient method for the enantioselective preparation of both the enantiomers of bepridil for the first time in an overall yield about 18% and ee>98% (*New J. Chem.* **2017**, *41*, 824).



New therapeutic indications

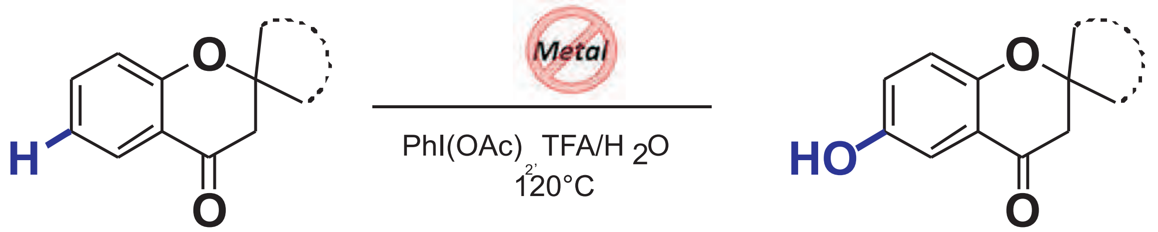
Alzheimer's (AD)
Neurological disorders
anti Ebola virus (EBOV)

Bepridil (Vascor^{TM})
Calcium channel blocker

Potency
R-isomer > *S*-isomer

Natural Products and Methodology

Development of synthetic methodologies: Transition metal free regio-selective C-H hydroxylation of chromanones towards the synthesis of hydroxyl-chromanones using PhI(OAc)$_2$ as oxidant: Chromones are privileged structural motifs; they are ubiquitous in plethora of natural products and pharmaceutically important compounds. They display exceedingly diverse range of biological activities such as antitumor, antioxidant, antibacterial, and anti-inflammatory properties. Incorporation of hydroxyl functionality into a chromone moiety (either natural or synthetically) often compliment with better activity profile than the parent molecules. Therefore, the regio and chemo selective introduction of hydroxyl into chromone framework especially chromanones and related complex molecules received considerable attention. However, late stage and selective introduction of hydroxyl into C-6 position of chromanones is unknown in the literature. Importantly, many chromanone molecules possessing C-6 oxygenation pattern are found to be biologically significant. We developed a novel, regioselective, transition metal free protocol for C-6 hydroxylation of chromanones. Using this late stage functionalization method, we synthesized diverse range of 6-hydroxy chromanones in good yields. This protocol can be easily utilized for the synthesis of those biologically relevant molecules (*Chem. Comm.* **2018**, *54*, 2252).



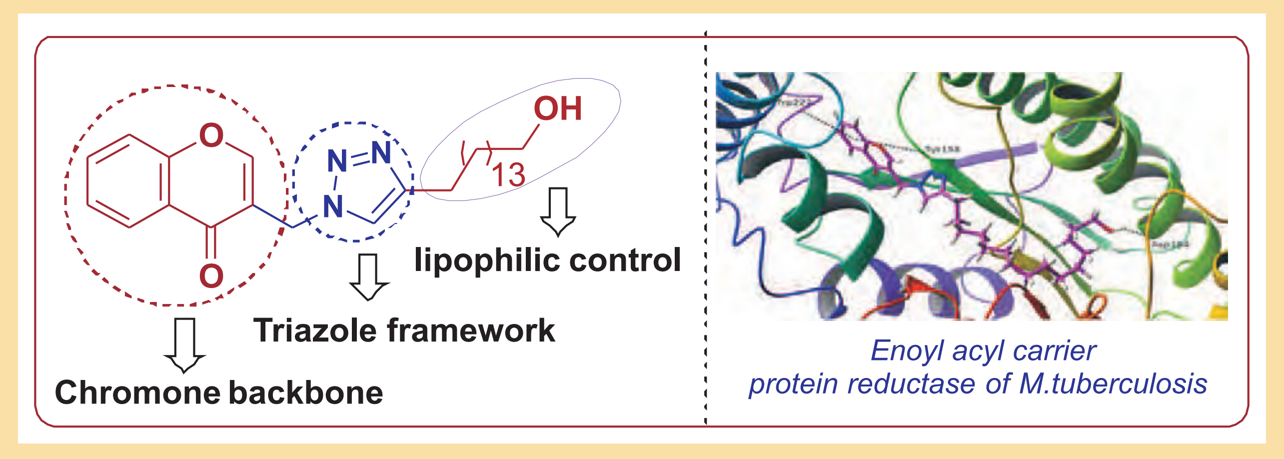
Transition metal free approach

Highly para selective hydroxylation

18 examples, yield upto 78%

Identification of potent chromone embedded [1,2,3]-triazoles as novel antitubercular agents: Natural products have a rich history as lead compounds for drug discovery. Further, natural products have contributed significantly to the current portfolio of anti TB drugs, with one first-line drug (rifampicin) and several second-line agents (kanamycin, viomycin etc) being either natural products themselves or being derived from a natural product lead. Chromone frameworks are frequently found in a diverse array of natural products, that includes natural flavone /isoflavone products, therapeutically active drugs such as anti-inflammatory, anti- platelet, anti-microbial, anti-obesity, anti-cancer agents, drug candidates for neurodegenerative diseases and adenosine receptors. We synthesized, a series of novel chromone embeded [1,2,3]-triazole derivatives via an easy and convenient synthetic protocol starting from 2-hydroxy acetophenone. The novel 20 analogues accomplished in four step synthetic sequences utilizing click chemistry in the key step and were fully characterized by their NMR and mass spectral data. The *in vitro* antimycobacterial evaluation study of all the compounds revealed seven compounds found to be active against *M.tuberculosis*

H37Rv. The compound 6s is the most potent compound in vitro with a MIC value of 1.56 μg mL-1.Cross docking studies revealed compound 6s to be more effective against the enoyl-acyl carrier protein reductase of Mtb. Molecular Docking and Chemoinformatics studies proved that compound 6s possesses drug-like properties (*Royal Soc. Open. Sci.* **2018**, *5*, 171750).



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Solid state auto inversion of C-centrochirality: Starting from dimethyl (*E*)-2-{[(1-*tert*-butoxycarbonyl)-1*H*-indol-3-yl]methylene}succinate and (*R*)-2,2,5,5-tetramethyl-1,3-dioxolane-4-carbaldehyde, facile synthesis of (−)-*epi*-claulansine D was accomplished via condensation and two intramolecular cyclizations. The (−)-*epi*-claulansine D in the solid state exists in a metastable form, and after an induction period of 30–90 days, it underwent complete epimerization to exclusively deliver the desired natural product (−)-claulansine D in quantitative yield. The witnessed inversion of C-centrochirality in the solid state is conceptually novel and takes place for relatively higher crystal stability reasons. Base-catalyzed ring expansion of both (±)/(−)-*epi*-claulansine D and (±)/(−)-claulansine D resulted in (±)/(+)-*epi*-claulansine C in very good yields (*J. Org. Chem.* **2018**, *83*, 382).

Total synthesis of (±)/(+)-subincanadine E and determination of absolute configuration: A facile synthesis of (±)-subincanadine E was described from tryptamine-based maleimide. 1,2-Addition of Grignard reagent to maleimide, internal activation of formed lactamol for in situ 1,4-addition of Grignard reagent, and associated position-specific allylic rearrangement in diastereoselective Pictet–Spengler cyclization were the key steps. Enantioselective first total synthesis of naturally occurring cytotoxic (+)-subincanadine E was also accomplished from (*S*)-acetoxysuccinimide via an unusual *syn*-addition of cuprate to the α,β-unsaturated lactam. *Sinister* absolute configuration was assigned to (+)-subincanadine E on the basis of total synthesis. (*S*)-Acetoxy group in the succinimide precursor was initially employed to impart regio- and stereoselectivity and then as a suitable leaving group to generate the desired conjugated lactam (*J. Org. Chem.* **2017**, *82*, 11126).

Natural Products and Methodology

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Lewis acid catalyzed cascade annulation of alkynols with a-ketoesters: A simple access for the synthesis of diverse unsaturated g-spiroketal-g-lactones was developed by employing $Bi(OTf)_3$ catalyzed cascade annulation of alkynols with a-ketoesters via dual (p and s) activation process for the first time. Highly sterically demanding products, ambient reaction conditions, cost-effective catalytic system, good yields, operational simplicity, atom and step-economies are salient features of this strategy. This developed synthetic methodology is useful in making biologically relevant natural and unnatural molecules (*Chem. Commun.* **2017**, *53*, 6641). ketoesters in a step and atom economic way.

Synthesis of furo [2,3-*b*] pyran-2-ones through Ag(I)- or Ag(I)–Au(I)-catalyzed cascade annulation of alkynols and α-ketoesters: The first catalytic protocol for the synthesis of furo[2,3-*b*]pyran-2-ones were reported using AgOTf or AgOTf and PPh_3PAuCl catalyzed cascade annulation of alkynols and a-diverse furo[2,3-*b*]pyran-2-ones were prepared and their synthetic utility is also well demonstrated. This cascade annulation strategy should find applications in the synthesis of biologically interesting natural products and also provides a platform for diversity-oriented synthesis in medicinal chemistry (*Org. Lett.* **2018**, *20*, 872).

Bismuth (III)- catalyzed cycloisomerization and (hetero) arylation of alkynois: The hydroalkoxylation (cycloisomerization) and hydro-(hetero)arylation cascade reaction of alkynols with (hetero)arenes mediated by main group element derived borderline metal catalyst $Bi(OTf)_3$ is identified. Diverse alkynols and electron rich arenes/ heteroarenes, which proceed cleanly under ambient reaction conditions and furnished a series of novel 2-(hetero)aryl tetrahydrofurans and tetrahydropyrans in good to excellent yields in an atom and step economic way. A further expansion of this work in building libraries related to pharmacologically active molecules and their biochemical evaluation is in progress (*Org. Biomol. Chem.* **2018**, *16*, 3229).

Screening methods and bioassays

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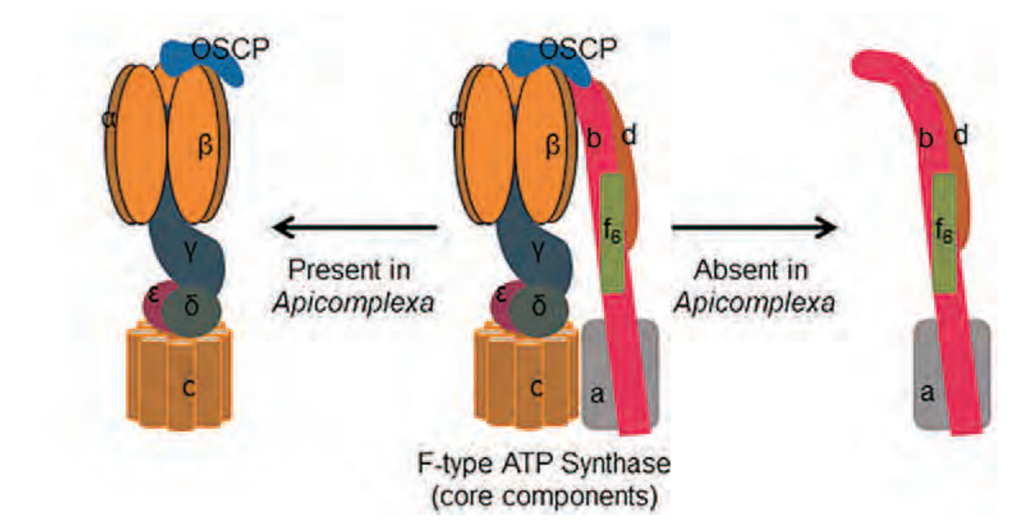
Highly diverged novel subunit composition of apicomplexan F-type ATP synthase identified from *Toxoplasma gondii*: The mitochondrial F-type ATP synthase, a multi-subunit nanomotor, is critical for maintaining cellular ATP levels. In *Toxoplasma gondii* and other apicomplexan parasites, many subunit components of this enzyme are missing. Here, we reported the identification of 20 novel subunits of *T. gondii* F-type ATP synthase from partially purified monomer (~600 kDa) and dimer (>1 MDa) forms of the enzyme. Discovery of these highly diversified novel components of parasite ATP synthase will facilitate the development of novel anti-parasitic agents (*PLoS Biol.* **2018**, *16, e2006128*).

Evaluating antimalarial efficacy by tracking glycolysis in *Plasmodium falciparum* using NMR spectroscopy: Glucose is an essential nutrient for *Plasmodium falciparum* and robust glycolytic activity is indicative of viable parasites. Using NMR spectroscopy, we have developed a method for real time analysis of the kinetics of glycolytic activity in live *P. falciparum* infected erythrocytes. Using this method we demonstrate the differential inhibitory effect of potent and mechanistically distinct antimalarial compounds on different developmental forms of blood stage malaria parasites. Our findings indicate that ring

Screening Methods and Bioassays



stage parasites are inherently more tolerant to antimalarial inhibitors, a feature which may facilitate emergence of drug resistance (*Sci. Rep.* **2018**, *8*, *18076*).

Chemical Biology

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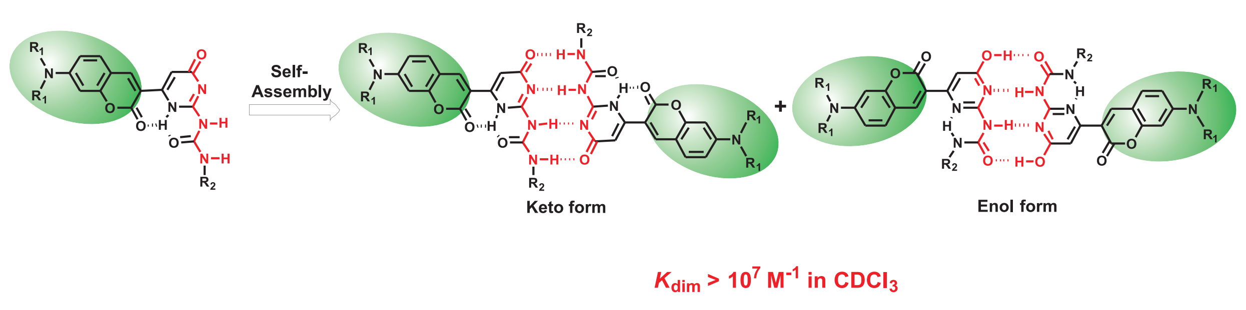
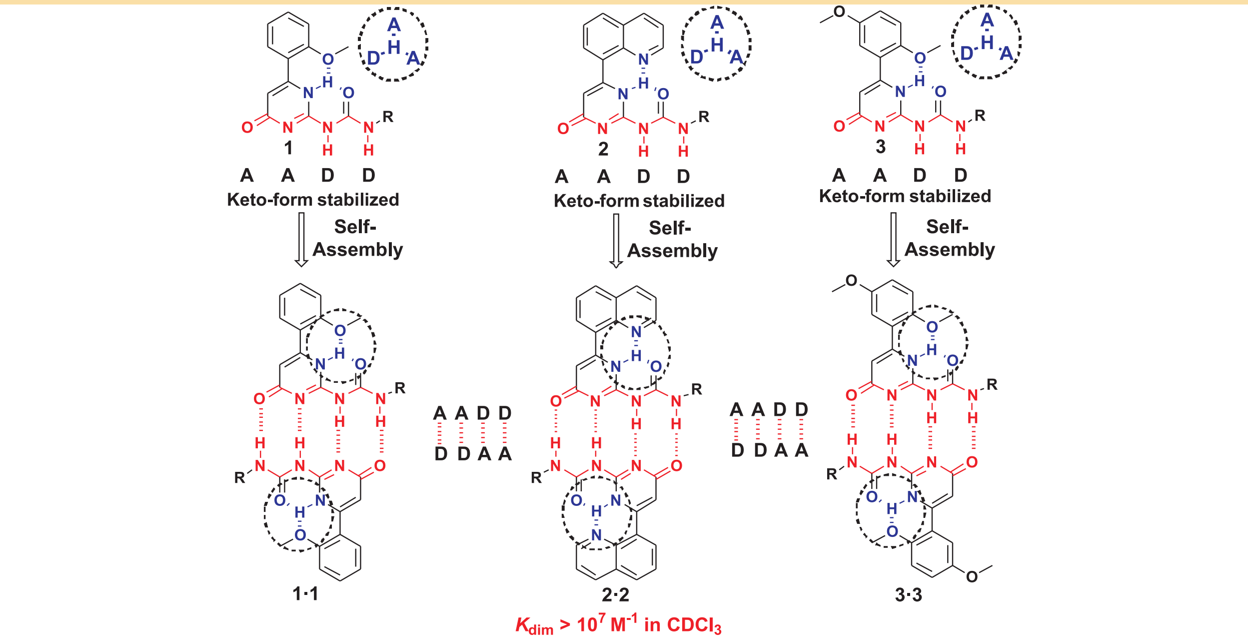
Highly stable self-complementary quadruple hydrogen systems with a built-in fluorophore: Coumarin-conjugated self-assembling system adorned with valuable features such as high duplex stability and a built-in fluorophore has been developed. This system forms a highly stable molecular duplex (Kdim > 1.9 × 10^7 M^{-1} in $CDCl_3$). Due to the fluorescent property of coumarin, these new structural motifs may find potential application in supramolecular chemistry (*J. Org. Chem.*, **2017**, 82, 6403).



Chemical Biology

De novo designed prototropy-free highly stable self-assembling systems: Prototropy limits the application scope of AADD-type self-assembling systems in material and biomedical science. An effective approach for addressing the prototropy-related problems in AADD-type self-assembling systems by freezing their H-bonding codes has been reported. This rational approach may find applications in supramolecular science, wherein proton shift-mediated structural changes become a detrimental factor (*Chem. Commun.* **2017**, 53, 2689; *Chem. Eur. J.* **2017**, 23, 783).



Modified ureidopyrimidinone-based duplexes, insensitive to prototropy (This work). Note: Prototropy issue arrested using intramolecular bifurcated H-bonding

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Two-dimensional infrared spectroscopy reveals cosolvent-composition-dependent crossover in intermolecular hydrogen-bond dynamics: Cosolvents have versatile composition-dependent applications in chemistry and biology. The simultaneous presence of hydrophobic and hydrophilic groups in dimethyl sulfoxide (DMSO) when combined with the unique properties of water, plays key roles in the diverse fields of pharmacology, cryoprotection, and cell biology. Moreover, molecules dissolved in aqueous DMSO exhibit an anomalous concentration-dependent nonmonotonic behavior in stability and activity near acritical DMSO mole fraction of 0.15. An experimental identification of the origin of this anomaly can lead to newer chemical and biological applications. We report a direct spectroscopic observation of the anomalous behavior using ultrafast two-dimensional infrared spectroscopy experiments. Our results demonstrate the cosolvent-concentration-dependent non-monotonicity arises from non-identical mechanisms in ultrafast hydrogen-bond-exchange dynamics of water above and below the critical cosolvent concentration. Comparison of experimental and theoretical results provides a molecular-level mechanistic understanding A distinct difference in the stabilization of the solute through dynamic solute–solvent interactions is the key to the anomalous behavior (*J. Phys. Chem. Lett.* ***2017***, *8*, *1604*).

Chemical Biology

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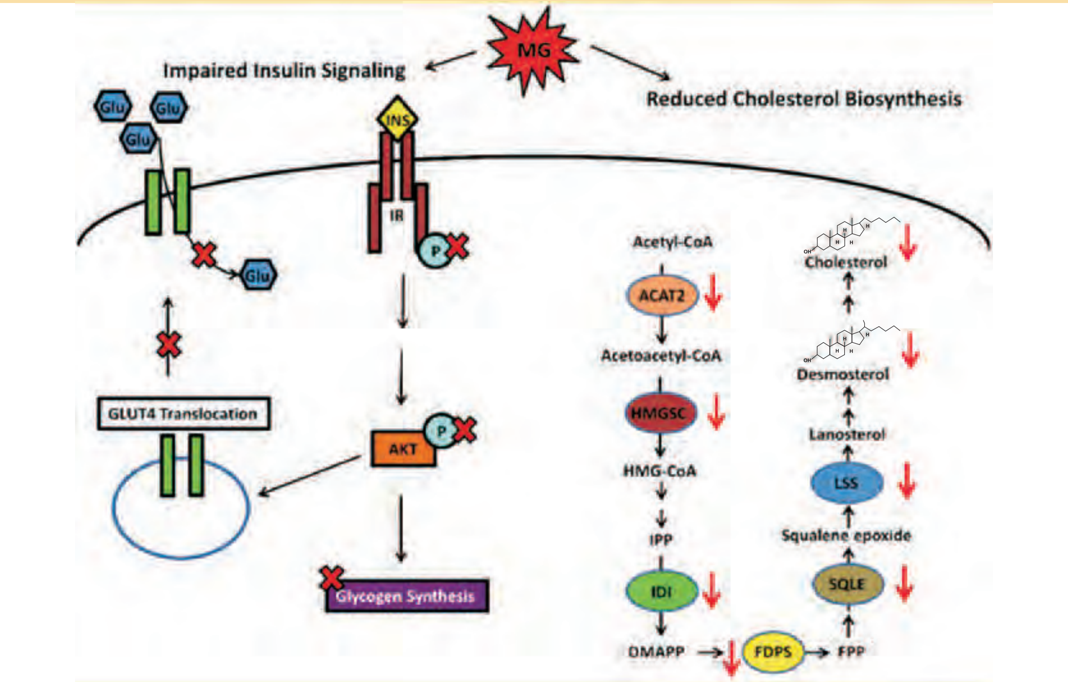
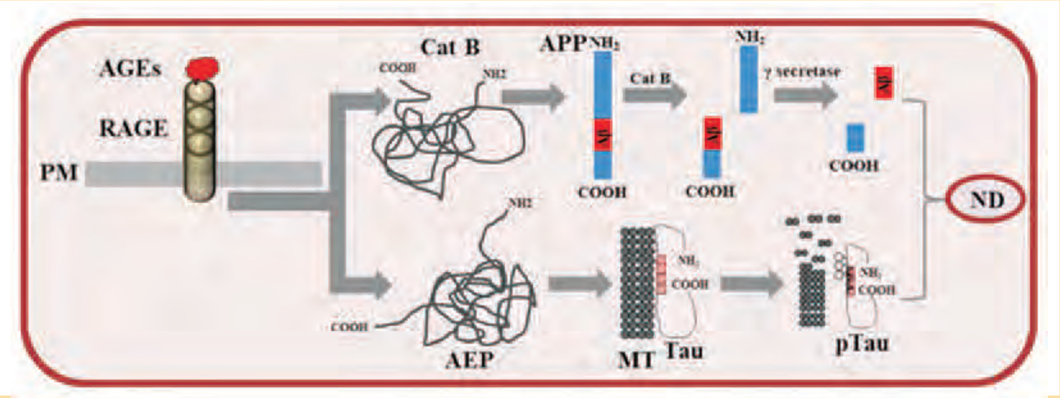
Methylglyoxal attenuates insulin signaling and downregulates the enzymes involved in cholesterol biosynthesis: Methylglyoxal (MG), a highly reactive dicarbonyl is implicated in the development of diabetic complications. In this investigation, we have observe that MG impairs insulin signaling, inhibits GLUT4 d translocation and reduces glucose uptake. Interestingly, aminoguanidine (AMG), a potent dicarbonyl scavenger, restored the deleterious effects of MG. For the first time, we report that MG induces down regulation of enzymes involved in cholesterol biosynthesis affecting cholesterol metabolism. Thus, MG leads to primary defects in insulin signaling and cellular abnormalities at the proteomic and metabolic levels. (*Mol. BioSyst.* **2017**, *13*, 2338).



Advanced glycation end products modulate amyloidogenic APP processing and Tau phosphor-ylation: Advanced glycation end products (AGEs) are implicated in the pathogenesis of Alzheimer's disease (AD).



Chemical Biology

In this study, the AGE-RAGE axis increased expression of cathepsin B and asparagine endopeptidase (AEP), which increased Aβ1–42 formation and tau phosphorylation, respectively. Elevated cathepsin B, AEP, RAGE, and pTau levels were found in human ADcoincident with enhanced AGEs. This study demonstrated that the AGE-RAGE axis regulates Aβ1–42 formation and tau phosphorylation via increased cathepsin B and AEP, providing a new molecular link between AGEs and AD pathology (*ACS Chem. Neurosci.* **2018**, **9**, 988).

Identification of Lead Molecules

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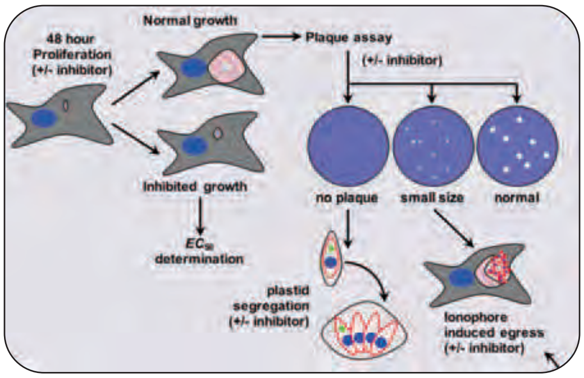
Targeted phenotypic screening in *Plasmodium falciparum* and *Toxoplasma gondii* identifies novel lead molecules: Widespread resistance to current drugs and the lack of a commercial vaccine necessitate novel pharmacological interventions with distinct modes of action against malaria and toxoplasmosis. The Malaria Box collection contains novel chemicals with proven anti-parasitic activities. Using targeted phenotypic assays on the Malaria Box molecules, we have identified potent inhibitors of plastid segregation and egress in both *Plasmo-dium. falciparum and Toxoplasma gondii*. This work has identified novel molecules with defined modes of action in multiple parasites and provided leads for new drugs (*mSphere* ***2018**, 3, pii:e00534-17*).



Synthesis of API

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TB drug with improved stability: The study claims a new cocrystal of fixed dose combination (FDC) of TB drug found to solve the problems of instability for 4FDC by applying Crystal Engineering principles. The improved stability of FDC cocrystal drug inhibits the cross-reaction reaction between Isoniazid (INH) and Rifampicin, thereby overcoming the formation of inactive by-products. The team showed that the pharmaceutically stable cocrystal of INH has improved stability of greater than 5 fold compared to the current 4FDC drugs. The conformer additives which stabilize the formulation are pharmaceutically accepted excipients. Stability studies were carried out under accelerated conditions of 40°C and 75% relative humidity (*J. Pharm. Sci.* **2018**, *107*, 1667).

Synthesis of API

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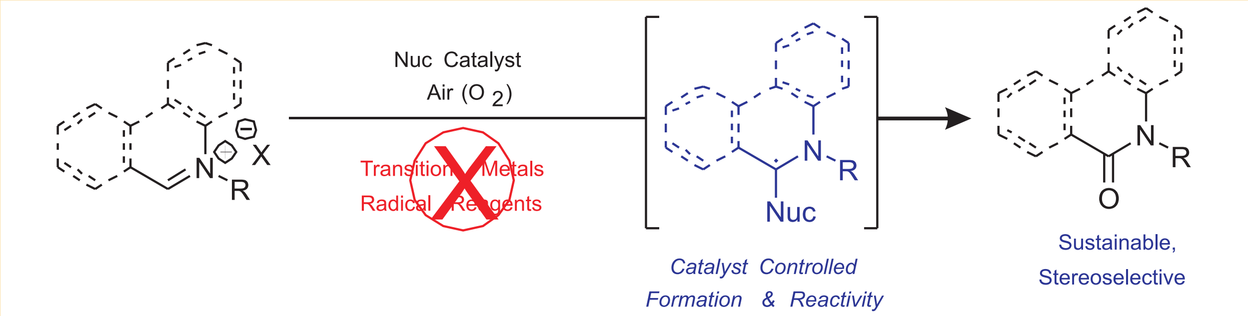
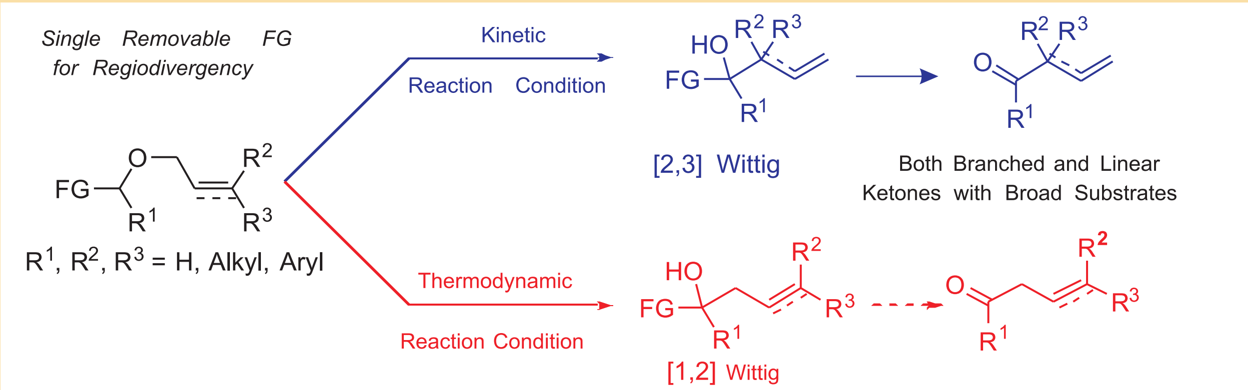
Organocatalyst bound α-aminoalkyl radical for controlled aerobic oxidation: A catalyst bound α-aminoalkyl radical intermediate from iminium is developed to control its formation and reactivity with aerobic oxygen. The catalyst influence was demonstrated, including the first catalyst controlled enantioselective aerobic oxidation. The proposed catalyst stabilization of radical intermediate was also exploited successfully for an alternative anionic auto oxidation of iminium to lactam and amide. This new avenue for catalyst bound α-radical holds the potential to be a general mode of radical (asymmetric) functionalization of polar sp^2 C-H bonds (*Org. Biomol. Chem.* **2018**, 16, 5081).



Vinylogous Pictet–Spengler cyclization for the total synthesis of (±)-Lundurine A: A novel vinylogous Pictet–Spengler cyclization has been developed for the generation of indole-annulated medium-sized rings. The method enables the synthesis of tetrahydroazocinoindoles with a fully substituted carbon center, a prevalent structural motif in many biologically active alkaloids. The strategy has been applied to the total synthesis of (±)-lundurine A (*Angew.Chem. Int. Ed.* **2018**, 57, 6888).

A removable functional group strategy for regiodivergent Wittig rearrangement products: [1,2] and [2,3] Wittig rearrangements are competing reaction pathways,often leading to uncontrollable product distribution. We employ a single removable functional group to fulfill the dual role of attaining a reversible [2,3] and stabilizing radical intermediate for the [1,2] path to obtain both the Wittig products selectively for a broad range of substrates (*Org. Biomol. Chem.* **2018**, 16, 8922).



Mathematical Modeling and Big Data Analytics

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Machine-learning to characterize diversity in protein-DNA binding: A high-throughput chromatin immunoprecipitation (ChIP) experiment identifies genomic regions bound by a protein in vivo. We have developed a new Bayesian method—DIVER SITY which asks what sequence component caused a specific region to be reported in a ChIP experiment? The answer, in combination with additional data such as conservation, SNPs, chromatin structure, downstream gene-expression, etc. can yield insights into the diverse regulatory mechanisms at play, something not attempted so far from ChIP. The added benefits of a web-server (http://diversity.ncl.res.in/) and a parallel version (https://github.com/NarlikarLab/DIVERSITY) make DIVERSITY a practical tool for discovering new biology from ChIP experiments (*PLoS Comput.Biol.* **2018**, *14*, doi.org/10.1371/image.pcbi.v14.i04).

Fast, sensitive detection of sequence features by clustering large datasets: We have developed a clustering-based approach- THICWEED—for efficiently analyzing transcription factor binding data from large high-throughput sequencing datasets, an effort led by Rahul Siddharthan (IMSc Chennai). THICWEED successfully recovers literature motifs, but also uncovers complex sequence characteristics in flanking DNA, variant and secondary motifs, all of which appear biologically relevant. We find recurring sequence patterns across diverse datasets, possibly related to chromatin architecture and looping. Significantly faster than standard motif-finding programs, THICWEED processes 30000 peaks in 1–2 hours, on a desktop computer (*Nucleic Acids Res.* **2018,** 46, e29).

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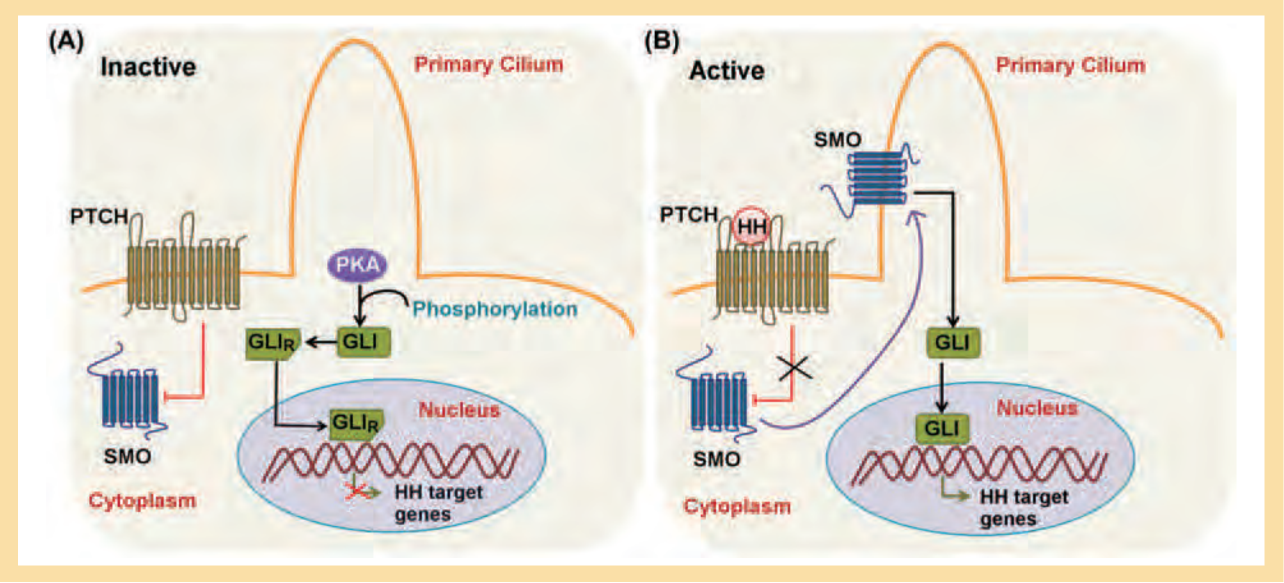
Development of a comprehensive database of biochemical pathways - BIOPYDB for a systems-level understanding of cellular functioning: A manually curated database called BIOPYDB: BIOchemical Pathway DataBase was developed to understand the complexities of biochemical pathways and to model the intracellular biochemical reactions (http://biopydb.ncl.res.in/biopydb). This database is a readily updatable, dynamic resource of human cell specific pathway information along with integrated computational platform to perform various pathway analyses. Presently, it comprises of 46 pathways, 3189 molecules, 5742 reactions and 6897 different types of diseases linked with pathway proteins, which are referred by 520 literatures and 17 other pathway databases. BIOPYDB is currently providing the biochemical, intra-cellular signaling pathway data under four different categories *viz.* i) Developmental Pathways, ii) Immunological Pathways, iii) Cell Proliferation Pathways, and iv) Disease Pathway. In the "Developmental Pathways" category, two important developmental pathways viz. Hedgehog and Notch pathways are included that have been implicated in the development of Cancer as well.

With its repertoire of biochemical pathway data, and computational tools for performing Topological, Logical and Dynamic analyses, BIOPYDB offers both the experimental and computational biologists to acquire a comprehensive understanding of signaling cascades in the cells. Automatedpathway image reconstruction, cross referencing of pathway molecules and interactions with other databases and literature sources, complex search operations to extract information from other similar resources, integrated platform for pathway datasharing and computation, etc. are the novel and useful features included in this database to make it more acceptable and attractive to the users of pathway research communities (*J. Integr. Bioinform.* **2018**, DOI:10.1515/jib-2017-0072).

Mathematical Modeling and Big Data Analytics

Identification of potential antagonists against smoothened protein and the study of their structural stability and binding mechanisms: Hedgehog (HH) pathway is an important pathway whose abnormal activation is implicated in cancers. Smoothened (SMO) is the key regulatory protein for activation of Hedgehog signaling (HH) pathway. SMO is a seven-pass transmembrane protein and belongs to the Class-F G-protein coupled receptors (GPCRs). The activation of the pathway occurs when HH ligands (e.g. SHH, DHH, or IHH) bind to the Patched receptor and release the inhibitory effect of Patched on SMO. Various knockout and mutation studies show that SMO functioning is essential for HH pathway regulation in cancer cells and hence considered as an important therapeutic drug target to reduce cancer progression. Hence with the aim to widen the scope of cancer chemotherapeutics, this study combines traditional *in silico* approaches of drug discovery (Homology Modelling, Virtual Screening and Docking), along with a novel integrative approach using molecular dynamics and dynamic graph theory analysis of the protein contact networks. This integrative approach helps in more precisely predicting and assessing the new potential drug-like molecule for SMO. From this study, ZINC12368305 (4-(9-anthryl)-4,5-dihydro-1H-pyrazol-3-yl](3-phenanthryl)methanone) is found as the best small molecule in terms of binding and stability among the entire dataset. The identified molecule is also comparable to other known reported inhibitors of SMO in terms of conformational fluctuations. It is found that a significant number of low fluctuating amino acid residues at the vicinity of the SMO drug binding site are making large clusters which drive the whole conformation toward a more stable state. Additionally, a unique and stable pi–pi interaction is also observed between the aromatic rings of ZINC12368305 and Phe484 amino acid residue of SMO, which in turn also provides structural insights behind the higher affinity of this drug molecule with SMO (Fig. 2). The physicochemical property of best identified hit (ZINC12368305) shows that the total number of Hydrogen Bond Donors, Acceptors, and Rotatable Bond Count are 1, 3, and 3, respectively. The cLogP value for the molecule is 6.1. This molecule is also reported to be absorbed in the human intestine and is able to cross the Blood–Brain Barrier (BBB+). Hence, these parameters clearly indicate that the reported compound could be a suitable drug to inhibit the membrane-bound receptor protein SMO in future cancer therapeutic studies (*J. Biomol. Struct. Dyn.* **2017**, *DOI:10.1080/07391102.2017.1372310*).



Mathematical Modeling and Big Data Analytics

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Exploring GPCR-lipid interactions by molecular dynamics simulations: This work highlights on the successes and challenges of computational methods to study the interaction of lipids with G protein-coupled receptors (GPCRs). GPCRs are seven transmembrane receptors that mediate a large number of cellular responses and are important drug targets. One of the current challenges in GPCR biology is to analyze the molecular signatures of receptor-lipid interactions and their subsequent effects on GPCR structure and function. It was showed that predicted cholesterol interaction sites appear to correspond well with experimentally determined binding sites and estimated time scales of association. The review will be an important step to benchmark molecular level understanding of GPCR-lipid interactions (*J. Phys. Chem. B* **2018**, 122, 5727).

Medicinal Chemistry

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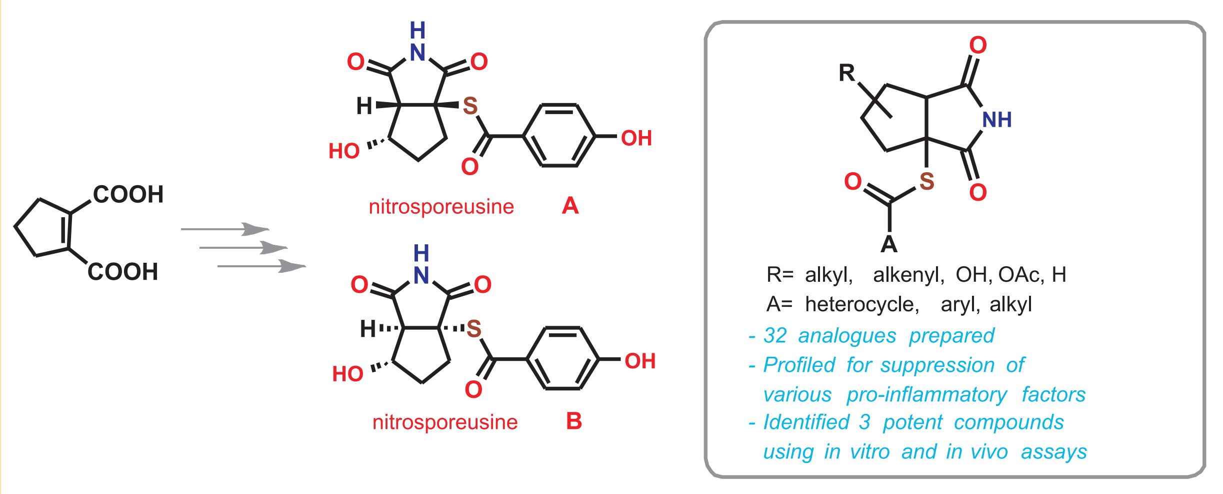
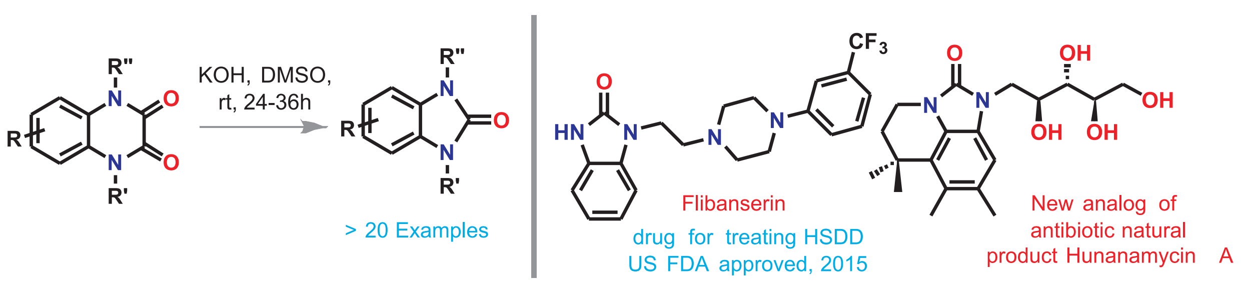
Identification of new anti-inflammatory agents based on nitrosporeusine, a class of marine natural products: Nitrosporeusines A and B are two recently isolated marine natural products with novel chemotype and exceptional as well as impressive biological profile. Interesting antiviral activity of nitrosporeusines and a promising potential in curing various diseases, evident from positive data from various animal models, urged us to investigate their anti-inflammatory potential. As per plan we successfully synthesized nitrosporeusines A and B in racemic as well as enantiopure forms, following which a library of analogues were synthesized as well. All the synthesized compounds were evaluated for *in vitro* and *in vivo* anti-inflammatory potential, among which, three compounds were found to be significantly active in reducing levels of nitric oxide (NO), reactive oxygen species (ROS) and pro-inflammatory cytokines. In addition, these compounds suppressed several pro-inflammatory mediators including inducible nitric oxide synthase (iNOS), cyclooxygenase-2 (COX-2), nuclear factor-κB (NF-κB), and thereby can be emerged as potent anti-inflammatory compounds. Furthermore, all possible isomers of lead compound were also synthesized, characterized and profiled in same set of assays and one of the enantiomer of the active analogue was found to be superior among them (*Eur. J. Med. Chem.* **2017**, 135, 89).

Medicinal Chemistry



Decarbonylative ring contraction of quinoxalinediones to access benzimidazol-2-ones: Benzimidazol-2-ones are a class of medicinally important and privileged heterocycles. They consist of cyclic urea fused with the aromatic backbone, which can potentially interact in a biological system by various noncovalent interactions such as hydrogen bonding and π stacking. This scaffolds exhibit a broad range of biological activities, and they are useful in treating various diseases including cancer, type II diabetes, central nervous system disorders, pain management, and infectious disease. Thus methods for synthesizing the same become an inevitable task. A simple and practical method to access a variety of benzimidazol-2-ones is reported here, where a series of *N*-alkyl `substituted benzimidazol-2-ones were synthesized by decarbonylative ring contraction starting from corresponding quinoxalinediones for the first time. The utility of the method has been demonstrated by synthesizing recently approved controversial drug flibanserin (Addyi®) and a urea analogue of marine antibiotic natural product hunanamycin-A (*ACS Omega* **2017**, 2, 5137).



Catalysis

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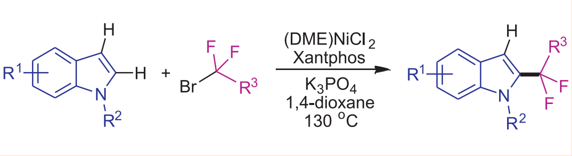
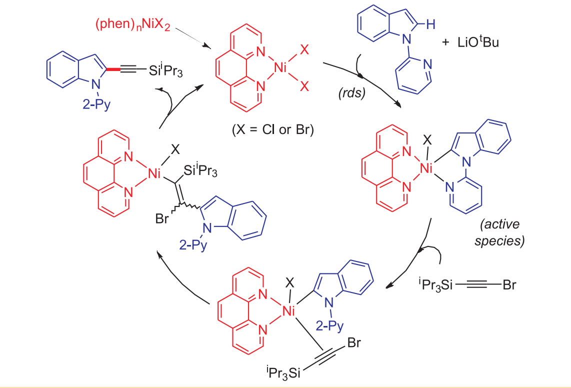
Nickel-catalyzed regioselective C(2)–H difluoroalkylation of indoles with difluoroalkyl bromides: Regioselective C(2)–H difluoroalkylation of C-3 unsubstituted indoles with commonly available fluoroalkyl bromides is successfully achieved employing a simple nickel catalyst system, (DME)$NiCl_2$/Xantphos. This methodology shows excellent regioselectivity and exhibits broad substrate scope (*Chem. Asian J.* **2018**, *13*, 2516).



Mechanism of nickel (II)-catalyzed C(2)–H alkynylation of indoles with alkynyl bromide: The mechanistic aspect of the nickel-catalyzed alkynylation of indoles with alkynyl bromide is demonstrated that proceeds through the coordinative insertion of alkynyl bromide involving the rate influencing C–H nickelation of indole (*Organometallics* **2018**, *37* 2037).



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Catalysts for sustainable process development

Single pot selective hydrogenation of furfural to 2-methylfuran: Amongst several catalysts screened, Ir/C showed complete furfural conversion and highest selectivity of 95% to 2-Methyl furan at very low H_2 pressure of 100 psig. Metallic (Ir) and oxide phases catalyzed first step hydrogenation of furfural and subsequent hydrogenation to 2-MF, respecively. At low temperature of 1400°C, almost equal selectivities of FAL (42%) and 2-MF (43%) were observed, while higher temperature favored selective hydrodeoxygenation. A plausible reaction pathway was proposed for selective formation of 2-MF. The selectivity to various other products in FFR hydrogenation can be manipulated by tailoring the reaction conditions over the same catalyst (*Green Chem.* **2018**, *20*, 2027; Patent: EP 2951165).

Bifunctional catalysis for direct transformation of furfural to 1,2-pentanediol: Complete conversion of furfural with 66% 1,2-PeDO was achieved over Pd/MMT-K10 catalyst. Brønsted acidity of the catalyst was responsible for C5-O cleavage of furan ring and the product selectivities could be tailored by varying H_2 pressure. The proposed reaction pathway to 1,2-PeDO involved FAL formation as the key step (*Catal. Today* **2018**, *309*, 195)

Mizoroki-heck cross-coupling in water: Mizoroki-Heck coupling reaction was successfully conducted in water in the absence of any additives under aerobic conditions using Pd based catalyst. The various key reaction parameters that affect the yield of desired cross coupling product were optimized. The Pd catalyst deactivation during Mizoroki-Heck coupling reaction was identified, which evolved a strategy for Pd-metal recyclability over ten times without appreciable loss of its activity. Thus, it provided access to variety of olefins in aqueous medium, making this protocol eco-friendly (*Green Chem.* **2017**, *19*, 5958).

Synthesis of furylmethane derivatives over -SO_3H functionalized ionic liquids: A new and effective unique two-phase reaction system for high yield production of tri(furyl)methane from furfural and furan was developed. This strategy involved acidic aqueous phase (water + -SO3H functionalized IL) and furan phase which significantly suppressed polymer

Catalysis

formation thereby increased the yield of tri(furyl)-methane. Increase in carbon chain length between imidazole/tri-ethylamine/pyridine and $-SO_3H$, increased the catalytic activity of respective ionic liquids. Strong acidic imidazolium based butylsulfonic acid showed the best activity with a maximum of 84% yield of condensation product. This strategy offered significantly high yield production of condensation products of furan and furfural as compared to the traditional mineral acid route and can be extended successfully for the condensation of furan derivatives (e.g. furan and 2-methylfuran) with several different aldehydes, ketones and alcohols (*Green Chem.* **2017**, 19, 4804; Patent: INV-NCL-0011, INV-NCL-009, 2017).

Reductive-etherification of bio-derived aldehydes over Zr-based catalysts: A single pot, efficient catalytic cascade sequence was developed for the production of value-added ethers from bio-derived aldehydes. Etherification of 5-(hydroxymethyl) furfural with different aliphatic alcohols over acidic Zr-Montmorillonite (Zr-Mont) catalyst, produced a mixture of 5-(alkoxymethyl) furfural and 2-(dialkoxymethyl)-5-(alkoxymethyl)furan. Later it was selectively converted back to 5-(alkoxymethyl) furfural by treating it with water over the same catalyst. Synthesis of 2,5-bis(alkoxymethyl)furan was achieved through a cascade sequence involving etherification, transfer hydrogenation and re-etherification over a combination of acidic catalyst (Zr) and CTH catalyst $[ZrO(OH)_2]$. This catalyst combination was further successfully explored for cascade conversion of 2-furfuraldehyde into 2-(alkoxymethyl) furan. The scope of this strategy was then extended for reductive-etherification of lignin derived arylaldehydes to get respective benzyl ethers in >80% yield (*ChemSusChem* 2017, 20, 4090; Patent: INV-NCL-065, 2017).

Diesel additives from fructose over PWA/SBA-15 catalyst: One pot synthesis of 5-(hydroxymethyl) furfural (5-HMF) and 5-(ethoxymethyl) furfural (EMF) was reported from fructose by successful incorporation of PWA into the SBA-15 framework that confirmed by ^{31}P NMR exhibited both Brønsted and Lewis acidity, large and well distributed three dimensional interconnected pores with high surface areas exhibiting excellent activity. The minimum loading of PWA in SBA-15 gave 78% fructose conversion with the highest yield of 70% towards 5-HMF (*Fuel* **2018**, 217, 38; Patent: INV-NCL-057, 2017).

Glycerol transesterification with propylene carbonate to glycerol carbonate: It was carried out efficiently under solvent-free conditions using solid base as catalysts involving non-noble metal oxide in combination with hydrotalcites. The best result obtained over Ca-HT catalyst giving 84% glycerol conversion and almost complete selectivity to glycerol carbonate were due to the crystal structure modification of hydrotalcite and the presence of highest basic site density (*Energ. Fuel.* **2017**, *31*, 4361; Patent: IN 2014DE00185, 2017).

Etherification of glycerol to potential fuel additives: Complete conversion of glycerol was achieved over montmorillonite clay catalyst to form a product containing mono-t-butyl, di-t-butyl, and tri-tert-butyl glycerol ethers (MTBGE, DTBGE, and TTBGE). The different parameters such as reaction temperature, catalyst loading, reaction time and molar ratio of glycerol to TBA were studied to optimize the operating conditions of glycerol etherification reaction (*Energ. Fuel.* **2017**, 31, 12272).

Domino synthesis of 3-Indolylquinones: A domino synthesis of 3-indolylquinones was achieved successfully via direct oxidative C-C coupling of hydroquinones with indoles over Ag_2O and Fe_3O_4/PVP-PWA catalysts at room temperature. Ag_2O catalyzed the in situ oxidation of hydroquinone and 3-indolylhydroquinone intermediates while, ferrite solid acid, with 1:4:1 ratio of Fe_3O_4, povidone and PWA catalyzed the activation of quinones. The efficiency of this catalytic domino approach was established by a broad scope of substrates involving a variety of hydroquinones and quinones to give high yields (81-97%) of 3-indolylquinones. Fe_3O_4/PVP-PWA was separated magnetically while a simple filtration could separate Ag_2O both of which could be recycled several times without losing their activities (ACS Omega **2017**, 2, 2238).

Biocatalytic route for direct conversion of bio-glycerol to C3-C4 diols: During screening of bacterial cultures *K. pneumoniae* and *E. aerogenes* were able to convert crude bio-glycerol to 2,3-butanediol (2,3-BDO) and 1,3-propanediol (1,3-PDO), as major compounds, ethanol and acetoin as minor compounds, with a utilization of 69% and 79% respectively. Process optimization achieved maximum conversion at pH 7.0, 37°C, 30-40 g/L glycerol and 1.5g of inoculum until 120 h. Mixed cultures led to complete glycerol conversion with optimal yield and productivity for products (*Curr. Env. Eng.* **2018**, 5, 4; Patent: INV-NCL-0097, 2017).

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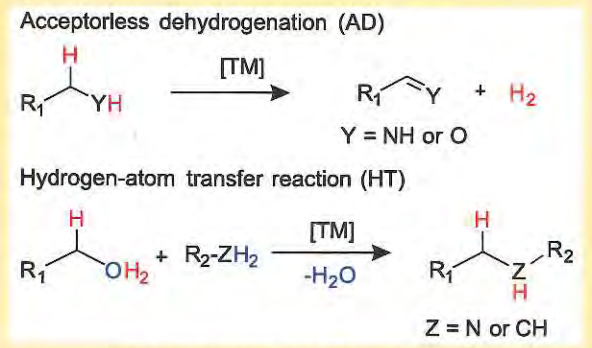
Dehydrogenation and hydrogen auto transfer reactions

Smart systems for acceptorless dehydrogenation strategy: Homogeneous catalysis: The catalytic dehydrogenation with concomitant removal of dihydrogen is a superior strategy and has enabled the direct access to valuable intermediates. In this regard, design and development of new catalytic systems for fundamentally important synthetic transformations and energy storage applications is an intellectually stimulating challenge. The group is working on catalyst design for various dehydrogenation and related reactions for both fundamental research and industrial application (*Org. Lett.* **2018**, *20*, 3381; *Chem. Commun.* **2018**, *54*, 90; *Catal. Sci. Technol.* **2018**, *8*, 428; *Synthesis* **2017**, *49*, 3957).



Dehydrogenation and related reactions.

Heterogeneous catalysis: The group has developed an unprecedented unique core–shell architecture of iron nanocatalyst with a shell comprising of oxide and a core mainly of carbide synthesized by thermally pyrolyzing Fe:N-rich ligand on a graphitic oxide support. Interestingly, the microstructure of the final catalyst showed a surface lacking the encapsulating sheath of carbon commonly observed in earlier works. The unique microstructure also resulted in an exceptional catalytic property in oxidant-free and acceptorless dehydrogenation of N-heterocycles, relatively abundant alcohols, and amines with the concomitant generation of hydrogen gas (*Nat. Commun.* **2017**, *8*, 2147; *Catal.Sci. Technol.* **2017**, *7*, 3177).

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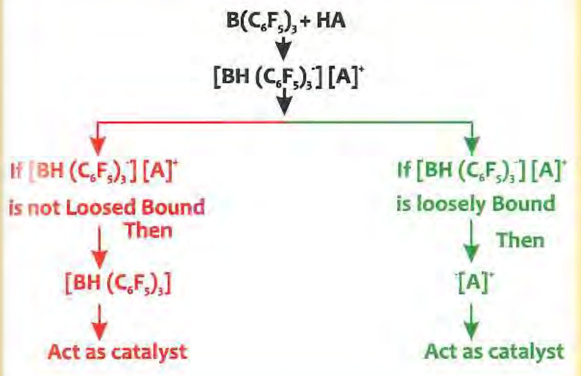
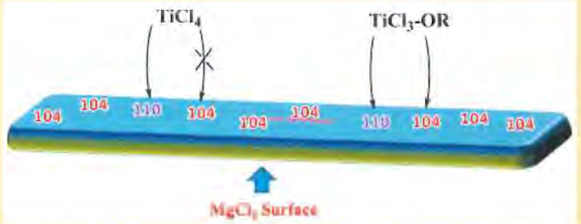
The unusual role of the aromatic solvent in single site Al(I) chemistry

Significance of autocatalysis in surrogate silicon chemistry: One of the most promising recent developments in catalysis has been the use of the metal-free Lewis acid $B(C_6F_5)_3$ as a catalyst for a range of different chemical transformations. Perhaps the most impressive achievement in this regard is the recently accomplished in situ generation of SiH_4 from surrogates (Simonneau and Oestreich, Nat. Chem. **2015**, *7*, 816). However, what the current computa-tional work, with density functional theory, reveals is that this process, in addition to being catalyzed by $B(C_6F_5)_3$, is also significantly dominated by a series of autocatalytic reactions. The results are further corroborated by the use of the energetic span model, which shows that the turnover frequency is higher for the newly proposed autocatalytic pathway in comparison to the conventional $B(C_6F_5)_3$-catalyzed pathway. The current work therefore provides interesting new insights into surrogate silicon chemistry. But, more importantly, the current studies indicate that $B(C_6F_5)_3$ is likely to function more as an initiator rather than a pure catalyst in many metal-free transformations that have been reported to date. This work provided important insights into metal free chemistry, and can therefore be expected to be of value for developing more environmentally friendly catalytic systems in the future (*ACS Catal.* **2018**, 8, 6163).



A schematic representation of the possibilities in surrogate silicon chemistry

Role of the (104) $MgCl_2$ lateral cut in Ziegler–Natta catalysis: Density functional theory (DFT) has been used for the study of ethylene polymerization in the Ziegler–Natta (ZN) olefin polymerization system for eight different alkoxy group containing titanium catalysts (Cat-A–H), Ti(III)Et(OR)(OR′) (where R = $-CH_3$, – Et, –*tert*-butyl, –cyclohexane, R′ = $-CH_3$, -Et, -*tert*-butyl, –cyclohexane). What is of significance is that the catalysts studied were all considered to be tethered to the (104) $MgCl_2$ surface, which has traditionally been considered a "dormant" surface in ZN catalysis systems, in contrast to the "more active" (110) $MgCl_2$ surface. Our calculations indicate that the binding of all the catalysts to the (104) surface is favorable, even after taking entropic effects into account. For purposes of comparison, ethylene polymerization has been investigated for the Cat-C ($TiEt(OEt)_2$) and the Cat-H ($TiEt(Cl)(OC_4H_8Cl)$) (OC_4H_8Cl = the chlorobutoxy group) cases, for both the (i) (110) and the (ii) (104) $MgCl_2$ surfaces. It has been seen that for both (i) and (ii) the energy gap between insertion and the termination barriers (ΔX) was nearly the same for both the Cat-C and Cat-H cases, which shows that ethylene polymerization on the (104) $MgCl_2$ surface is likely to be a prominent occurrence in Z–N catalysis, when alkoxy groups are bound to the titanium center. Additionally, for the Cat-C and the Cat-H cases, the regio- and stereo-selective behavior of the propylene monomer on the titanium species present on the (110) and the (104) $MgCl_2$ surfaces has also been investigated, and the results indicate that the (104) $MgCl_2$ surface is only slightly less effective than the (110). However, the calculations also indicate that for Cat-H the (104) $MgCl_2$ surface significantly improves the molecular weight of polypropylene in comparison to the (110) surface, further showcasing how the (104) surface (ignored until date) might be a major player in ZN catalysis. Given that a major portion of the $MgCl_2$ support is made up of (104) lateral cuts, the current findings are of considerable relevance in developing and understanding how more efficient systems for Ziegler-Natta catalysis can be developed in the near future (*J. Phys. Chem. C* **2018**, 122, 285).



Possibilities of coordination of different potential catalytic species on the different lateral cuts on the $MgCl_2$ surface in

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Novel catalytic pathways to valorize biomass

Valorization of lignin: By-product in 2G ethanol industry: A novel methodology was reported for depolymerization of high molecular weight lignin (60,000 Da) to low molecular weight substituted phenolic compounds using various recyclable solid base catalysts at 250 °C in 1 h. Most of the zeolytic catalysts (NaX, NaY, NaP) showed very high yields (~51%) of low molecular weight products than other catalysts (MgO, CaO, HT, HAP). Identification and quantification of products was done by various analytical techniques. FT-IR studies revealed retention of most of functional groups from lignin into products. The efficiencies of catalysts were dependent on pH, cation, type and concentration of basic sites etc (*GreenChem.* **2017,** 19, 778).

Ambient condition hydrogenation of furfural to furfuryl alcohol: Biomass derived furfural (FAL) can be hydrogenated to yield industrially important platform chemical, furfuryl alcohol (FOL). Bimetallic PtCo/C catalysts with varying metal concentrations were employed to achieve maximum possible FOL yield (100%) at 35°C under 0.1 MPa H_2 in water. With concentrated FAL (40wt%) at 50°C and under 1 MPa H_2 pressure, 86% yield for FOL was observed. Efficient recycling of catalyst with marginal loss in activity due to handling error and isolation of FOL in pure form confirmed by NMR and HPLC is attractive (*GreenChem.* **2017,** 19, 1144).

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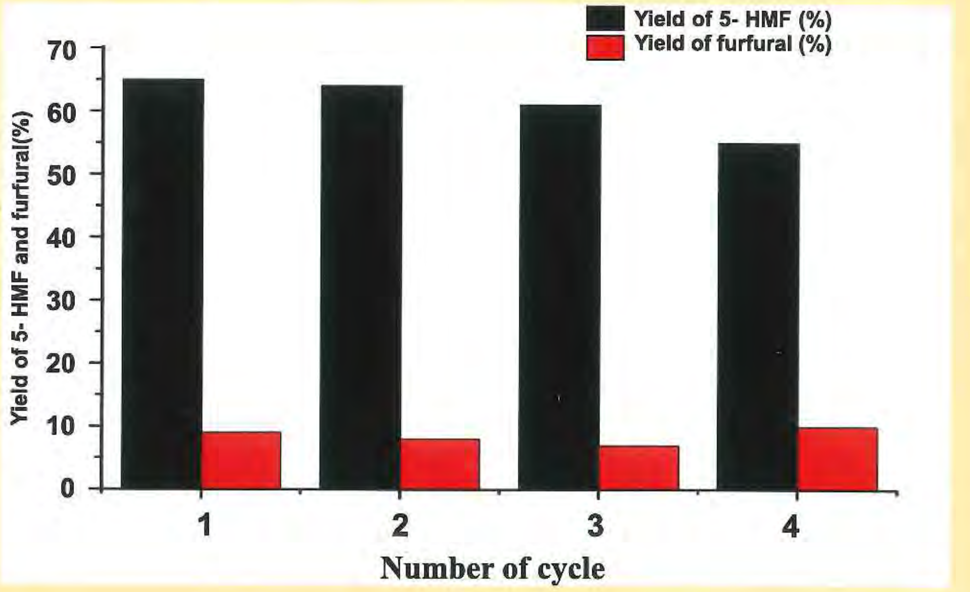
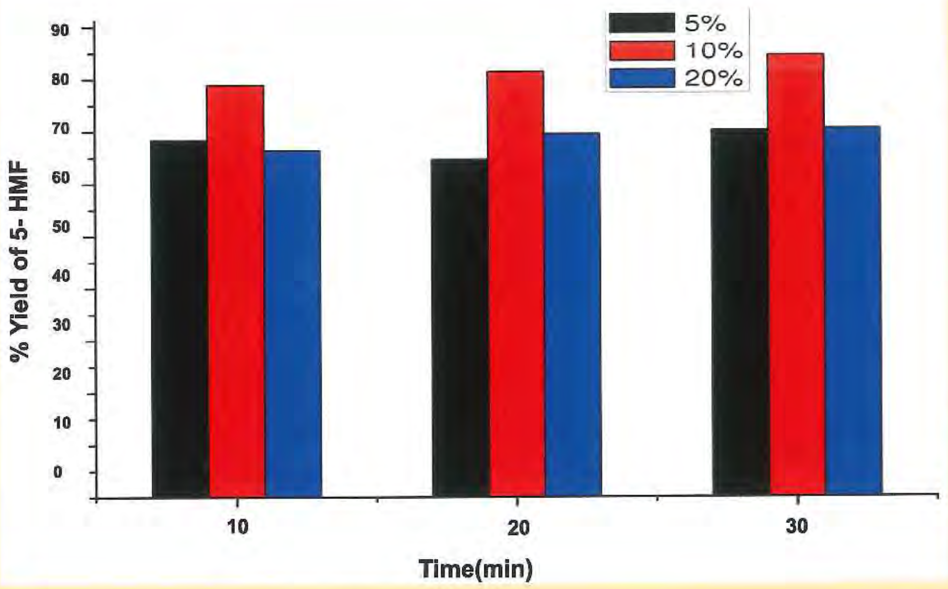
Acid modified zeolite for fructose to 5-hydroxymethyl furfural: Commercially available solid acid catalyst, H-USY zeolite was modified by treating with aqueous solution of H_3PO_4 and H_2SO_4 (10-30 wt %). Its catalytic performance was evaluated for the fructose conversion to 5-HMF in methyl isobutyl ketone (MIBK)-water system. Modified H-USY zeolite was identified to have potential in enhancement of 5-HMF yield up to 65% from 32% (parent H-USY) with minimum formation of furfural (8%). Best performance of 10P-Y is associated with the optimum combination of moderate acidity (both weak as well as strong), moderate dealumination of Al from extra-framework sites as well as from framework sites of H-USY, formation of new Al-O-P bonds between framework Al and elemental monomeric phosphorus, presence of Brønsted as well as Lewis acidity and creation of mesopores (*Energ. Fuel.* **2018,** 32, 3783).





$H_xZr_{3-x}PW_{12}O_{40}$ as new heteropolyacid for fructose dehydratio: Dehydration of fructose is a way to produce an important platform chemical such as 5-hydroxymethylfurfural (HMF which is widely used to synthesize variety of renewable chemicals and fuel). Heteropoly acid, H3PW12O40 is highly soluble strong acidic catalyst with well-defined structure. This study reports the modification of soluble heteropoly acid to insoluble and reusable heteropolyacid (HxZr3-xPW12O40) by exchanging with Zr and investigation of its catalytic performance in selective transformation of renewable fructose to 5-HMF in Dimethyl sulfoxide (DMSO) system. At optimized reaction condition, 5-HMF yield of 85% with 100% selectivity was achieved with H1Zr2 PW12O40 catalyst at much lower reaction time of 10 min than reported. The catalyst was observed to be recoverable, reusable as compared to parent H3PW12O40. Effect of catalyst loading is given below (*Chemistry Select* **2018,** 3, 832).

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o-alkylation of hydroquinone to hydroquinone monomethyl ether: The selective synthesis of monoalkylated products is subject of high industrial importance because these products play a vital role in manufacturing of fine and speciality chemicals. The monomethyl ether of hydroquinone, commonly named mequinol, is an important building block which is also used as polymerization inhibitor for acrylic compounds, stabilizer for photo sensitive materials, lubricating agent, and key intermediate in many pharmacological applications. Traditionally, 4-methoxyphenol is synthesized by methylation of hydroquinone with dimethyl sulphate or halomethane in presence of sodium hydroxide which are hazardous and highly polluting and thus there has been high demand to reduce negative environmental impacts of chemical process and to discover clean and economical process based on green catalysis system. We are working on methylation of dihydroxybenzene by using ionic liquid as catalyst which yields single product formation. The main focus is on obtaining high extent of reaction and maximum selectivity towards desired product with good catalyst recyclability.

Catalysis

The heterogenization of ionic liquid is one of most aspiring area of heterogeneous catalyst. The design and development of a new type of heterogeneous catalysts using ionic liquid with both high activity and good stability for the o-alkylation reaction is, still, a significant challenge of scientific research. The main objective of this work is to understand the fundamental of *o*- alkylation reactions, investigate the kinetics of the reaction and develop suitable reactor for similar reactions. The mechanistic and kinetic aspects will be advantageous for migration of process from lab scale to pilot or commercial scale and to make improvement in selectivity.

Multiphase Reactors and Flow Processes

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Four phase hydrogenation system: The heterogeneous catalytic hydrogenation processes are commonly used in fine and speciality chemical industry. There is an extensive research done in this regard for optimising the three phase hydrogenation processes from laboratory to pilot plant scale. But addition of the fourth immiscible liquid phase to such processes brings in system specific benefits. This form the gas-liquid-liquid-solid, [G-L-L-S], four phase hydrogenation systems. The benefits of adding the fourth phase include- increased selectivity towards the desired product by adjusting pH of secondary liquid phase (Cinnamaldehyde to Cinnamyl alcohol), separation of the product on virtue of difference in product solubility in two liquid phases (Benzene to Cyclohexene), in situ rearrangement of products in secondary liquid leading to increased selectivity to desired product (Nitrobenzene to Para-aminophenol). The current work aims at understanding the thermodynamic, reaction engineering and mass transfer aspects of G-L-L-S systems leading to development of multifunctional, intensified hydrogenation processes. The case of cinnamaldehyde hydrogenation has been selected to develop general guidelines for optimization of G-L-L-S systems through experimentation and modelling.

Mathematical and Computational Modeling

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Correlation between structure, thermodynamics, dynamics and role of locally favored structures in the glass forming ability and slow dynamics

Role of the pair correlation function in the dynamical transition predicted by mode coupling theory: It was found that for a large number of systems the configurational entropy at the pair level S_{c2}, which is primarily determined by the pair correlation function, vanishes at the dynamical transition temperature T_c. Thus, it appears that the information of the transition temperature is embedded in the structure of the liquid. In order to investigate this, we describe the dynamics of the system at the mean field level and, using the concepts of the dynamical density functional theory, show that the dynamical transition temperature depends only on the pair correlation function. Thus, this theory is similar in spirit to the microscopic mode coupling theory (MCT). It predicts a transition temperature that is similar to T_c. This implies that the information of the dynamical transition temperature is embedded in the pair correlation function (*Phys. Rev. Lett.* **2017**, 119, 265502).

Mathematical and Computational Modeling

Analysis of the anomalous mean-field like properties of Gaussian core model in terms of entropy: We investigated the entropies, namely, the excess entropy (S_{ex}) and the configurational entropy (S_c) and their different components. The study corroborates most of the earlier observations and also sheds new light on the high and low temperature dynamics. We found that unlike in standard glass former where high temperature dynamics is dominated by two-body correlation and low temperature by many-body correlations, in the GCM both high and low temperature dynamics are dominated by many-body correlations. We also found that many-body entropy which was usually positive at low temperatures and was associated with activated dynamics was negative in the GCM suggesting suppression of activation. Interestingly despite the suppression of activation, the Adam-Gibbs (AG) relation that describes activated dynamics holds in the GCM, thus suggesting a non-activated contribution in AG relation. We also find an overlap between the AG relation and mode coupling power law regime leading to a power law behavior of S_c. We predicted that in the GCM the high temperature dynamics will disappear at dynamical transition temperature and below that there will be a transition to the activated regime. Our study further reveals that the activated regime in the GCM is quite narrow(*J. Chem. Phys.* **2018**, 148, 34504).

Determination of onset temperature from the entropy for fragile to strong liquids: We established a connection between the onset temperature of glassy dynamics with the change in the entropy for a wide range of model systems. The crossing temperature of pair and excess entropies was identified as the onset temperature. Below the onset temperature, the residual multi particle entropy, the difference between excess and pair entropies, becomes positive. The positive entropy can be viewed as equivalent to the larger phase space exploration of the system. The new method of onset temperature prediction from entropy is less ambiguous, as it does not depend on any fitting parameter like the existing methods (*J. Chem. Phys.* **2017**, 147, 24504).

Fickian yet non-Gaussian behaviour: A dominant role of the intermittent dynamics: A study of the dynamics of small solute particles in a solvent medium was done where the solute is much smaller in size, mimicking the diffusion of small particles in crowded environment. The solute exhibits Fickian diffusion arising from non-Gaussian Van Hove correlation function. It shows that there are at least two possible origins of this non-Gaussian behaviour. The decoupling of the solute-solvent dynamics and the intermittency in the solute motion, the latter playing a dominant role. In the former scenario when averaged over time long enough to explore different solvent environments, the dynamics recovers the Gaussian nature. In the case of intermittent dynamics the non-Gaussianity remains even after long averaging and the Gaussian behaviour is obtained at a much longer time. The study further shows that only for an intermediate attractive solute-solvent interaction the dynamics of the solute is intermittent. The intermittency disappears for weaker or stronger attractions (*J. Chem. Phys.* **2017**, 146, 134504).

Process Intensification and Engineering

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Flow process and intensification

Multi-step continuous flow synthesis of ivacaftor: Continuous flow safe ozonolysis method combined with multi-step flow sequence was developed for the drug ivacaftor for the first time. The work was done in collaboration with the group of Dr. D. S. Reddy from Org. Chem. Division. Quadruple reaction to construct quinolone scaffold, in-line extraction followed by continuous phase separation in the multi-step integrated continuous flow are the key features of present work. Feasibility of using a continuous mixed

Process Intensification and Engineering

flow reactor commonly referred as CSTR for integrated flow setup is also investigated for reaction approach with long reaction time. The current integrated multi-step flow synthesis can achieve 7.2 g/day of the Ivacaftor drug at lab scale, which is sufficient to treat 50 patients per day. The present route can also be used as a general route for the synthesis of other related drugs such as quinolone antibiotics (*React. Chem. Eng.* **2018**, *3*, 520).

Continuous flow synthesis of silica particles Monodispersed micron size (0.5- 2.5μm) silica particles were synthesized in semi batch mode using Stober process. Systematic parametric study and effect of solvent on particle size was checked. Kinetic parameters were estimated and process was transformed into continuous process. A Mono-dispersed submicron size (0.2-1.5μm) silica particle is synthesized in helical coil tubular reactor in a shorter reaction time with complete conversion of limiting reactant. Various process parameters were optimized to obtain monodispersed particles of size up to 0.85 μm and conversion over 90% within 60 min of residence time. Further growth of particles was achieved by theaddition of precursor (TEOS) to the reactor via multipoint injection approach. Clogging in tube was observed after long time and hence it is necessary to achieve PFR effect using CSTR in series (*J. Flow Chem.* **2018**, *8*, 59).

Continuous flow microwave synthesis of NiPt alloy nanoparticles: NiPt alloy nanoparticles of variable composition were synthesized by a novel microwave assisted route. The method alowed tuning of the alloy composition based on residence time and initial concentration of the precursors. The material was tested for hydrogen evolution reaction and methanol oxidation reactions. The work was done in collaboration with the group of Dr. B. L. V. Prasad (Physical Materials Division). The particular optimized alloy composition showed the specific current density for HER and methanol oxidation to be enhanced by 3 and 2 times higher, respectively as compared with commercial Pt/C (Cryst. Growth Des. **2017**, 17,5163).

Design and scale-up guidelines for continuous flow nitration of biaryl aromatic compounds: The efficacy of using CSTRs in series for exothermic aromatic nitration reactions was studied and experimentally demonstrated. The reaction kinetics were determined and used in the design equations of CSTR including energy balance. Lab scale experiments were performed and results were compared with that of numerical. Numerical results found to predict the nature of the temperature profile in CSTR, % conversion and the isomer yielded within ±3.2%. Effect of different parameters such as mole ratio, initial concentration, jacket temperature, the volume of the reactor and residence time on the overall process was studied in detail. Different scale-up strategies (viz. parallel CSTRs, Series of CSTRs of equal or different volumes, multipoint dosing) were studied to maximize the production (150 – 520 Kg/day). The simulations indicated that the multipoint dosing with variable volume reactors can be used for maximizing the production with safe operation (Application Number: WO2015011729A1).

Batch and continuous flow antisolvent based production of small sized metformin hydrochloride crystals under sonication: A liquid anti solvent precipitation based continuous flow high throughput process was developed for production of small sized metformin hydrochloride crystals. Enhanced mixing from the integration of ultrasound and impinging jet reactor helped to yield small sized particles. The effect of process parameters (viz. solvent to antisolvent ratio, solute concentration, antisolvent temperature and mixing) on precipitation was investigated systematically to optimize conditions for smaller sized metformin hydrochloride crystals. L-histidine was used as a biocompatible additive to suppress growth and agglomeration of the particles. 15 μm sized MHC particles can be obtained in a continuous and clogging free manner using an impinging jet reactor.

Crop Protection

Ashok P. Giri ap.giri@ncl.res.in

Plant defense mechanisms, crop protection strategies

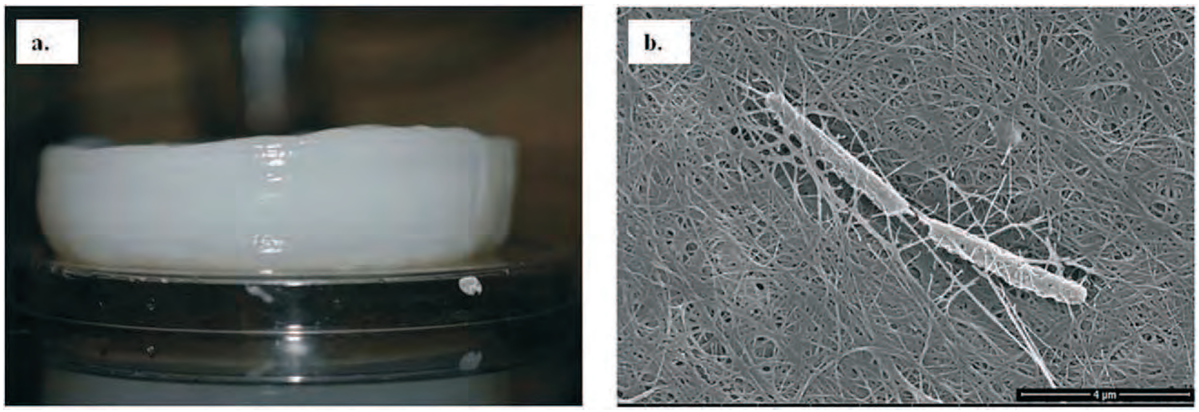
Metabolic reprogramming of metabolites in blight resistance in wild tomato: Exploration with high throughput leaf metabolomics along with functional genomics in wild tomato unravels potential role of steroidal glycoalkaloids (SGA) and phenylpropanoids during early blight (EB) resistance. Total 2047 potential metabolite were detected of which 681 and 684 metabolites revealed significant modulation and clear differentiation in resistant and susceptible accessions, respectively. Majority of the EB-triggered metabolic changes were active from SGA, lignin and flavonoid biosynthetic pathways. Overall, this study highlights vital roles of SGAs as phytoalexins, phenylpropanoids and lignin accumulation in EB resistance (*Plant Molec. Biol.* **2017**, 95, 411).

Tripeptides from reactive centre loop of protease inhibitors inhibit proteases of *Helicoverpa armigera*
We demonstrated serine protease inhibition by reactive center loop (RCL) of plant Pin-II inhibitors. RCL tri-peptides selectively inhibited *Helicoverpa armigera* midgut proteases at alkaline pH. Further elucidated of RCL-protease binding mechanism by crystal structure and modelling. We reported negative impact of RCL tripeptides on growth and digestive physiology of *H. armigera*. These peptides are suitable molecules for the development of sustainable pest management strategies for crop protection (*Insect Biochem. Molec. Biol* **2018**, 95, 17).

Plant Diversity and Bio-prospecting

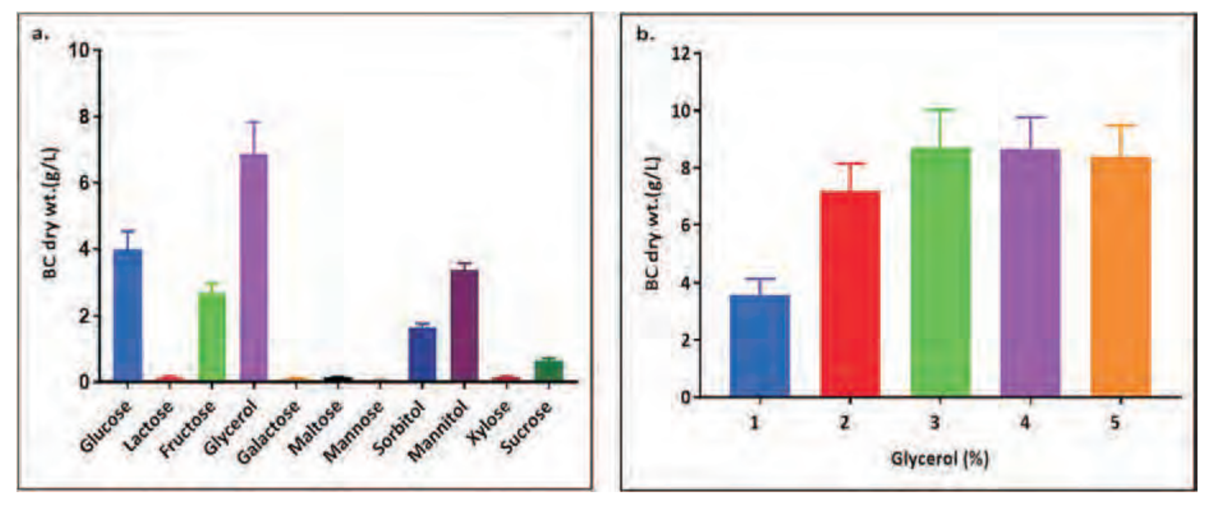
Syed Dastager sg.dastager@ncl.res.in

High yield production of cellulose by a *Komagataeibacter rhaeticus* PG2 strain isolated from pomegranate as a new host: Cellulose is the chief constituent of several dental materials and finds application in dentistry for isolation in the form of cellulose wafers for isolation, paper points in endodontics, medicated paper points. These products have high consumption value in dentistry. Also, its application can be diversified as it is biodegradable and can hold medicaments for varied niches and wounds in the oral cavity. We have developed bacterial cellulose from an indigenous bacterial source. This has several advantages over plant cellulose (*RSC Adv.* **2018**, *8*, 29797).



(a) The pure wet BC membrane produced by the K. rhaeticus strain PG2 using glycerol as the carbon source after 15 days of incubation at 28 $^{-}$C under static cultivation. **(b)** A FE-SEM image of the bacterial cellulose membrane network with the entrapped K. rhaeticus strain PG2

Plant Diversity and Bio-prospecting



BC membrane production by the K. rhaeticus strain PG2 $(g\ L^{-1})$
(a) from different carbon sources, and **(b)** with different glycerol % (w/v)

Plant Secondary Metabolic Pathway Analysis

Ashok P. Giri ap.giri@ncl.res.in

Transcriptional transitions in Alphonso mango during fruit development: We analyzed the transcriptome of Alphonso mango through Illumina sequencing from seven stages of fruit development and ripening as well as flower. Importantly, 20,755 unique transcripts were annotated and 4,611 were assigned enzyme commission numbers, which encoded 142 biological pathways. Novel 79 transcripts of inhibitors of cell wall modifying enzymes were simultaneously detected throughout Alphonso fruit development and ripening, suggesting controlled activity of these enzymes involved in fruit softening (*Sci. Rep.* **2017**, *7*, 8711).

Resource Centers

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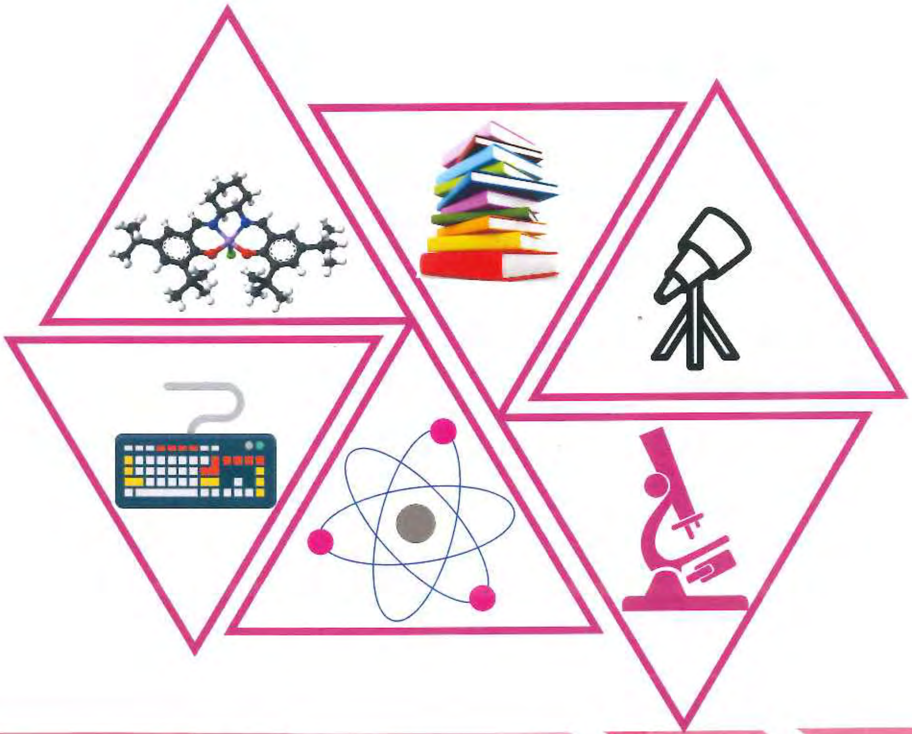

Catalyst Pilot Plant

Catalyst Pilot Plant (CPP) is well equipped with all the catalyst scale-up facilities such as wide range of batch reactors from 250mL to 50L capacity to perform step wise scale up from gm level to 4kg/batch level. CPP is also equipped with other wet and dry processing units required for filtration; centrifugation; drying; calcinations and extrusion of the catalyst up to 1kg level. These wide ranges of reactors are also suitable for translating batch process from Laboratory scale to Pilot Plant scale. It also houses the micro-fixed bed reactors for the performance evaluation of the catalysts in various reactions of academic and industrial importance.

CPP is also involved in various industrial as well as government projects for the development of catalyst and catalytic process in batch and continuous mode. In one of the activity, new catalyst development and process optimization for converting biomass derived C_5 sugars to valuable chemicals such as 5-HMF; Levulinic acid; Ethoxymethyl furfural; furfural; levulinic esters in single/one step is a continuous activity under Dept of Biotechnology sponsored project. CPP also made an attempt to prepare and supply the catalysts for the R & D purpose at client's end. Moreover, we also focussed our activities in the following research areas :

- Synthesis and modifications of different zeolites to alter the physico-chemical properties.
- One step pretreatment of biomass with selective extraction of lignin by steam explosion and dilute acid treatment as a function of biomass particle size.
- Catalytic epoxidation of renewable feed-stocks for CSIR-CNR, Italy Bilateral Exchange Programme.
- Synthesis of zeolites, its optimization, modification and application for Industrial Client.
- Development of catalytic process for converting Indian and Russian origin biomass to Levulinic acid and GVL for DST-RFBR, Russia project.

National Collection of Industrial Microorganisms

NCIM is dedicated to the isolation, identification, collection, preservation, and distribution of authentic microbial strains to industries and academia for biotechnological applications. It is also one of the unit generating bio based economy in recent times utilizing microbiology and biotechnological interventions to preserve Indian microbial wealth and diversity. It has generated the cash flow of Rs 275 lakh through supply of 8000 microbial strains. Around 400 microbial strains were lyophilized for their long-term preservation. Nearly 45 new microbial strains were received for deposition. New services of sequencing and phenotypic identification were initiated. About 200 in-house strains were authenticated by molecular methods like sequencing. Standardized certificate of analysis of microbial cultures was given. Latest catalog of microbial strains were made available in the form of hard copy and online version. Updated deposit forms, and sequencing forms as per global standards are available.

Digital Information Resource Center

Digital Information Resource Center maintained two data centers consisting of more than two hundred server/storage and network devices as well as required non-IT infrastructure consisting of high end UPS, PAC, VESDA, Surveillance, fire detection, access control systems, etc. located at DIRC. It Manages AMC for more than thousand desktop/laptop PCs, printers and other computer peripherals in the lab.

It has installed four Visitor management system (VMS) kiosk machines and two nos. of Barcode visitors slip readers at the reception for the visitors to make the

Digital Information Resource Center

entry gate pass. – DIRC procured, installed, commissioned and tested 26 new Aadhar enabled biometric attendance system (AEBAS) in the lab for marking of central attendance of all the regular NCL staff members. It has also procured, installed, commissioned and tested two high end servers for the on-line registration of the candidates appearing for the CSIR-NET Exam, from all across the country. It has provided/altered about hundred new LAN ports at various locations in the lab/hostel. DIRC has maintained surveillance system consisting of more than 50 IP based Indoor and Outdoor cameras in the lab, guest house as well as hostel DIRC also manages Wi-Fi services provided in most of the corridors in the lab as well as some of the areas in the colony campus.

Knowledge Resource Center

Knowledge Resource Centre (KRC) manages both print and digital resources. KRC subscribes to various journals in print and e-journals format. During the year KRC subscribed to more than 276 journals out of which around 250 are electronic journals and 26 are print journals.

It provides access to various journals and databases through NKRC consortia which covers 39 CSIR labs and 26 DST institutes. Through the consortia users get access to wide range of e-journals. During the year library users were provided access to various databases such as ithenticate plagariasm software, Web of Science, Sci-Finder, Questal/Orbit, Thompson/ Innovations. Users were also provided trial access to Grammarly Software, Bentham Press Journals, Proceedings of the National Academy of Sciences, Healthcare and Biological Sciences Package. More than 100 documents were added in the library collection of which 70 are print books, 30 Hindi Books and around 70 theses. During the year 20 casual visitors, 33 students, 6 corporate members, 13 retired scientists availed services of the library.

KRC/Library is part of CSIR-KNOWGATE project which is initiated by CSIR to initiated use of Koha : an open source library automation software. Under KNOWGATE project KRC/Library has procured new HP ProLiant DL380 Generation9 (Gen9) – 2U rack server with RAID 5 configuration. KRC/Library has transferred all bibliographic data of books/bound volumes on new Koha. The new Koha webopac is now made live through http://krclib.ncl.res.in/opac.

S & T Support Services

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Publication and Science Communication

Publication and Science Communication (PSC) Unit is a channel that communicates between the laboratory and its stakeholders. It uses the facilities like web, print, electronic media and social media. It takes care of the video conference facility, external and internal websites; prepares annual reports and brochures. The unit communicates the impact making work from the laboratory in the form of R&D features, prepares and issues press releases and also coordinates the videos for its stakeholders. It supports to organize conferences. The unit participates in exhibitions, organizes the interviews with scientists on request of the reporters.

PSC coordinated/ participated in following exhibitions during the year both organised by CSIR and also by CSIR-NCL.

- 5th Bharatiya Vigyan Sammelan (BVS) and Expo, Pune (11–14 May 2017)
- Bioenergy-Urja Utsav, Pune (7-8 July 2017)
- Exhibition at Parliament House Annexe, New Delhi (27 July- 11 August 2017)
- Platinum Jubilee Mega Exhibition at CSIR-NCL (20-24 August 2017)
- Platinum Jubilee Mega Exhibition at CSIR-IICT, Hyderabad (1-6 September 2017)
- 5th Industrial Green Chemistry & Engineering World (IGCW) Convention, Mumbai (5-6 October 2017)
- India International Science Festival (IISF), Chennai (13-16 October 2017)
- India Water Week-2017 (IWW), , New Delhi (10-14 October 2017)
- India Centric R&D, Mumbai (12-13 January 2018)
- Be an Entrepreneur of Science & Technology (BEST), Visakhapatnam (25 January 2018)
- CHEMTECH + WATEREX Gujarat World Expo 2018, Ahmedabad (23-25 January 2018)
- 105th Indian Science Congress (ISC), Imphal (16–20 March, 2018)

Posters relevant to the theme of the exhibition were prepared and exhibited along with the models and prototypes.

Engineering Services Unit

Engineering services unit is providing all basic services related to Civil, Electrical, Mechanical engineering and Glass blowing. It is playing an important role in research activities. Institute has a major engineering infrastructure of buildings and related engineering services such as Water reservoir, Pump house and water distribution system, drainage system. It includes electrical substation and electricity distribution, backup power supply, mechanical workshop for all kind of mechanical requirement, fitting and fabrication setup, air conditioning setup, LN2 supply and distribution, Glass blowing etc.

Along with laboratory activities, it is equally important to provide engineering backup for Colony and other outside laboratory area activities, such as Medical centre, Community centre, Guest house, Hostels etc.

Air-conditioning & Lab. furniture: Under the energy conservation drive, Survey was carried out as per guidelines of committee. About 250 air conditioners were disconnected. Other various major A.C installations like, Split, Package, Duct-able, Precision etc. were maintained.

Electrical Engineering works: Maintenance of major electrical installations like sub-stations, D.G. sets, Street lights, major pilot plants, Pump house, Liquid nitrogen, All common installations like Auditorium, Lecture hall, conference hall, board rooms etc. were carried out.

Human Resource Management

Project Training: More than 450 intern students pursuing the courses like M.Sc., M.Pharm., B.E., M.E., B.Tech., M.Tech. at various colleges, universities and Indian institutes including IITs, IISERs, and NITs as well as foreign institutes completed their Summer/Winter Projects at CSIR-NCL.

Guest workers: One guest-worker and two from abroad were trained worked at CSIR-NCL.
Institutional visits: Nine institutional visits were coordinated mainly of students pursuing professional courses in chemical sciences, medical sciences, agricultural sciences, engineering sciences, besides basic and applied sciences from postgraduate colleges located across the India.

CSIR-UGC NET Examination: The tests were conducted at Pune centre on June 18, 2017 and December 17, 2017 for 16678 and 19906 registered candidates respectively.

वित्त एवं लेखा

1.	**निधि की उपयोगिता 2016.17**	
	सीएसआईआर अनुदान राशि	
	परियोजनाएँ	(रु. लाख में)
	नेटवर्क (सी/एफ सहित)	2059.670
	गैर–नेटवर्क	20673.272
	NMITLI परियोजनाएँ	474.403
	ईएमआर एवं वैज्ञानिक पूल	193.796
	प्रयोगशाला आरक्षित निधि	453.648
	बाहरी वित्तपोषित परियोजनाएँ	2462.868
	विविध जमा राशि	66.757
	बाहरी निकायों की ओर से भुगतान	599.785
	प्रायोजित सम्मेलनों/संगोष्ठियों हेतु अमानत	17.438
	कुल	**27001.637**
2.	**प्रयोगशाला आरक्षित निधि का अर्जन**	(रु. लाख में)
	वर्ष के दौरान अतिरिक्त निधि (सीएसआईआर के अलावा) के निवेश पर अर्जित ब्याज के माध्यम से प्रयोगशाला आरक्षित निधि का अर्जन	93.394
	अन्य लेखाशीर्षों से	797.703
	कुल	**891.097**
3.	**31.3.2017 को अतिरिक्त निधि का निवेश (रु. लाख में)**	4000.000
4.	**आपत्ति–पुस्तिका मदों का निपटारा**	
	वर्ष के दौरान किए गए समायोजन	(रु. लाख में)
	निजी	1976.492
	यात्रा भत्ता /छुट्टी यात्रा रियायत	29.700
	स्थानीय	16.904
	कुल	**2023.096**
	कुल मदें	
5.	**निम्न लिखित प्रकार के वाउचर तैयार किए गए**	
	भुगतान	14154
	प्राप्त राशि	4567
	टी.ई.	334
	कुल	**19055**

FINANCE & ACCOUNTS

1.	**Funds Utilization**	
	CSIR Grant	
	Projects	(₹ in lakh)
	Network (including C/F)	2059.670
	Non-network	20673.272
	NMITLI Projects	474.403
	EMR & Scientist Pool	193.796
	Laboratory Reserve	453.648
	Externally Funded Projects	2462.868
	Misc. Deposits	66.757
	Payment on behalf of outside bodies	599.785
	Deposits for Sponsored conf. / seminars	17.438
	Total	**27001.637**
2.	**Generation of Lab Reserve**	(₹ in lakh)
	Through earning of interest on investment of surplus funds (other than CSIR) during the year	93.394
	From other heads	797.703
	Total	**891.097**
3.	**Investment of surplus funds as on 31.3.2011 (Rs. in lakh)**	4000.000
4.	**Clearance of OB items**	
	Adj. made during the year	(₹ in lakh)
	Private	1976.492
	TA/LTC	29.700
	Local	16.904
	Total	**2023.096**
	No. of items	
5.	**Following types of vouchers were generated**	
	Payment	14154
	Receipt	4567
	TE	334
	Total	**19055**

भंडार एवं क्रय

उपलब्धियां

मद	संख्या		मूल्य (रू. करोड़ में)	
	2016.17	2017.18	2016.17	2017.18
कुल प्राप्त एवं निष्पादित मांगपत्रा	2427	1490	51.93	48.70
कुल दिए गए ऑर्डर (आयातित)	144	142	30.21	21.35
कुल दिए गए ऑर्डर (स्वदेशी : ऑनलाइन आरसी ऑर्डर सहित)	2283	1348	21.72	5.92
स्थानीय खरीद ;ऑनलाइन आरसी ऑर्डर सहित)	4229	3397	10.22	6.07
वित्तीय वर्ष के दौरान समायोजित बकाया शेष	-	579	15.99	29.18
वित्तीय वर्ष 2017.18 के दौरान सीमा शुल्क से छूट प्राप्त राशि का उपयोग	-	-	0.41	0.87

Stores & Purchase 2017-18

Accomplishments

Item	Numbers		Value (₹ In Crores)	
	2016-17	2017-18	2016-17	2017-18
Total indents received and Processed	2427	1490	51.93	48.70
Total orders placed(imported)	144	142	30.21	21.35
Total orders placed (indigenous : including on line RCorders)	2283	1348	21.72	5.92
Local purchases (including. On-line RC)	4229	3397	10.22	6.07
O.Bs adjusted during the financial year 2015-16.	-	579	15.99	29.18
Utilization of Custom Duty Exemption during	-	-	0.41	0.87

Skill Development Program

Skill India' is an initiative of the Government of India that has been launched to empower the youth with particular skill sets that will not only enhance their chances of employability but also make them more productive in their work environment. Today, India has a formidable task of skilling 500 million people as only 2% of its total population are a skilled worker. At CSIR-NCL we thought that this twisted figure needs to be corrected through various result oriented quality skilling programs. Recognizing the need towards skill development, we have embarked on implementing CSIR's Skill Integrative initiative and started its first skill development course from 11th September 2017 in the area of Industrial Microorganism. Since then the skill development program is running successfully. By the end of financial year 2017-2018,

CSIR-NCL conducted skilling in areas such as:

- Industrial Microorganism (11th September 2017 to 27th September 2017)
- Gas Chromatography and GC-Mass Spectrometry (31st October 2017– 17th November 2017)
- Mass Spectrometry and Proteomics (1st September 2017 to 17th November 2017)
- Embedded Systems (11th December 2017 – 29th December 2017 (1st batch) and 20th December 2017 to 9th January 2018 (2nd batch)
- Biocompatible and Biodegradable Polymers (19thFebruary 2018 to 9thMarch 2018).

During the year 2017-2018, a total of 46 candidates were trained under various skill development programs. The main aim of our courses is to create the high-quality skilled workforce relevant to current and emerging industry needs in the S&T sector through skilling/training in diverse areas at different National Skill Qualification Framework. It further aims at promoting technopreneurship /entrepreneurship through skilling, training of the trainers and facilitation of incubation center.

We are in accessing in the capacity to skill about 1000-2000 candidates every year. Most of these courses are of 120 hours duration while some of these are 200 hours duration and charges per candidates are Rs. 10000. Additionally, CSIR-NCL also provides accommodations to the course participants on a nominal charge basis at its premises to make their training comfortable and affordable.

Finally, the sustainability of any venture or scheme depends on how it generates its own sources of finances to keep up the float. However, the training and development program has maximum share of the social cause in which poor and unemployed youth will get an opportunity to develop the skills they'll need to succeed "both in their career and beyond" and cannot afford to pay high course fees. Therefore, most of the training and development courses offered at CSIR-NCL have a nominal fee structure.

Analytical Facilities

CSIR-NCL has several state-of-the-art analytical facilities which cater its research community within the lab. The analytical facilities at CSIR-NCL include instruments for biochemical, mass spectrometric, chromatographic, elemental, magnetic, thermal, X-ray, spectroscopic, and microscopic methods of analysis. The analytical facilities are also extended to users from individuals, industries, and students/researchers from colleges, universities and other academic as well as research organizations on a payment basis.

The Centre for Materials Characterization (CMC) is a central facility for routine and advanced characterization of materials. X-ray diffraction is the basic characterization technique used for identification of solid materials and X-ray crystallo-graphy is the most powerful method for determining crystal structures of small as well as macromolecules. The mass spectrometry facility at CSIR-NCL is used for qualitative, semi quantitative and quantitative studies. The mass spectrometers are routinely used for molecular weight determina-tion/characterization of different materials.

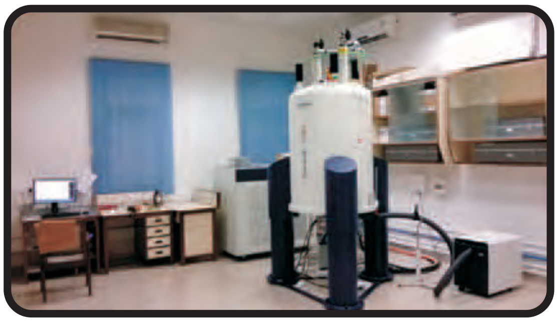
The Central NMR (Nuclear Magnetic Resonance) Facility is a resource centre providing support to all the scientific activities of the laboratory. The scientists associated with this centre also carry out research activities on application of solid state and solution state NMR spectroscopy in diverse areas of chemical, biological and materials sciences.

The National Collection of Industrial Microorganisms (NCIM) Resource Centre provides biochemical characterization services to in-house researchers, industries and academia.

Further details are available at: http://www.ncl-india.org /Analytical Facilities.

Division / center-wise earnings by technical services for 2017-18 is as follows:

Division/ Centers	**Earnings (₹ in Lakh)**
Chemical Engineering and Process Development	7.63
Catalysis and Inorganic Chemistry	27.73
Organic Chemistry	18.04
Physical and Materials Chemistry	2.86
Polymer Science and Engineering	18.88
Biochemical Sciences	6.35
Centre for Materials Characterization	33.30
Nuclear Magnetic Resonance	73.64
Total	**188.43**



Foreign Patents Granted

Title	Inventor(s)	Country: Patent No
[R/S-(2-Amino-3-Methoxy) Propyl] (R-Amp And S-Amp) Nucleic Acids	Vaijayanti A Kumar; Venubabu Kotikam	US: 9920319
A Mild And General Process For The Synthesis Of Aryl Sulfones	Santosh B Mhaske; Virat Pandya	US: 9650330
A New Method For Formation Of Ortho Alkynyl Anilines A Key Intermediate Of Dihydroquinolines System Via Copper Catalyzed Multi Component Reactions (Mcr) Of Terminal Alkynes / Arynes / Azodicarboxylate	Gurunath Suryavanshi; Anil MarutiShelke	US: 9758476
A New Organocatalytic Process For The Total Synthesis Of Stagonolide E And (-)-(6r,11r,14r)-Colletallol	Soumen Dey;Varun Rawat; Arumugam Sudalai	US: 9765048 US: 9809566
A New Organocatalytic Route For The Asymmetric Synthesis Of Novel Kainic Acid Analogs	A Sudalai ; Ravindra Dattatray Aher; Boopathi Senthil Kumar	US: 9718773
A Novel Approach In The Design Of Electrode-Electrolyte Interface Towards High A Performance All-Solid-State-Supercapacitor With Very Low Esr	Sreekumar Kurungot; Manohar Virupax Badiger; Bihag Anothumakkool; Arun Torris	US: 9905371
A Novel Aromatic Stacked Metal Oxide Nano Layer Based Nucleating Agent For Polyolefins	Chellaswamy Ramesh; Mohan Raj Mani; Vijayamohanan Kunjikrishnan Pillai	AT: 2938667 EP: 2938667 FR: 2938667 DE: 2938667
A Nucleotide Sequence Encoding Enone Oxidoreductase From 'Alphonso' Mango	Vidya Shrikant Gupta; Ram Shridhar Kulkarni; Ashok Prabhakar Giri; Keshav H Pujari	US: 9790526 US: 9650683
A One Pot And Single Step Hydrolytic Process For The Conversion Of Lignocellulose Into Value Added Chemicals	Dhepe Paresh Laxmikant; Sahu Ramakanta	DE: 2529036 FR: 2529036 EP: 2529036 ES: 2529036
A Process For Deacidification Using Membranes	Ulhas Kanhaiyalal Kharul; Ramchandra Vitthal Gadre; Vithal Venkatrao Jogdand; Yogesh Jayasing Chendake	EP: 2401066 GB: 2401066 FR: 2401066 AU: 2010217356 DE: 2401066
A Process For The Solvent-Free, Sterically Congested Passerini	Akkattu T Biju; Trinadh Kaicharla; Santhivardhana Reddy Yetratony Roy	US: 9783496
A Process For The Transition- Metal-Free N-Arylation Of Tertiary Amines	Akkattu T Biju; Sachin Suresh Bhojgude; Trinadh Kaicharla	EP: 3013787 GB: 3013787 DE: 3013787 US: 9650329
A Process For The Transition-Metal-Free Three-Component Coupling Involving Arynes, Phosphines And Aldehydes	Akkattu T Biju; Anup Bhunia; Trinadh Kaicharla	US: 9902746

Foreign Patents Granted

Title	Inventor(s)	Country: Patent No
ABPBI Based Porous Membranes	Ulhas Kanhaiyalal Kharul; Harshada Ramesh Lohokare	GB: 2539057 NL: 2539057 FR: 2539057 DE: 2539057 US: 9757696 EP: 2539057 ES: 2539057
Acidic Ionic Liquids Catalyzed Depolymerization Of Lignin	Paresh Laxmikant Dhepe; Ashutosh Anant Kelkar; Babasaheb Mansub Matsagar; Sandip Kumar Singh	SE: 2994505 EP: 2994505 FI: 2994505
Algorithm For Label Free And Internal Standard Free Maldi MS/MS Quantitation Of Structural Isomers	Venkateswarlu Panchagnula; Nivedita Bhattacharya; Avinash Dattatraya Ghanate	US: 9659759
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An Improved Process For The Preparation Of Membrane Electrode Assemblies (Meas)	Vijayamohanan Kunju Krishna; Ulhas Kanhaiyalal Kharul; Sreekumar Kurungot; Harshal Dilip Chaudhari; Sreekuttan Maraveedu Unni; Bipinlal Unni; Husain Noman	JP: 6148663 EP: 2692004 FR: 2692004 BE: 2692004 GB: 2692004 DE: 2692004
Applied Potential And Inherent Roughness Driven Reversible Switching Between Superhydrophobic And Superhydrophilic States	Kothandam Krishnamoorthy	US: 9624381
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Copper Catalyzed Carbonylation Of Halides With Cyanide: New Process For The Production Of Carboxylic Acid Derivatives.	Arumugam Sudalai; Pragati Kishore Prasad	US: 9656927
Curcumin Coated Superparamagnetic Iron Oxide Nanoparticles For Biomedical Applications	Pattayil Alias Joy; Jayaprabha Kunnoth Naduvilidam	US: 9775919
Cystine Mediated Reduction Allows Tunable Synthesis Of Different Size Of Fluorescent Au Quantum Clusters	Pankaj Poddar; Puneet Khandelwal; Dheeraj Kumar Singh	US: 9857376 GB: 2976644 DE: 2976644 EP: 2976644 FR: 2976644

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Detection Of Fluoride Ions	Satishchandra B Ogale Debanjan Guinpooja Singh	US: 9651491
Development Of NMR Chemical Shift Fingerprints And Applications	M Karthikeyan; Renu Vyas; Pattuparambil R Rajamohanan	JP: 6211182 EP: 3014504 DE: 3014504
Development Of Tricycle Structure Of Substituted Sugar Drived 1, 2, 3-Triazol Derivatives :A (Small-Molecule Library) For Screening Against Various Cancer Cell Lines And Other Related Targets	Pradeep Kumar; Anand Harbindu; Brijesh Sharma	EP: 2948454 DE: 2948454 GB: 2948454
DNA Loaded Supported Gold Nanoparticles, Process For The Preparation And Use Thereof	Prasad L V Bhagavatula; Periyasamy Shanmugham, Vijaykumar; Othalathara Usharraj, Abhilash; Bashir Mohammad Khan	KR: 10-1784904
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Iso-DNA For G-Rich Functional Oligomers	Vaijayanti Anil Kumar; Anita D Gunjal ; Moneesha Fernandes	US: 9914928

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Method For The Preparation Of Biofuels From Glycerol	Dharbha Srinivas; Lakshmi Saikia; Paul Ratnasamy	MY: 162898-A
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Methodology For The Continuous Flow Manufacturing Of Beta-Amino Crotonate	Amol Arvind Kulkarni; Ramesh Anna Joshi; Rohini Ramesh Joshi	EP: 2702035 GB: 2702035 FR: 2702035
Nanoporous Graphene Through Chemically Assisted Chipping Of Graphene Quantum Dots And Its Conversion To Efficient Oxygen Reduction Electrocatalyst Through Nitrogen Doping	Sreekumar Kurungot; Thangavelu Palaniselvam	KR: 1018358790000 JP: 6211687 US: 9637388
N-Doped Porous Carbon Derived From Graphitic C3n4-Mof Composite As An Efficient Non-Platinum Electrocatalyst	Sreekumar Kurungot	JP: 6174790
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PIP 3 Antagonist	Ramana Venkata Chepuri; Alexei Degterev	US: 9701646
Polymeric Form Of Ionic Liquids	Ulhas Kanhaiyalal Kharul Santosh Chandrakant Kumbharkar,; Rupesh Sudhakar Bhavsar	KR: 10-1845108
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Probiotic Properties From Diverse Habitant / Organisms	Archana V Pundle; Hrishikesh Vinayak Mungi; Pooja Vijay Ghushe ; Avinash Nellore Sunder	DK: 3035945 EP: 3035945 GB: 3035945 DE: 3035945 FR: 3035945
Process For Making Dimethyl Carbonate	Darbha Srinivas; Pulikkeel Unnikrishnan	JP6305989
Process For Preparing Amides	Darbha Srinivas; Anuj Kumar; Nepak Devadutta	JP: 6251691 EP: 2819994 DE: 2819994
Process For Preparing Biodegradable Lubricant Base Oils	Darbha Srinivas; Mehejabeen Kotwal	JP: 6174130
Process For Producing Furan	Darbha Srinivas; Bhogeswararao Seemala	US: 9650354
Pyrrole Derivatives With Silicon Incorporation	D Srinivasa Reddy; N Vasudevan; Sachin Bhausaheb Wagh; Remya Ramesh	US: 9657037
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Solomonamides Analogues And Synthesis Thereof	Mahalingappa Hengne Dumabala Srinivasa Reddy; Kashinath Kormirishetty;	US: 9751911
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Surface Modified Porous Polyethylene As Reservoir Scaffolds For Pancreatic Cells	Anup Bhunia; Tony Roy B L V Prasad	US: 9617280 KR: 10-1776977
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Synthesis Of Dimethyl Carbonate (Dmc) From Methanol And Urea In Presence Of Stripping With Inert Gas	Vivek Vinayak Ranade; Ashutosh Anant Kelkar; Vilas Hari Rane; Kisan Kinage; Savita Kiran Shingote; Lalita Sanjib Roy	US: 9920000
Synthesis Of Disuphonic Acids Starting From Cashew Nut Shell Liquid: Crosslinking Catalysts For Silane Functionalized Polyolefins	Prakash P Wadgaonkar; Bhimrao D Sarwade; Bhausaheb Vilas Tawade	EP: 2788319 FR: 2788319 DE: 2788319
Synthesis Of Indazole Derivatives And Uses Thereof	D Srinivasa Reddy; Chaitanya Saxena; Kashinath Komirishetty	ES: 3027605 US: 9737510 DK: 3027605 EP: 3027605 DE: 3027605 GB: 3027605 FR: 3027605 IE: 3027605 IT: 3027605 CH: 3027605 BE: 3027605 NL: 3027605
Synthesis Of Spherical And Fluorescent Nanostructures Using Sophorolpids	Asmita Ashutosh Prabhune; Pradeep Kumar Singh; Ruchira Arup Mukherji; S. B. Ogale	FR: 2844304 EP: 2844304 GB: 2844304
Synthesis Of Tamiflu Employing Stereospecific Amidoalkylation Protocol And Ramberg-Backlund Reaction	Subhash Prataprao Chavan ; Prakash Narsing Chavan	US: 9757481 EP: 3052473 DE: 3052473
Synthesis Of Tricyclic Compounds And Uses Thereof	Dumbala Srinivasa Reddy Kashinath Komirishetty; Prakash Daulat Jadhav	GB: 3052473 US: 9771325
Synthesis, Gas Separation And Fluorescence Properties In A Polybenzimidazole Based Poly(Yionic Liquid)S With Pyrene And Anthracene Fluorophore	Ulhas Kharul ; Sayali Vinayak Shaligram; Prakash Purushottam Wadgaonkar	EP: 3110874 FR:3110874 GB: 3110874 DE:3110874
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Tube In Tube Continuous Glass-Lined Reactor	Amol Arvind Kulkarni; Vivek Vinayak Ranade	DE: 3079805 NL: 3079805 CH: 3079805 FR: 3079805 EP: 3079805
Useful Compounds From Anisomeles	Swati Pramod Joshi; Roshan Rajan Kulkarni; Ketki Dilip Shurpali; Sampa Sarkar; Dhiman Sarkar	US: 9801918
Utilization Of Long-Chain Branched (Lcb) Polypropylene In Extrusion Film Casting Or Extrusion Coating Processes	Ashish K Lele; Harshawardhan V Pol; Kalyani Chikhalikar	DE: 2800764 EP: 2800764 IT: 2800764 FR: 2800764
Vortex Diodes As Reactors And Effluent Treatment Devices	Vivek V Ranade; Amol A Kulkarni; Vinay M Bhandari	US: 9725338
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Aryl Phosphonates And Process For The Preparation Thereof	Santosh B Mhaske; Ranjeet Ashokrao Dhokale	295285
Aziridination Of Olefins	Pratibha Uttam Karbal; Pandurang Vilasrao; Tanveer Mahamadali; Gurunath Mallappa Suryavanshi; Arumugam Sudalai	295227
Catalytic Dehydration Of Lactic Acid To Acrylic Acid	Mohan K Dongare; Shubhangi Umbarkar; Samadhan Lomte	291730
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Silica Encapsulated Au Clusters	R Nandini Devi; Anupam Samanta	292982
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Patil, S. S.	Exploitation of controlled/living Polymerazation Methods and Click Chemistry Approach for Sythesis of Designed macromolecular Archetectures	Wadgaonkar, P. P.
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Savitribai Phule Pune University

Author	Title	Guide(s)
Negel, A.	Conceptually new approach to the total synthesis of (-) - lycorine and (-) - alpha -lycorane	Pandey, G. C.
Ghugare, Suhas B.	Design and development of computational intelligence based methodologies for chemical engineering and technology application	Tambe, Sanjeev S.
Baravkar, S. B.	Developing novel bioactive peptides featuring alpha, beta hybrid peptides and investigations of competing folding in synthetic oligomers	Sanjayan, G. J.
Kheria, S.	Exploring non - covalent interactions in developing synthetic zipper structure and prototropy - free self - complementary quadrupal H-bonding arrays	Sanjayan, G. J.
Sardessai, R. S.	Inositol 1,3 -acetals as versatile intermediates for the synthesis of cyclitol derivatives	Shashidhar, M. S.
Upasani, M. L.	Molecular characterization of chickpea - fusarium oxysporum f. sp. ciceri interaction	Gupta, Vidya S.
More, Snehal Vijay	Production optimization and applications of industrially important enzymes from beauveria Sp. MTCC 5184	Prabhune, Asmita A.
Phatake, Ravindra S.	Unexplored olefin oxidations with oxone and application of alpha-diazocarbonyl compounds in the synthesis of N-heterocycles	Ramana, C. V.

CSIR-NCL Customers

Indian

- Aditya Birla Science & Tech. Co. Ltd
- Ajeet Seeds Ltd.
- AltReal Bio- Innovations P. Ltd.
- Amar Equipments P. Ltd.
- Analytical Solutions
- Apothecon Pharmaceuticals P. Ltd.
- Aquapharm Chemicals P. Ltd.
- Aura Innovations P. Ltd.
- Bharat Forge Ltd.
- Biocon India Ltd.
- Cadila Healthcare Ltd.
- Centaur Pharmaceuticals P. Ltd.
- Currency Note Press (SPMCIL- CNP)
- Deccan Nutraceuticals P. Ltd.
- Delta Finochem P. Ltd.
- Dr. Reddy's Laboratories Ltd.
- E.I. DuPont India P. Ltd.
- Emcure Pharmaceuticals Ltd.
- Glenmark Pharmaceuticals Ltd.
- Godavari Sugar Mills Ltd.
- Godrej Agrovet Ltd.
- Godrej Industries Ltd.
- GSP Crop Science P. Ltd.
- Gulbrandsen Chemicals P. Ltd.
- Indofil Industries Ltd.
- Macleods Pharmaceuticals Ltd.
- Mallak Specialties P. Ltd.
- Multi Vaccines Development Program
- Mysore Paints and Varnish Ltd.
- Nayam Innovations P. Ltd.
- Nichem Solutions
- North Maharashtra University
- OmiX Research & Diagnostics Lab P. Ltd.
- PET Packaging Asso. for Clean Environ.
- Praj - Matrix
- Praj Industries Ltd.
- Ratnamani Biochemicals & Pharmaceuticals P. Ltd.
- Redox Pharmachem P. Ltd.
- Reliance Industries Ltd.
- Renault Nissan Tech & Business Centre India P. Ltd.
- Sarna Chemicals P. Ltd.
- Sudarshan Chemical Industries Ltd.
- Tata Chemicals P. Ltd.
- Torrent Pharmaceuticals P. Ltd.
- Ventri Biologicals
- Vivira Process Technologies P. Ltd.
- Watson Pharma P. Ltd.

Foreign

- Chem-Impex International Inc.
- Kraton Polymers LLC
- Exxon Mobil Res. & Engg. Company
- General Cable Corporation
- General Mills Inc.
- GlaxoSmithKline LLC
- Kraton Polymers LLC

Publicly Funded

- Bharat Petroleum Corporation
- GAIL (India) Ltd.
- Hindustan Petroleum Corporation Ltd.
- Mangalore Refinery and Petrochemicals Ltd.
- Rajiv Gandhi Sci. & Tech. Commission

Dateline CSIR-NCL

Date	Event
May 11, 2017	National Technology Day Celebrations
June 08, 2017	Conference on Sustainable Catalytic Technologies at CSIR-NCL
June 18, 2017	Visit of Ethiopian Delegation
August 20, 2017	CSIR Platinum Jubilee Mega Exhibition, Pune
August 29, 2017	Crystallography and Society: Satellite conference in Pune at CSIR-NCL
September 29, 2017	75th CSIR Foundation Day Celebration
December 11, 2017	Symposium on “Modern Trends in Inorganic Chemistry”
Januray 5, 2018	68th CSIR-NCL Foundation Day Celebration
January 18, 2018	Indo-Japan International Conference (IJC-2018)
February 28, 2018	National Science day Lecture by Prof. Anil K. Bhowmick Professor of Eminence & INAE Chair Professor IIT, Kharagpur on "Sustainable Materials in the Polymer Industry : Science & Technology
March 06, 2018	Safety week celebration and Safety day Lecture by Mr. Sanjay Nirgudkar on Safety in Chemical Handling
March 25, 2018	Ramanujan Conclave - 2018

Awards/ Recognitions

Name	Award
Dr. D. Srinivasa Reddy	The ‘Sun Pharma Research Award’ (also known as ‘Ranbaxy Research Award’) in the field of Pharmaceutical Sciences
Dr. D. Srinivasa Reddy	A Fellow of the National Academy of Sciences (NASI), India.
Dr. Sakya S. Sen	The CSIR Young Scientist Award for the year 2017 in Chemical Sciences.
Dr. Sakya S. Sen	Young Associate of the Indian Academy of Sciences, Bangalore
Dr. Pankaj Poddar	Electron Microscope Society of India (EMSI) Fellow Award for the year 2017
Dr. Dinesh Jagadeesan	INSA Young Scientist Award 2017
Dr. Rahul Bhambure	Early Career Research Award from the Department of Science and Technology, New Delhi
Dr. Magesh Nandagopal	Chevening Rolls-Royce Science Innovation and Leadership Programme (CRISP) Fellowship 2017

Outreach Program

CSIR- National Chemical Laboratory and Indian Institute of Science, Education and research, Pune conducts an Outreach Programme which is the science activity for science popularization and awareness. The purpose is to boost the excitement of science and technology with school children. Following talks were organized during the year.

Date	Topic	Speaker
16 April, 2017	Polynomials that no one can solve!	Dr. Supriya Pisolkar, IISER, Pune
28 May, 2017	Exciting Photochemistry	Dr. Jayaraj Nithyanandan, CSIR-NCL, Pune
11 June, 2017	Nuclear Research Reactors and their Utilization	Dr. Dilip Kumar Lahiri, Retired from BARC, Mumbai
23 July, 2017	Mix it Up! The science of mixtures and separation techniques	Dr. Rahul Bhambure, CSIR-NCL, Pune
20 August, 2017	Euler, Plato and balloons	Dr. Tejas Kalelkar, IISER-Pune
24 September, 2017	Cell Migration: The voyage of building blocks of life	Dr. Kiran Kulkarni, CSIR- NCL, Pune
29 October, 2017	Wave particle duality: Some exciting experiments with ultra-cold matter	Dr. Umakant Rapol, IISER-Pune
19 November, 2017	Plant-Insect Interactions	Dr. Sagar Pandit, IISER-Pune
17 December, 2017	Behavior and Natural History: What we can learn from the birds and the bats!	Dr. Anand Krishnan and Dr. Rohit Chakravarty, IISER-Pune
21 January, 2018	The Afterlife of Your Water Bottle? The Story of how PET bottles are recycled into t-shirts, pillows and soft-toys	Dr. Magesh Nandagopal, CSIR-NCL, Pune
4 Febraury, 2018	Light, colors and action	Prof. Arnab Bhattacharya, TIFR, Mumbai
18 February, 2018	Excursions through Science, Technology and Medicine, employing Case Studies	Prof. John Mathew, IISER-Pune
18 March, 2018	When electrons dance in pairs - the story of superconductivity	Dr. Sunil Nair, IISER-Pune

CSIR HARIT

CSIR-800 program has objective to achieve the inclusive growth and improved quality of life and bring smiles to the faces of 800 million citizens of India through socially and economically relevant science and technology interventions.

CSIR-NCL deployed 32 water filtration units having capacity of 50 LPH in the rural areas of Kada Taluka (District- Beed, Maharashtra) through NAAM foundation. These units were deployed primarily in Zilla parishad schools. NAAM foundation through NCL research students assisted in identifying the beneficiary schools. It has also deployed 172 water filtration units of same capacity in tribal areas of Kalyan and Vikramgad. Twenty portable concrete Toilets were installed in schools of Wada and Vikramgad Talukas. The portable concrete toilets were installed in girl schools.

Osmanabad and Nandurbar are aspirational districts assigned to CSIR-NCL. In a meeting with DM of Nandurbar, the technologies available with CSIR were briefed. DM and VSTF representatives showed interest in Water filtration unit and Shudh-Jal plant. Accordingly guidance is being provided. The work has been started for the installation of Shudh-Jal Plant at North Maharashtra University, Jalgaon and discussions have been initiated for its installation at Swami Ramanand Teerth Marathwada University, Nanded and IIT Bhilai.

हिन्दी कार्यशाला रिपोर्ट

सीएसआईआर – एनसीएल में हिन्दी अनुभाग द्वारा राजभाषा हिन्दी के कार्यान्वयन को बढ़ावा देने तथा स्टफ सदस्यों की हिन्दी में कार्य के प्रति रुचि बढ़ाने के उद्देश्य से दिनांक 1 मार्च, 2018 को तकनीकी तथा प्रशासनिक स्टाफ के लिए हिन्दी कार्यशाला का आयोजन किया गया। कार्यक्रम में प्रशिक्षण देने के लिए सीएसआईआर – एनआईओ (CSIR & NIO) के हिन्दी अधिकारी डॉ. राकेश शर्मा उपस्थित थे।

कार्यक्रम के आरंभ में हिन्दी अधिकारी ने अतिथि व्याख्याता डॉ. राकेश शर्मा का स्वागत किया तथा कार्यक्रम के उद्देश्य के बारे में जानकारी देते हुए बताया कि केंद्र सरकार की राजभाषा नीति का कार्यान्वयन प्रत्येक केंद्रीय कर्मचारी / अधिकारी का संवैधानिक कर्तव्य है। इस संबंध में राजभाषा विभाग द्वारा प्रत्येक वर्ष वार्षिक कार्यक्रम जारी किया जाता है तथा क्षेत्रवार लक्ष्य निर्धारित किए जाते है। समय समय पर संसदीय राजभाषा समिति तथा मुख्याालय से प्राप्त निर्देशानुसार सभी विभागों को राजभाषा हिन्दी में कार्य करना अत्यंत आवश्यवक है। ईमेल या कम्प्युटर पर सभी भाषाओं में कार्य करने के लिए अद्यतन सुविधाएं उपलब्ध है जिनके द्वारा कम्प्युटर पर राजभाषा हिन्दी में कार्य करना सरल और रुचिकर हो गया है, किन्तु जानकारी के अभाव और अभ्यास की कमी के कारण इन सुविधाओं का उपयोग नहीं हो पाता । इसी अभ्यास की निरंतरता को बनाये रखने तथा अधिक से अधिक कार्य राजभाषा में करने के लिए हिन्दी विभाग द्वारा इस कार्यक्रम का आयोजन किया गया है ।

डॉ. राकेश शर्मा ने कंप्यूटर पर यूनिकोड सक्रिय करने, कंप्यूटर पर हिन्दी के उपयोगी सॉफ्टवेयर और उनका उपयोग तथा मोबाईल के माध्यम से गूगल वॉयस टायपिंग के बारे में विस्तृत जानकारी देते हुये प्रत्यक्ष मार्गदर्शन दिया। उपस्थित सभी कर्मचारियों / अधिकारियों ने प्रयोग करके प्रत्यतक्ष अनुभव लिया। प्रशिक्षण में सभी विभागों के कर्मचारियों ने उत्सानहपूर्वक हिस्सा लिया। कार्यक्रम के दौरान प्रतिभागियों की व्येवहारिक कठिनाईयों का समाधान भी किया गया।

कार्यक्रम के अंत में हिन्दी् अधिकारी ने धन्यवाद ज्ञापन प्रस्तुत किया तथा सभी विभाग प्रमुखों से राजभाषा कार्यान्वरयन में अपना सहयोग प्रदान करने का अनुरोध किया।

हिन्दी पखवाड़ा

एनसीएल में दिनांक 14 से 27 सितंबर, 2017 के दौरान हिन्दी पखवाड़ा समारोह आयोजित किया गया। हिन्दी पखवाड़े के अंतर्गत राजभाषा हिन्दी के प्रयोग को बढ़ावा देने की दृष्टि से विभिन्न हिन्दी प्रतियोगिताएं, हिन्दी संबंधी गतिविधियों का आयोजन किया गया, जिनमें स्टाफ एवं शोध छात्रों ने बड़ी संख्या में उत्साहपूर्वक प्रतिभाग लिया।

दिनांक 14 सितंबर, 2017 को हिन्दी पखवाड़ा शुभारंभ एवं गृहपत्रिका 'एनसीएल आलोक' का लोकार्पण किया गया। इस अवसर पर मुख्य अतिथि के रूप में गरवारे कॉलेज के हिन्दी विभाग प्रमुख तथा प्रसिद्ध लेखक डॉ. ओमप्रकाश शर्मा तथा अध्यक्ष के रूप में डॉ. एस. पी. चव्हाण (अध्यक्ष– कार्बनिक रसायन प्रभाग एवं प्रमुख वरिष्ठ वैज्ञानिक) उपस्थित थे।
मुख्य अतिथि डॉ. ओमप्रकाश शर्मा ने अपने संबोधन में कहा कि 'आज विभिन्न क्षेत्रों में हिन्दी का प्रयोग निरंतर और लोकप्रियता बढ़ रही है। अपनी सरलता–सहजता के बल पर हिन्दीा मीडिया, वाणिज्यो, उद्योग–व्यापार इत्यादि क्षेत्रों में केवल भारत ही नहीं बल्कि समूचे विश्वय में अपने पंख पसार रही है। हिन्दी हमारे देश की केवल संपर्क भाषा नहीं बल्कि जन भाषा है। इसके बावजूद भी हम सभी भारतीयों को इस भाषा के प्रचार–प्रसार में अपना योगदान देने की आवश्यकता है ताकि शिक्षा, रोजगार और प्रशासन के क्षेत्र में इस भाषा को अच्छी तरह से लागू किया जा सकें।' उन्होंने एनसीएल द्वारा राजभाषा पत्रिका एनसीएल आलोक के प्रकाशन पर प्रसन्नता व्यक्त करते हुए कहा कि 'विभिन्न प्रकार के वैज्ञानिक एवं तकनीकी लेखों को जन मानस की सरल भाषा में प्रस्तुत किया जाना एक बहुत बड़ी उपलब्धि है, इससे निश्चय ही हिन्दी भाषा का प्रचार–प्रसार होगा एवं विज्ञान के क्षेत्र में भी इस भाषा का उपयोग बढ़ेगा।'

कार्यक्रम के अध्यक्ष तथा प्रमुख वैज्ञानिक डॉ. एस. पी. चव्हाण ने अपने संबोधन में कहा कि – 'हिन्दी हमारे राष्ट्र की भाषा है, हमारे देश की पहचान है। इस अवसर पर हम सभी यह संकल्प करें कि केवल हिन्दी ही नहीं बल्कि सभी भारतीय भाषाओं के माध्यम से देश की अखण्डता बनाए रखेंगे। हमारे एनसीएल में हिन्दीभाषा का प्रशासन तथा अन्य सभी क्षेत्रों में संतोषजनक प्रयोग हो रहा है। हिन्दी पत्रिका का प्रकाशन, वेबसाईट का द्विभाषीकरण तथा हिन्दी माध्यम से संगोष्ठियों का आयोजन हमारी हिन्दी भाषा के प्रति निष्ठा का प्रमाण है।' उन्होंने उपस्थित स्टाफ सदस्यों् से अपील की कि 'सभी वैज्ञानिक/अधिकारी/कर्मचारी अधिक से अधिक राजभाषा हिन्दीं में कार्य करें और अपने राजभाषा संबंधी दायित्वों को निभाएं। यह अत्यंत आवश्यक है कि अनुभाग/प्रभाग प्रमुखों को इस दिशा में पहल करनी होगी, वे स्व यं भी हिन्दीह में कार्य करें तथा अपने अधीनस्थन कर्मचारियों को हिन्दी में कार्य करने एवं हिन्दी पखवाड़ा के दौरान सभी गतिविधियों में प्रतिभागिता के लिए प्रोत्साहित करें'।
तत्पश्चात हिन्दी अधिकारी डॉ. श्रीमती स्वाति चढ्ढा द्वारा हिन्दी पखवाड़े की प्रस्तावना प्रस्तुत की गई। कार्यक्रम के अंत में हिन्दी पखवाड़ा आयोजन समिति की अध्यक्ष तथा वरिष्ठ प्रधान वैज्ञानिक डॉ. श्रीमती शुचिश्वेता केंदुरकर ने सभी के प्रति आभार व्यक्त किया।

हिन्दी पखवाड़े के दौरान एक दिवसीय हिन्दी कार्यशाला, एक दिवसीय वैज्ञानिक परिचर्चा 'समाज हेतु विज्ञान', हिन्दी शुद्धलेखन प्रतियोगिता, हिन्दी काव्यपाठ प्रतियोगिता, सामान्य ज्ञान प्रतियोगिता, शब्द ज्ञान प्रतियोगिता एवं हिन्दी निबंध लेखन प्रतियोगिताओं का आयोजन किया गया।

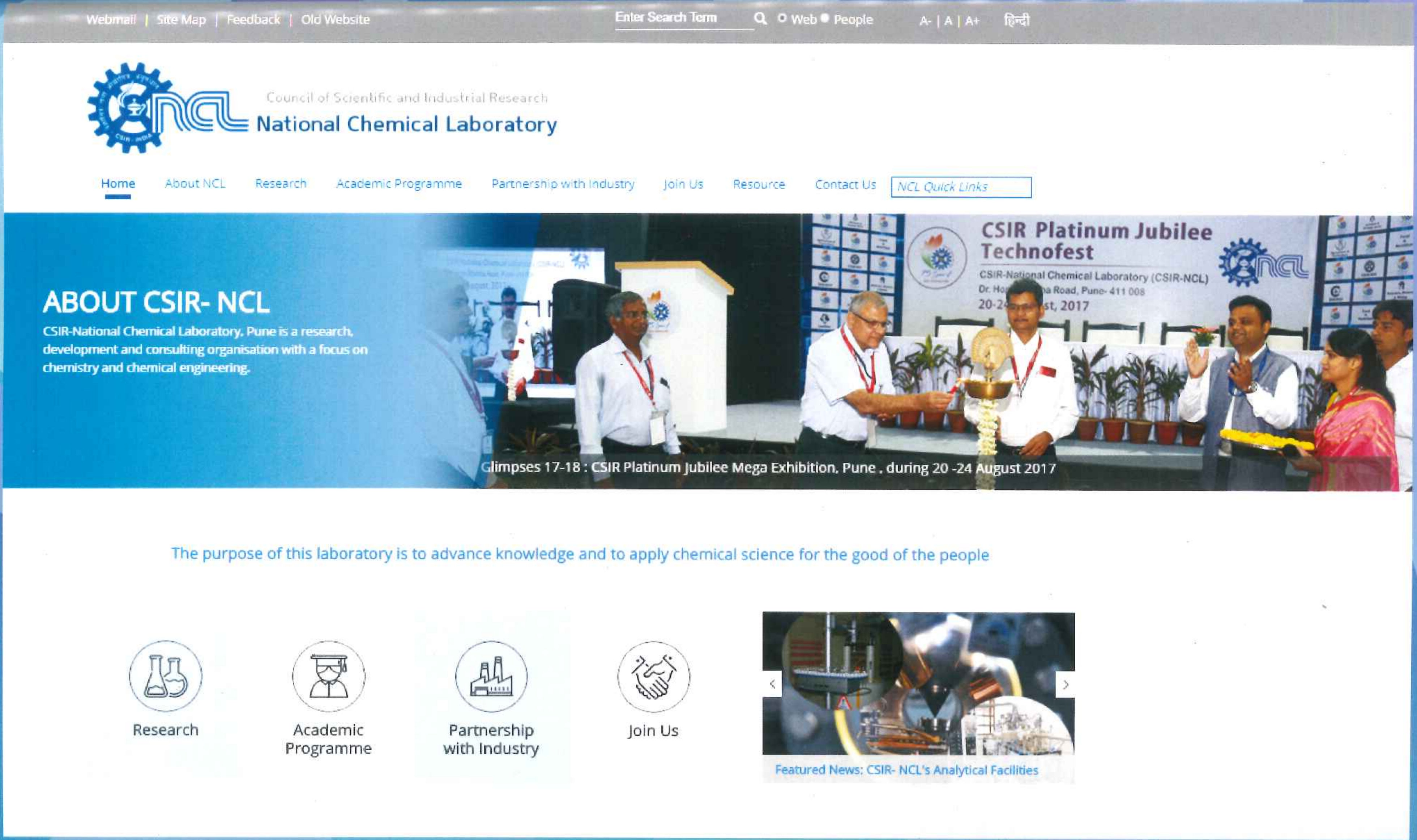
हिन्दी कार्यशाला रिपोर्ट

इन सभी प्रतियोगिताओं के पुरस्कार दिनांक 27 सितंबर, 2017 को आयोजित पुरस्कार वितरण समारोह में प्रदान किए गए। इस अवसर पर अध्यक्ष के रूप में प्रा. अश्विनी कुमार नांगिया, मुख्य अतिथि के रूप में आई.आई.टी.एम. के प्रमुख वैज्ञानिक डॉ. गुरफान बेग तथा सम्मानित अतिथि के रूप में आई.आई.टी.एम. के हिन्दी अधिकारी तथा नगर राज. समिति के सचिव डॉ. ओंकारनाथ शुक्ला, हिन्दीं पखवाड़ा आयोजन समिति की अध्यक्ष डॉ. श्रीमती शुचिश्वेता केंदुरकर, प्रशासन अधिकारी श्रीमती पूजा कुलकर्णी एवं हिन्दी अधिकारी डॉ. श्रीमती स्वाति चढ्ढा उपस्थित थी।

समारोह के आरंभ में डॉ. श्रीमती शुचिश्वेता केंदुरकर ने हिन्दी पखवाड़े की प्रासंगिकता एवं इस दौरान आयोजित गतिविधियों की जानकारी दी। मुख्य अतिथि डॉ. गुरफान बेग ने अपने उद्बोधन में कहा कि "हमें यह नहीं भूलना चाहिए कि हमारी अपनी भाषा हिन्दीं का मान देश का मान है। विश्वस्तर पर हमारी अपनी पहचान हमारी राष्ट्रभाषा, राष्ट्रध्वज एवं राष्ट्रगान से ही होती है। विश्व के अनेक देशों ने अपनी भाषा के माध्यम से ही सभी स्तरों पर प्रगति की है। हम भारतीयों को उनसे सीख लेने की जरूरत है।" कार्यक्रम के अध्यक्ष निदेशक प्रो. अश्विनी कुमार नांगिया जी ने कहा कि जिस प्रकार हम अपने राष्ट्रध्वज और राष्ट्र गीत का सम्मान करते हैं, उसी तरह हम सबको अपनी राजभाषा– राष्ट्रभाषा हिन्दी का भी सम्मान करना चाहिए और अपनी भाषा का अधिक से अधिक प्रयोग करके उसके विकास में अपना योगदान देना चाहिए। मुझे विश्वास है कि हमारी प्रयोगशाला के सभी वैज्ञानिक और अधिकारी/कर्मचारी अपना अधिकाधिक कार्य हिन्दी में करके राष्ट्रसेवा में अपना अमूल्य योगदान देंगे।'

इस कार्यक्रम में विभिन्न प्रतियोगिताओं के विजेताओं तथा सरकारी कामकाज में राजभाषा हिन्दी का उल्लेखनीय प्रयोग करने वाले अधिकारियों/कर्मचारियों को अध्यक्ष एवं मुख्य अतिथि के करकमलों द्वारा पुरस्कृत किया गया। साथ ही विभिन्न प्रतियोगिताओं में आंतरिक निर्णायक की भूमिका निभाने वाले पदाधिकारियो को भी स्मृति चिन्ह देकर सम्मानित किया गया।

अंत में श्रीमती पूजा कुलकर्णी, प्रशासन अधिकारी ने सभी के प्रति धन्यवाद ज्ञापित किया। समारोह की कार्यवाही का संचालन हिन्दी अधिकारी डॉ. श्रीमती स्वाति चढ्ढा ने किया। इस संपूर्ण आयोजन में हिन्दी पखवाड़ा समिति की अध्यक्ष डॉ. श्रीमती शुचिश्वेता केंदुरकर तथा सदस्य श्रीमती गौरी मांडे, श्री वी. आर. पाटिल, श्री सुभाषचंद्र मिश्र, श्री योगेश महाजन ने महत्वपूर्ण भूमिका निभाई।



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