

ANNUAL REPORT 2015-16



सीएसआईआर-राष्ट्रीय रासायनिक प्रयोगशाला  
**CSIR-National Chemical Laboratory**  
 वैज्ञानिक तथा औद्योगिक अनुसंधान परिषद

**Published by**  
**Prof. Ashwini Kumar Nangia**  
Director, CSIR-NCL

**Compiled and Edited by**  
**Dr. P. K. Ingle**  
Head,  
Publication & Science Communication Unit,  
CSIR-NCL

**Editorial Assistance**  
**Mr. G. S. Mane**  
Publication & Science Communication Unit,  
CSIR-NCL

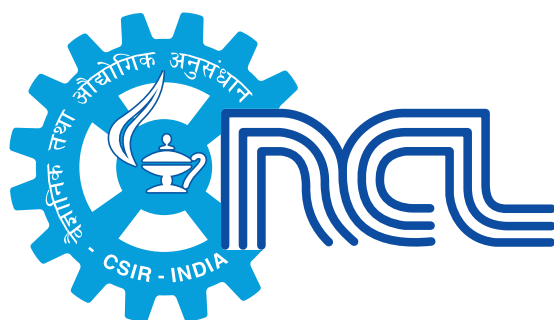
**Designed by**  
**Ms. Sonali Shinde**  
Publication & Science Communication Unit,  
CSIR-NCL

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सीएसआईआर – राष्ट्रीय रासायनिक प्रयोगशाला

**CSIR - National Chemical Laboratory**

वार्षिक प्रतिवेदन 2015 - 16



With Best Compliments from●

**Prof. Ashwini Kumar Nangia**  
**Director**

**CSIR-National Chemical Laboratory**

Dr. Homi Bhabha Road, Pune - 411 008, India Ph: (Off) +91 20 2590 2600; Fax: +91 20 2590 2601  
Email: [director@ncl.res.in](mailto:director@ncl.res.in); URL: [ncl-india.org](http://ncl-india.org)

# CONTENT

निदेशक की कलम से	.....	04
From The Director's Desk	.....	06
Vision, Mission & Guiding Principles & Values	.....	08
Organization Chart	.....	09
Research Areas	.....	10
Research Council	.....	11
Management Council	.....	12

## PERFORMANCE INDICATORS

Science Performance Indicators	.....	14
Technology Performance Indicators	.....	15
Human Resource Indicators	.....	16
Financial Performance Indicators	.....	20
Outputs and Outcomes	.....	23

## Research & Development Reports

Research Highlights	.....	26
<b>Advanced Materials</b> (Nanostructured materials, Materials for energy, Functional materials, Polymers, Composite materials, Biomaterials, Materials for environmental & healthcare applications )	.....	42
<b>Agriculture, Food &amp; Nutrition</b> (Crop protection, Plant diversity and bio-prospecting, Plant secondary metabolites & pathway analysis)	.....	63
<b>Energy &amp; Environment</b> (Conventional energy coupled with CO <sub>2</sub> capture, storage & utilization, Renewable & alternative energy technologies, Emission & effluent control including water & soil management, Water: treatment, disinfection, purification)	.....	68
<b>Healthcare</b> (Natural products & methodology, Screening methods & bioassays, Chemical biology, Medicinal chemistry, Synthesis of API, Identification of lead molecules)	.....	76
<b>Sustainable Chemical Industry</b> (Process intensification & engineering, Process development & scale-up, Process separations, Catalysis, Biochemical processes & engineering, Multiphase reactors & flow processes, Mathematical & computational modeling, Chemical engineering science)	.....	110



## RESOURCE CENTERS

Catalyst Pilot Plant	.....	134
Central NMR Facility	.....	134
Center for Materials Characterization	.....	135
Digital Information & Knowledge Resource Center	.....	135
National Repository of Molecules	.....	136
National Collection of Industrial Microorganisms	.....	136

## S & T SUPPORT SERVICES

Business Development	.....	138
Publication & Science Communication	.....	138
Engineering Services	.....	139
Instrumentation & Communication	.....	139
Human Resource Management	.....	139
वित्त एवं लेखा	.....	140
Finance & Accounts	.....	141
भण्डार एवं क्रय	.....	142
Stores & Purchase	.....	142

## ANNEXURES

Patents Granted: Foreign & Indian	.....	144
PhD Theses	.....	148
Network Projects	.....	152
CSIR-NCL Customers	.....	155
Dateline CSIR-NCL	.....	156
Awards / Recognitions	.....	157
Outreach Programme	.....	158
राजभाषा रिपोर्ट	.....	159

## निदेशक की कलम से...

अत्यंत प्रसन्नता का विषय है कि वर्ष 2015-16 के लिए सीएसआईआर-राष्ट्रीय रासायनिक प्रयोगशाला की वार्षिक रिपोर्ट प्रस्तुत करने का सुअवसर मुझे प्राप्त हुआ। यह 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। इस प्रयोगशाला का बाहरी नकदी आय हमारे बजट का लगभग 20 प्रतिशत है, जो सीएसआईआर-प्रयोगशालाओं के आत्मनिर्भर बनने के लक्ष्य की दिशा के अनुरूप है।

वर्ष के दौरान बहुत से महत्वपूर्ण कार्यक्रमों का आयोजन हमारे द्वारा किया गया। भारतीय प्रौद्योगिकी संस्थान, पवई, मुंबई के निदेशक डॉ. देवांग खरखर ने सीएसआईआर-स्थापना दिवस समारोह में “A New Era for R&D in India: The Role of CSIR” नामक विषय पर व्याख्यान दिया। प्रो. रामागोपाल राव, प्राध्यापक-विद्युत अभियांत्रिकी विभाग, भारतीय प्रौद्योगिकी संस्थान, पवई, मुंबई द्वारा एनसीएल-स्थापना दिवस समारोह में “Bridging Chemistry with Nanoelectronics- A Roadmap for Future Smart Electronic Systems” नामक व्याख्यान प्रस्तुत किया गया। राष्ट्रीय विज्ञान दिवस के उपलक्ष्य में प्रो. ए. बी. पंडित, रासायनिक प्रौद्योगिकी संस्थान, मुंबई द्वारा “Chemical Engineering Forays in Rural India” विषय पर व्याख्यान प्रस्तुत किया गया।

वर्ष के दौरान प्रयोगशाला के द्वारा इंडस्ट्रियल ऑटोमेशन एवं प्रोसेस कंट्रोल, सिंथेसिस, कैरेक्टराइजेशन, एवं एप्लीकेशन ऑफ नैनोपार्टिकल्स एसेंबलीज कार्यशालाओं का भी आयोजन किया गया। रिसर्च स्कालर्स सम्मेलन में प्रो. के. एन. गणेश, निदेशक, आईसर, पुणे ने अपना व्याख्यान प्रस्तुत किया।

प्रयोगशाला द्वारा राष्ट्रीय तथा अंतर्राष्ट्रीय स्तर के जर्नल्स में 600 से भी अधिक शोधपत्र प्रकाशित किए गए, जो कि वैज्ञानिक प्रकाशन के क्षेत्र में हमारी एक बड़ी उपलब्धि है। प्रयोगशाला ने प्रौद्योगिकियों को विकसित करने एवं उन्हें उद्योगों को स्थानांतरित करने के अपने प्रयास को जारी रखा है। इन प्रक्रियाओं और प्रौद्योगिकियों के कुछ उदाहरण हैं- batch to continuous nitration process for the production of pendimethalin, modelling framework for underground coal gasification, parametric effect on continuous flow nitration and photobromination reaction, scale-up preparation and characterization of molecular sieves, process for p-aminophenol from nitrobenzene, and hydrothermal conversion of lipid oils. औद्योगिक अपशिष्ट जल (industrial effluent) के लिए वोस्टेक्स डायोड हाइड्रोडायनामिक केविटेशन डिजाइन से संबंधित तकनीकी जानकारियों के व्यवसायीकरण के लिए लाइसेंस प्रदान किया गया।

इन गतिविधियों 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।

मैं अपने पूर्ववर्ती निदेशकों डॉ. सौरव पाल एवं डॉ. विजयमोहनन पिल्लै के सहयोग एवं समर्थन का उल्लेख करना चाहता हूँ कि उन्होंने इस रिपोर्ट की कालावधि के दौरान अनुसंधान संबंधी गतिविधियों तथा वैज्ञानिकों एवं स्टाफ के कार्यनिष्पादन को दिशा प्रदान की। मैं सीएसआईआर-एनसीएल के अनुसंधान परिषद और प्रबंधन परिषद के साथ ही महानिदेशक, सीएसआईआर एवं सीएसआईआर मुख्यालय, नई दिल्ली के स्टाफ को उनके सतत समर्थन एवं सहयोग के लिए धन्यवाद देना चाहता हूँ। अंत में मैं सीएसआईआर-एनसीएल के विभिन्न हितधारकों, वैज्ञानिकों, स्टाफ एवं विद्यार्थियों के प्रति अपनी कृतज्ञता प्रगट करता हूँ, जिनके उत्कृष्ट कार्यनिष्पादन को सम्मिलित करके इस वार्षिक रिपोर्ट को बनाया जा सका।

आश्विनी कु. नांगिया

(अश्विनी कु. नांगिया)



## From the Directors Desk...

I take this opportunity to present the Annual Report of CSIR-National Chemical Laboratory, Pune for the year 2015-16. This report summarizes the achievements in the areas of basic sciences as well as processes and technologies developed during the year. The laboratory has progressed in the number and quality of publications and strengthened its association with industry partners. The external cash flow stood at about 20% of our budget, which is in line with the goal of CSIR labs to attain self-sufficiency.

Several important events took place during the year. Prof. Devang Khakhar, Director, IIT Powai, Mumbai delivered the CSIR Foundation Day lecture on the topic "A New Era for R&D in India: The Role of CSIR". The CSIR-NCL Foundation Day Lecture was presented by Professor Ramgopal Rao, P. K. Kelkar Chair Professor, Department of Electrical Engineering, IIT Powai, Mumbai on the topic "Bridging Chemistry with Nanoelectronics - A Roadmap for Future Smart Electronic Systems". The National Science Day lecture was given by Prof. A. B. Pandit, Institute of Chemical Technology, Mumbai on the theme of "Chemical Engineering Forays in Rural India".

The Laboratory hosted workshops on Industrial Automation and Process Control and Synthesis, Characterization and Application of Nanoparticle Assemblies during the year. The Research Scholars meet was addressed by Prof. K. N. Ganesh, Director, Indian Institutes of Science Education and Research, Pune.

The laboratory achieved major milestones in scientific publications having published more than 600 research papers in national and international peer reviewed journals. The laboratory has continued its efforts to develop technologies and transfer them to the industries. Some of the processes and technologies include batch to continuous nitration process for the production of pendimethalin, modelling framework for underground coal gasification, parametric effect on continuous flow nitration and photobromination reaction, scale-up preparation and characterization of molecular sieves, process for p-aminophenol from nitrobenzene, and hydrothermal conversion of lipid oils. The process know-how for Vortex diode hydrodynamic cavitation design for industrial effluent was out-licensed for commercialization.

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.

I wish to acknowledge the support and cooperation of my predecessor Directors Dr. Sourav Pal and Dr. Vijayamohanan Pillai during the report period for directing the research and output of scientists and staff. I wish to thank the Research Council and Management Council of CSIR-NCL as well as DG-CSIR and the staff at CSIR, 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 this 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 balance 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

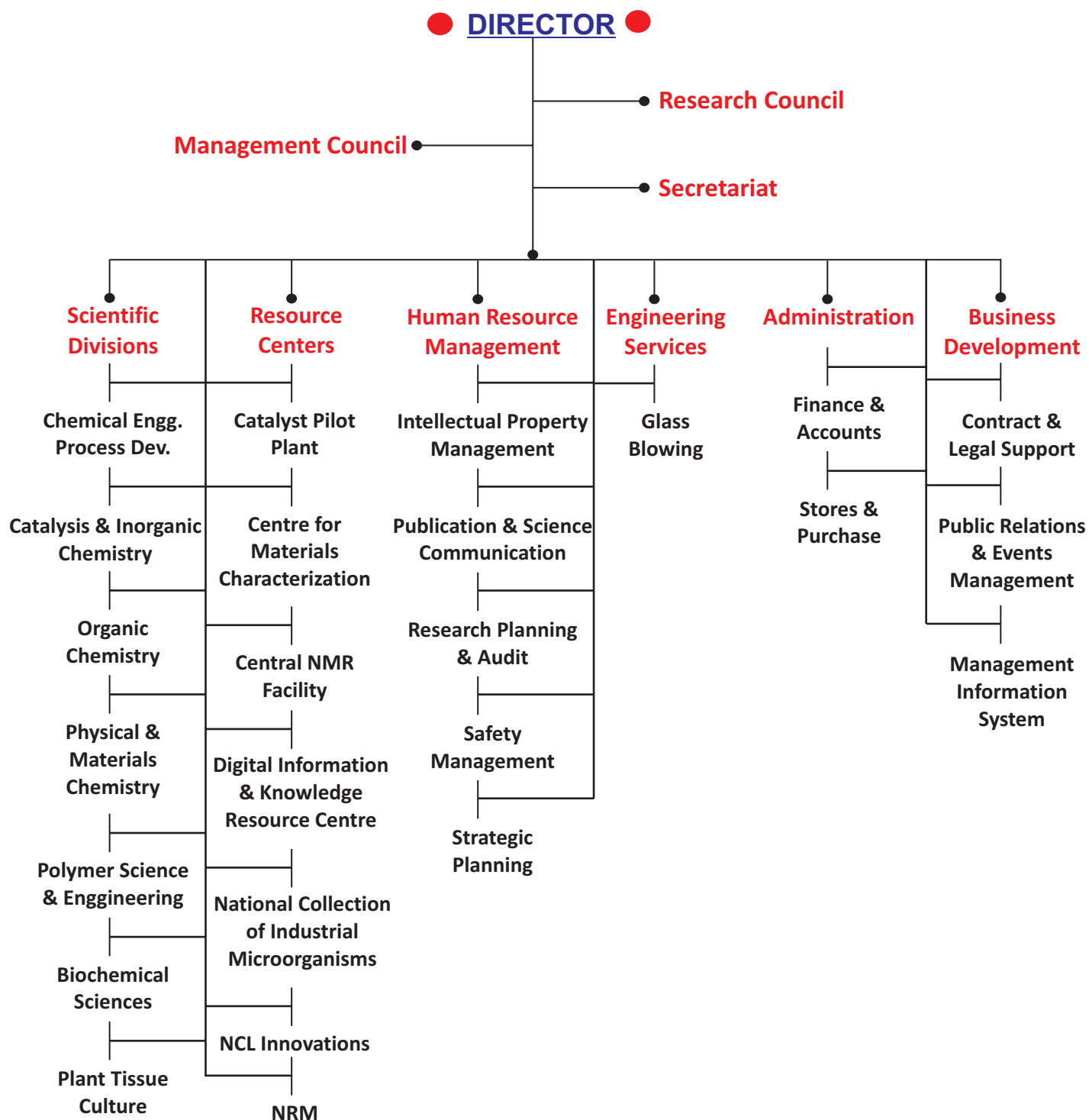
To create and sustain a self - driven and self - managed learning organization with a high degree of internal and external transparency

To encourage a culture of collective and principle-centred leadership

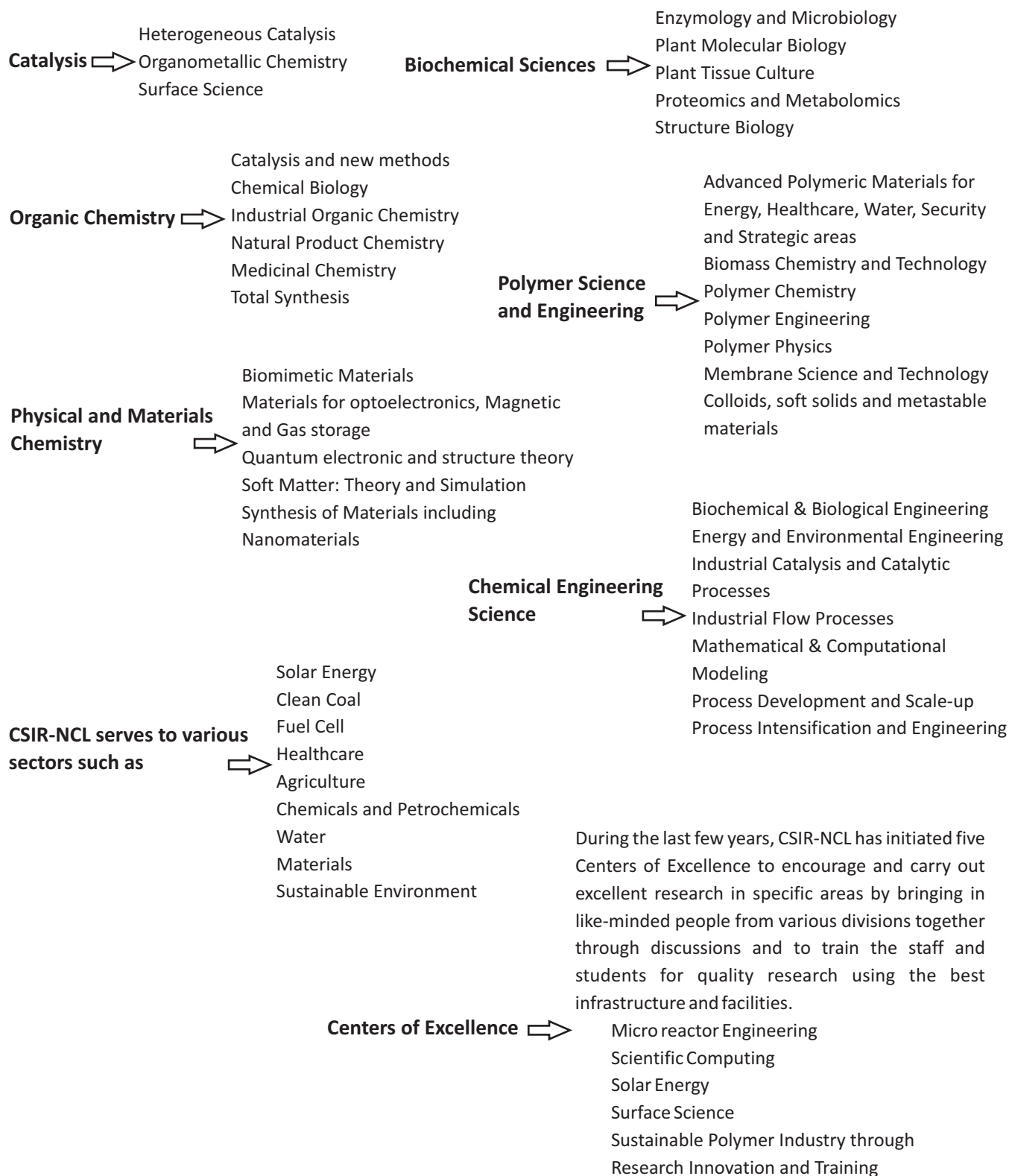
To value the dignity of the individual and deal with people with a sense of fairness and without bias, prejudice or favour

To nurture the highest standards of integrity and ethical conduct

## Organisation Chart



## Research Areas



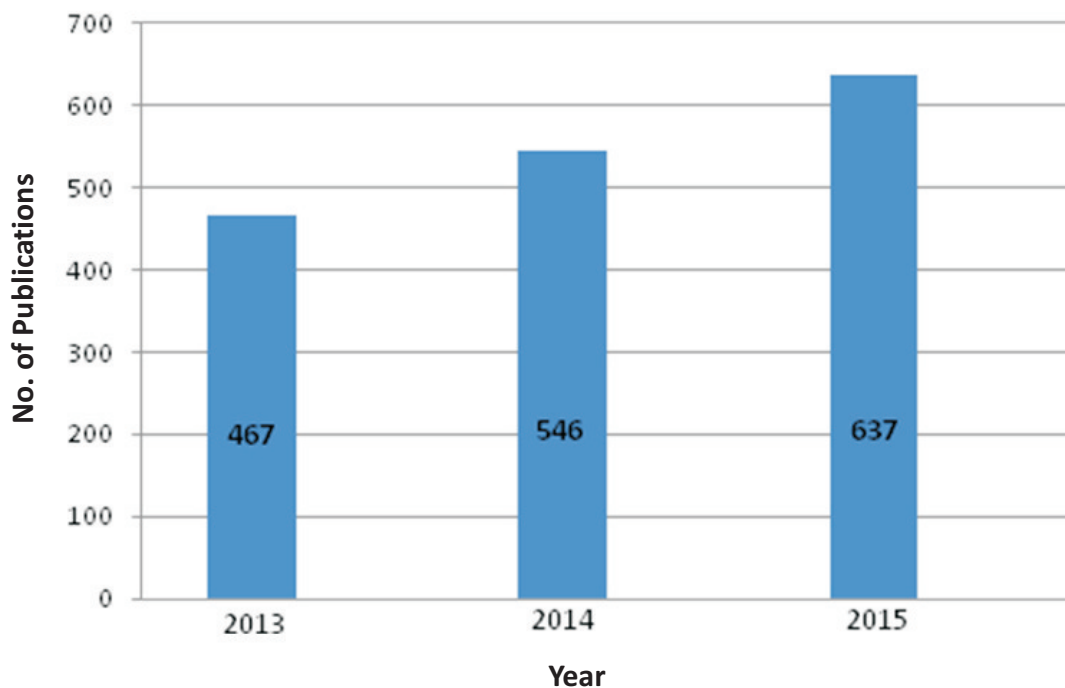


## Performance Indicators

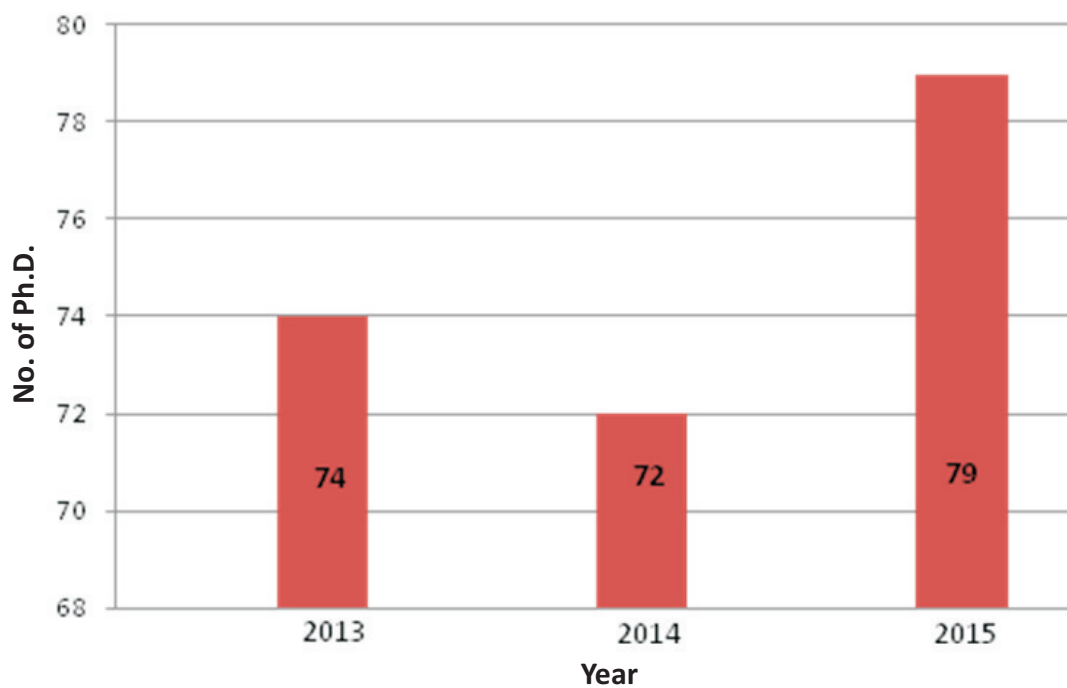
▶ Science Performance Indicators	14
▶ Technology Performance Indicators	15
▶ Human Resource Indicators	16
▶ Finance Performance Indicators	18
▶ Outputs and Outcomes	21

## Science Performance Indicators

### Research Output: Publications



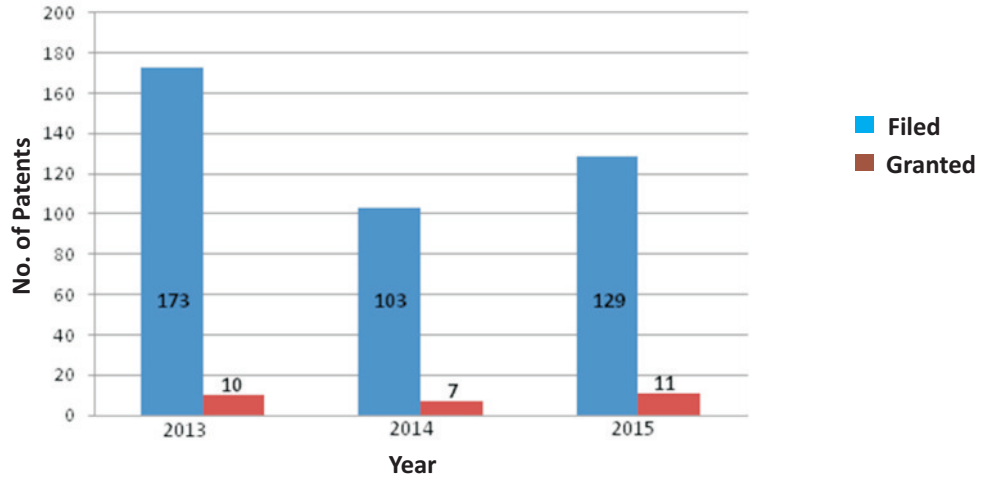
### Ph. D. Theses



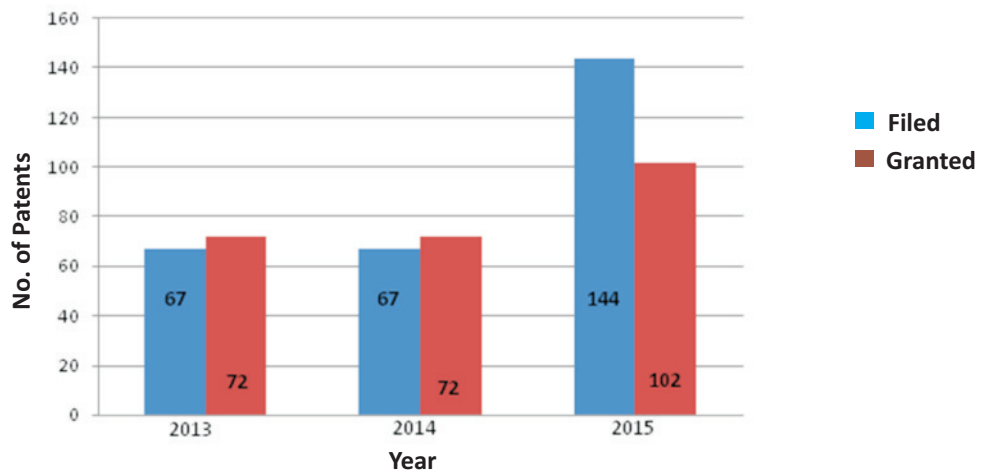


## Technology Performance Indicators

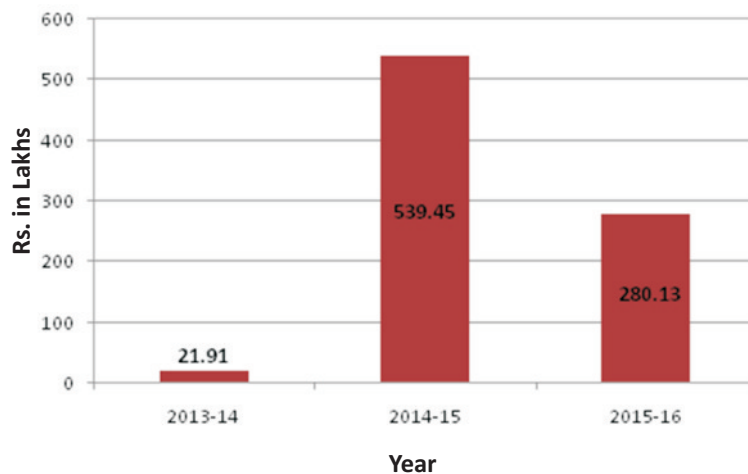
### Indian Patents: Filed & Granted



### Foreign Patents: Filed & Granted

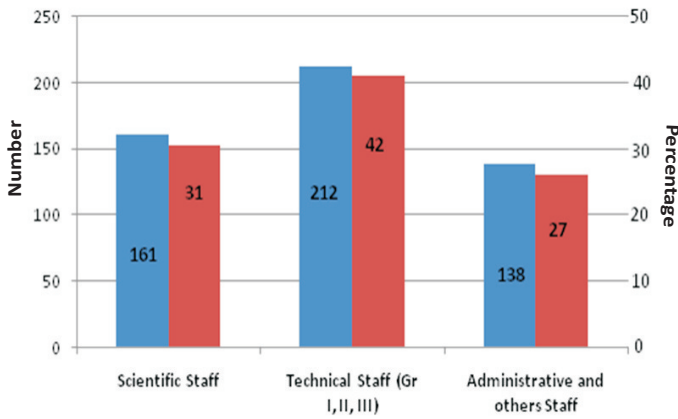


### Premia/Royalty Earnings

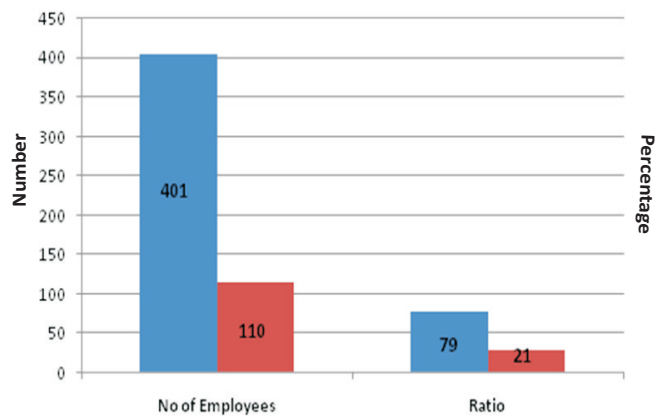


## Human Resource Indicators

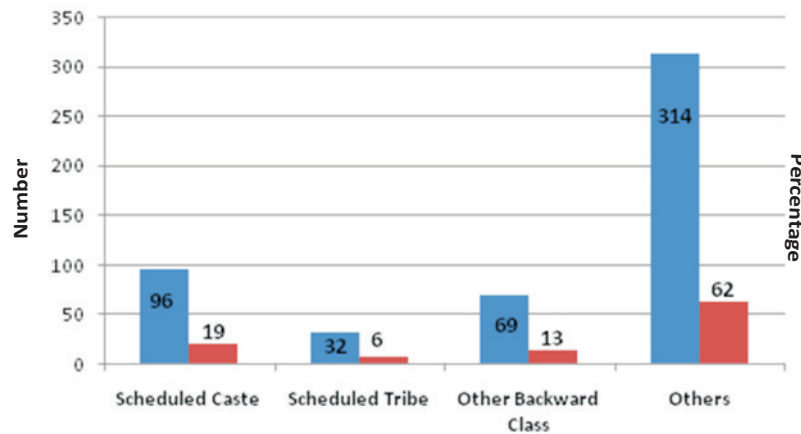
### Total Staff : 511



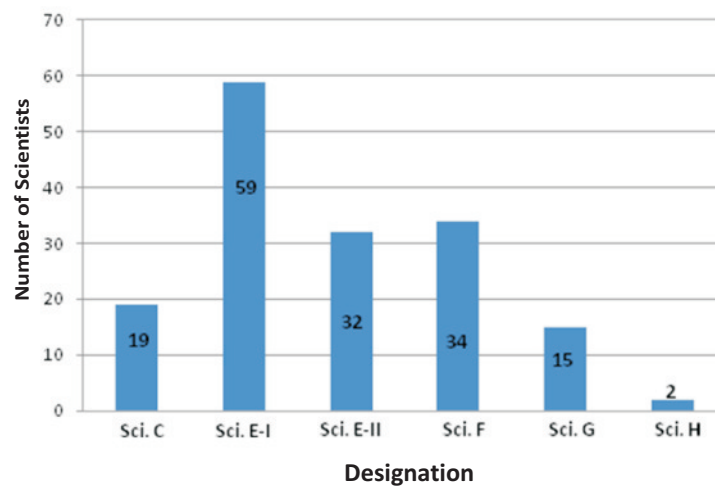
### Male & Female Employees



### SC, ST, OBC & Others



### Scientific Staff Distribution



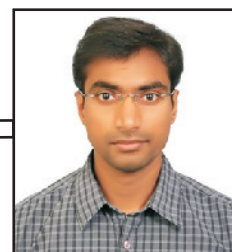
## We Welcome



### **In-vivo exploratory /efficacy studies, regulatory registration, value added bioactive molecules for biochemistry**

- Junior Scientist/Scientist/Sr. Scientist, CSIR-Indian Institute of Toxicology Research, Lucknow (2002-2015)
- Research Officer, Jai Research Foundation, Vapi, Gujarat (2001-2002)
- Ph.D, Jamia Hamdard Univesrity, New Delhi (2012)

**Dr. Bhushan Choudhary**  
(23 April 2015)



### **Peptide Chemical Biology and NMR Spectroscopy Applications**

- Postdoctoral Researcher, Department of Organic Chemistry, Technical University Munich (TUM), Germany (2010-2012, 2013- 2015)
- Postdoctoral Researcher, Structural and Computational Biology Unit, European Molecular Biology Laboratory, Heidelberg, Germany (2012-2013)
- Ph.D., CSIR-Indian Institute of Chemical Technology, Hyderabad (2005-2010)

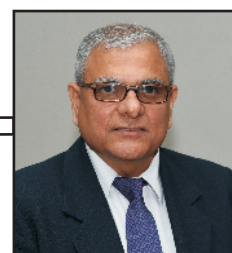
**Dr. Udayakiran Marelli**  
(15 July 2015)



### **Materials Chemistry, Nanotechnology, Polymer Chemistry, Catalysis & Optoelectronics**

- Scientist, CSIR-Central Salt & Marine Chemicals Research Institute, Bhavnagar (2011- 2015)
- IRCSET-EMPOWER Postdoctoral Fellow, Trinity College, Dublin, Ireland (2012-2013)
- CSIR-Nehru Postdoctoral Fellow, CSIR-NCL, Pune (2010-2011)
- Deputy Manager (Scientist), Tata Chemicals Innovation Centre, Pune (2007-2009)
- Ph. D., University of Hyderabad (2002-2007)

**Dr. Shatabdi Mukherjee**  
(29 Sept 2015)



### **Crystal Engineering, Supramolecular Chemistry, Host-guest Compounds, Hydrogen Bonding Polymorphism, Cocrystals, Eutectics**

- Professor, School of Chemistry, University of Hyderabad (2001-2016)
- Lecturer, School of Chemistry, University of Hyderabad (1989-2001)
- Ph. D., Yale University, USA (1988)
- M. Sc. Chemistry, Indian Institute of Technology, Kanpur (1983)

**Prof. Ashwini Kumar Nangia**  
(29 Feb 2016)



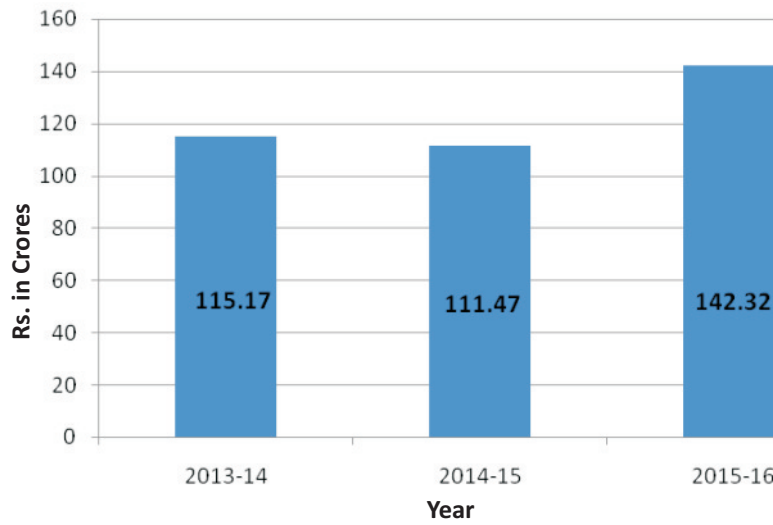
### **Biochemical Engineering, Bioprocess Technology, Chromatography, Adsorptive Separation**

- Associate consultant, Merck-Millipore, USA and University of Delaware, USA (2015-2016)
- Post-Doctoral Fellow, Department of Chemical and Biomolecular Engineering, University of Delaware, Newark, USA (2013-2015)
- Ph. D. Indian Institute of Technology, Delhi (2010-2012)

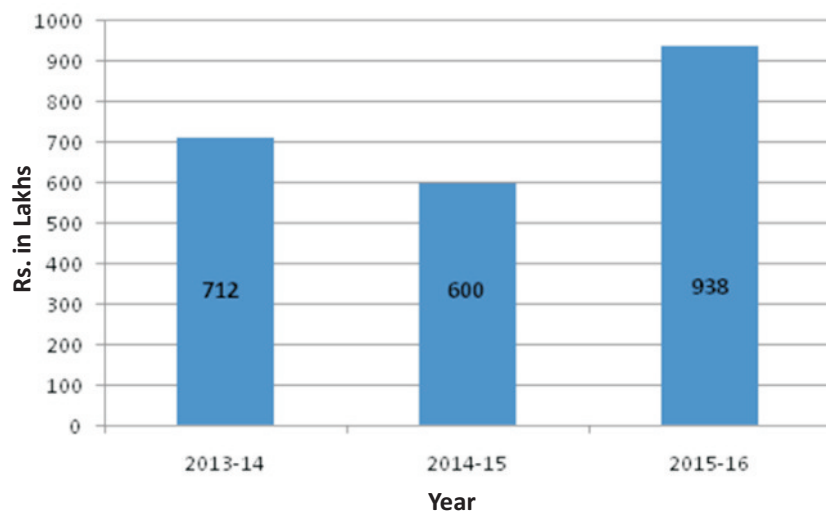
**Dr. Rahul Bhambure**  
(3 March 2016)

## Financial Performance Indicators

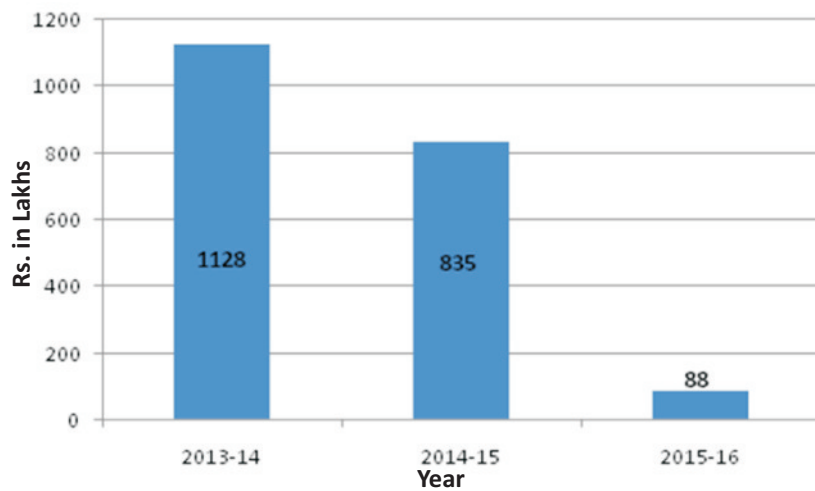
### CSIR Budget



### Laboratory reserve: Receipts

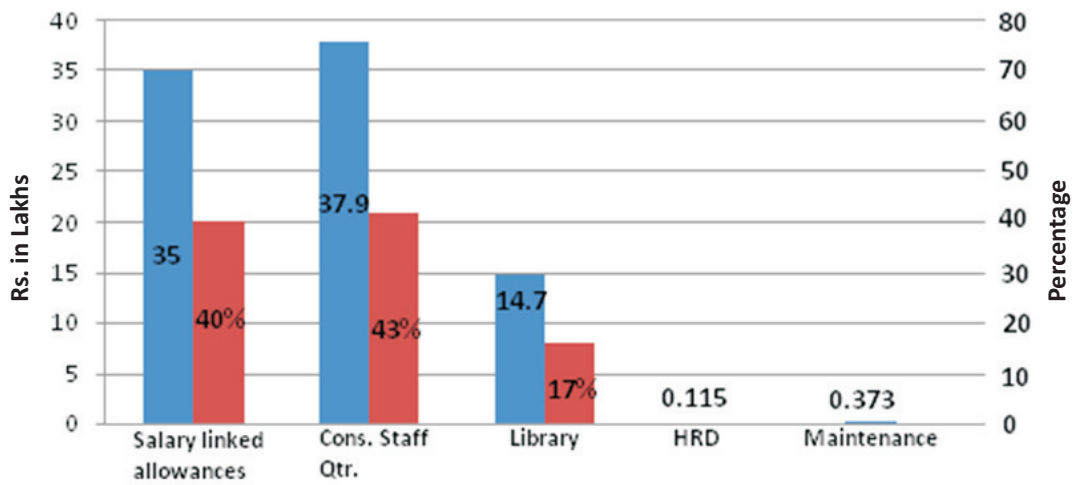


### Laboratory reserve: Expenditure

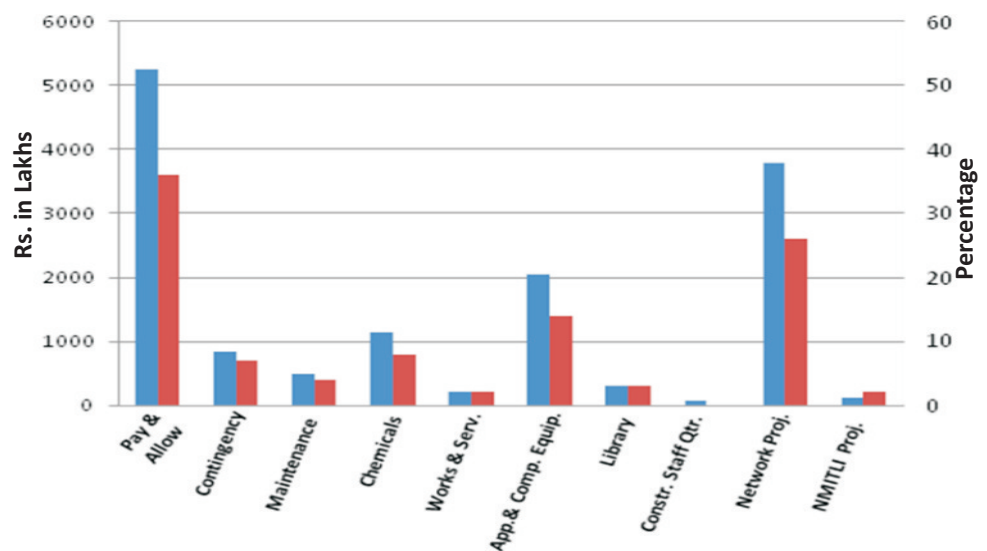


## Financial Performance Indicators

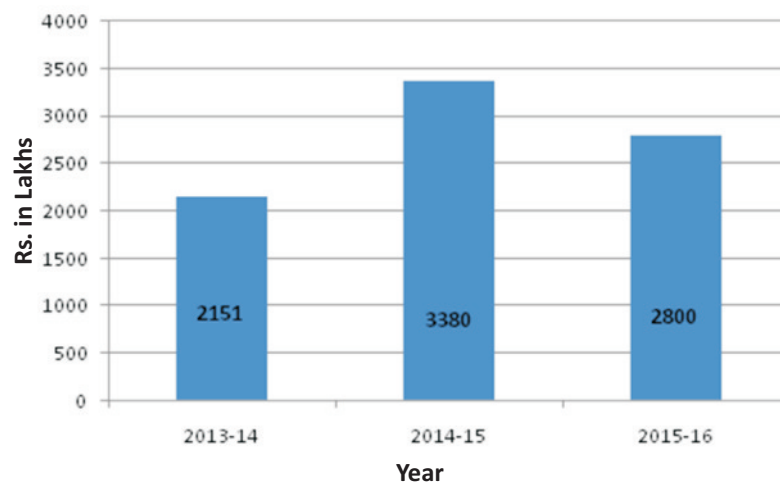
### Expenditure: Laboratory reserve(2015-16)



### Expenditure: CSIR & Network Projects



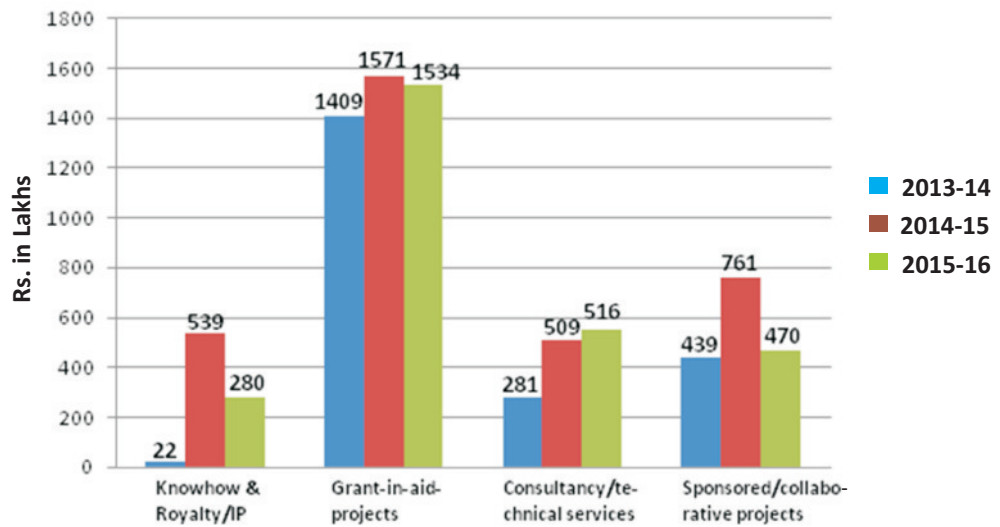
### External Income



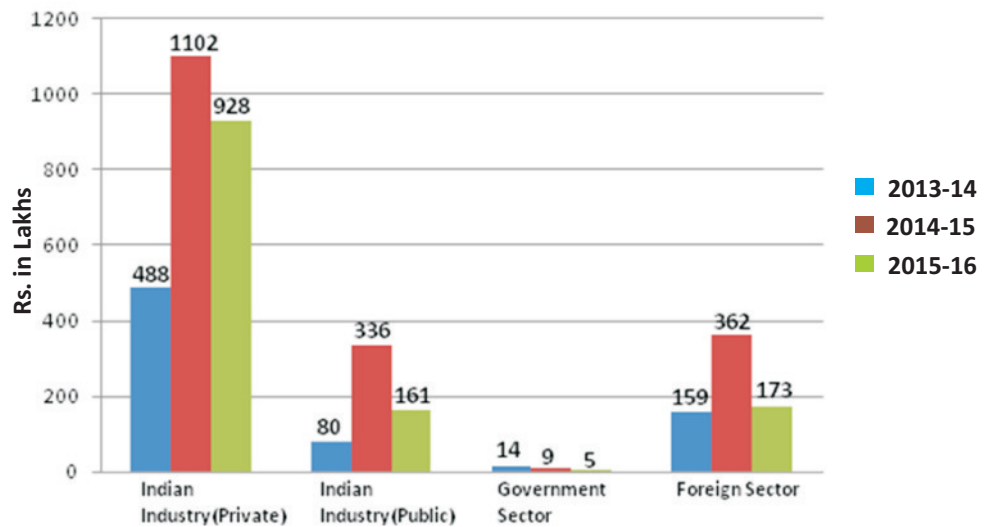


## Financial Performance Indicators

### ECF by Source



### ECF from Industry



## Outputs and Outcomes

Category of Benefits	Benefit	Indicators	2013-14	2014-15	2015-16
Public and social goods	Generation of and dissemination of generic knowledge	Number of papers published (Calendar year)	447	540	637
		Number of invention disclosure (Calendar year)	176	150	105
		Number of patents filed in India (Calendar year)	118	112	97
		No of foreign patents filed ** (Calendar year)	66	78	120
		Number of PCT applications filed (Calendar year)	55	77	44
		No of US applications filed	24	50	58
	Highly trained man-power	Number of PhDs produced (Calendar year)	73	68	58
		Number of NET/GATE qualified students joined (including DBT JRF)	118	88	57
	Science awareness, popularization etc.	Number of popular S&T articles published (in all languages)	-	3	-
		Number of national and regional workshops, seminars organized	4	7	2
	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)	62	49	88
	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)	6	6	8

1 Crore = 10 Million

## Outputs and Outcomes

Category of Benefits	Benefit	Indicators	2013-14	2014-15	2015-16
Public and social goods	Generation of and dissemination of generic knowledge	Number of papers published (Calendar year)	447	540	637
		Number of invention disclosure (Calendar year)	176	150	105
		Number of patents filed in India (Calendar year)	118	112	97
		No of foreign patents filed ** (Calendar year)	66	78	120
		Number of PCT applications filed (Calendar year)	55	77	44
		No of US applications filed	24	50	58
	Highly trained man-power	Number of PhDs produced (Calendar year)	73	68	58
		Number of NET/GATE qualified students joined (including DBT JRF)	118	88	57
	Science awareness, popularization etc.	Number of popular S&T articles published (in all languages)	-	3	-
		Number of national and regional workshops, seminars organized	4	7	2
	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)	62	49	88
	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)	6	6	8

1 Crore = 10 Million

## Outputs and Outcomes

Category of Benefits	Benefit	Indicators	2013-14	2014-15	2015-16
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)	7.42	18.09	12.67
	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)	0.22	5.39	2.80
Strategic goods and options	Other tactical and strategic developments	Total earnings from patent related transaction (₹ in crore)	-	-	-
		No. of patents in new Licensing /assignment/ option arrangements	1	1	-
		No. of unique Licensing /assignment/ option cases	1	-	-
		No. of Indian patents granted (Calendar year)	10	7	8
	No of foreign patents granted** (Calendar year)	68	49	88	
	Contributions to projects involving valuable opportunities in the form of technology options	Money in flow from NMITLI projects and other similar strategic projects (₹ in Crore)	5.21	1.65	0.13
		Money inflow from Technology Mission & GIA projects (other than NMITLI) projects (₹ in Crore)	14.09	15.71	15.34
Intellectual assets and reputation	Quality, reputation and standing of scientific man-power	No. of Indian patents granted (Calendar year)	10	7	14
		No. of foreign patents granted** (Calendar year)	68	49	88
		Number of scientists who are members of editorial boards of international peer-reviewed journals, covered by SCI	NA	NA	NA

\*- 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

## Advanced Materials

### Biomaterials

Manohar V. Badiger | mv.badiger@ncl.res.in

**Enhanced drug release by selective cleavage of crosslinks in hydrogels:** Redox sensitive double cross linked poly (acrylic acid) hydrogels were synthesized and characterized using two different cross linking agents namely, jeffamine and cystamine. The amount of two cross linking agents was varied in order to synthesize hydrogels with different mechanical strengths. The

swelling controlled release of Doxorubicin (anti cancer drug) by selective cleavage of cystamine bonds in hydrogels using dithiothreitol (DTT) was demonstrated. The antibacterial properties were induced by incorporating silver nanoparticles in hydrogels to further enhance their application in tissue engineering (*RSC Adv.* **2016**, *6*, 102453).

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

**Self - assemblies of isomannolipids:** The group has synthesized isomannide lipids (IMLs) of three fatty acids namely oleic, elaidic and stearic acid. Out of them, oleic and elaidic IMLs self - assemble into spherical like

structure. The fluorescent dye loaded self - assembled spheres were efficiently taken up by the cancer cell lines enabling their usage in medical applications (*RSC Adv.* **2016**, *6*, 72074).

G.V.N. Rathna | rv.gundlori@ncl.res.in

**Bioactive thermoresponsive polyblends of nanofiber formulations for wound healing:** Thermosensitive non-woven nanofiber formulations were designed and fabricated using polymeric blends of poly (N-isopropyl acrylamide), polycaprolactone and egg albumen. The morphology of nanofibers was influenced by concentration of polymer, drug, and polymer blend composition. Gatifloxacin hydrochloride was used as an antibacterial drug. *In vitro* release study of nanofibers showed initial rapid release of drug up to 10 h, followed by slow and controlled release for 696 hours. Nanofiber mats with drug exhibited antibacterial properties to *Staphylococcus aureus*, supported suitable controlled drug release with *in vitro* cell viability and *in vivo* wound healing (*Mater. Sci. Eng. C* **2015**, *48*, 126).

**Blends of shellac as nanofiber formulations for wound healing:** Blends of shellac, gelatin, and poly(N-isopropylacrylamide) with nadifloxacin and fabricated nanofiber mats were developed using electrospinning. The morphology of nanofiber formation was influenced by the concentration of polymer, drug, and polymer blend composition. Drug release studies recorded slow, constant and sustained drug release for 140 hours. Release kinetics and mechanism confirmed zero order release with resultant  $r^2$  values greater than 0.99 and Korsmeyer-Peppas release exponent ( $n$ ) was slightly higher than 0.8, which indicated drug diffusion was non-Fickian type and drug release followed diffusion involving chain stretching. Nanofiber mats were cell viable and antibacterial. *In-vivo* studies demonstrated that the bioactive nanofiber formulations were more suitable for faster tissue regeneration as compared to nanofiber mats without drug and commercial nadifloxacin cream (*J. Bioact. Compat. Pol.* **2015**, *30*, 472).



## Advanced Materials

### Biomaterials

Asmita A. Prabhune | aa.prabhune@ncl.res.in

**Pulsed laser-driven molecular self-assembly of Cephalexin: Utility as a mercury ion sensor:** A fluorescent self-assembly of cephalexin obtained by pulsed laser irradiation process emitted intense fluorescence due to occurrence of a typical aggregation-induced emission in cephalexin molecules. It was observed that fluorescence quenching of the self-assembled fluorescent nanostructures occurred in the presence of extremely low  $Hg^{2+}$  ion concentrations (107 M) as compared to other heavy metal ions e.g. Ferrous ( $Fe^{2+}$ ), Manganese ( $Mn^{2+}$ ), Magnesium ( $Mg^{2+}$ ), Cobalt ( $Co^{2+}$ ), Nickel ( $Ni^{2+}$ ) and Zinc ( $Zn^{2+}$ ) at the same concentrations. These compounds showed a wide range of applications due to their unique optical properties and non-toxic synthesis. Aggregation induced fluorescence presented opportunities for constructing various sensor probes like water purification, dental applications, detection of mercury in fish etc. (*Photochem. Photobiol.* **2015**, *91*, 1340).

**Quorum sensing antagonists: glycomonoterpenols synthesized using linalool and alpha terpineol:** Quorum sensing showed the potential to regulate a plethora of bacterial virulence phenotypes. Monoterpene alcohols like linalool and alpha terpineol were shown to possess anti microbial and anti-biofilm activity. These glycomonoterpenols were synthesized using *Candida bombicola* ATCC 22214. The advantage of these molecules over their parent compound was their additional surfactant like property, increased solubility and enhanced QSI potential. These glyco moieties inhibited virulence phenotypes of the gram negative pathogens, simply by impeding QS (quorum sensing). It led to the development of next generation of antimicrobials. Additionally, with the ever increasing surge of drug resistant organisms, newer drug targets with significantly decreased propensity of development of resistance are the need of the hour and quorum sensing fitted this prerequisite perfectly (*World J. Microb. Biot.* **2015**, *31*, 841).

**Sophorolipid assisted rapid gelation of silk fibroin for biomedical scaffolds:** The gelation of SF was accelerated

under physiological conditions using a biosurfactant, sophorolipid (SL) as a gelling agent. These hydrogels showed pore architecture, porosities and mechanical stability ideally suited for tissue culture applications. The fibroblast cells proliferation on these SF-SL scaffolds was studied. The SF-SL hydrogels showed applications in wound dressing, while the SF-SL 3D scaffolds have potential use in tissue regeneration (*RSC Adv.* **2015**, *5*, 33955).

**Antibacterial activity of *Lantana camara* leaf extract synthesized silver nanoparticles:** The size controlled silver nanoparticles (AgONPs) were synthesized by using leaf extract from the weed plant *Lantana camara*. Characterization of AgONPs by optical absorption, photoluminescence, dynamic light scattering (DLS), zeta potential, infrared spectroscopy, X-ray diffraction measurements, FE-SEM and TEM analysis were performed. The synthesis of AgONPs via this green approach showed high antibacterial activity against *E. coli* (Gram -ve) and *S. aureus* (Gram +ve) at very low concentration (50 ppm Ag nanoparticles). The use of such eco-friendly nanoparticles helped to develop new range of bactericidal agents (*RSC Adv.* **2015**, *5*, 24513).

***Staphylococcus epidermidis* RM1: Quorum quencher and bile salt hydrolase producer:** *Staphylococcus epidermidis* RM1 was isolated from fermented soy curd and possessed both potent bile salt hydrolase (BSH) and N-acyl homoserine lactone (AHL) cleavage activities. The genetic basis of this dual-enzyme activity was explored by means of specific primers designed using *S. epidermidis* ATCC 12228 genome as the template. Two different genetic elements corresponding to each of the enzymatic activity were successfully amplified from the genomic DNA of the isolate. All the findings highlighted the uniqueness of the isolate especially in terms of a potential probiotic organism. Since *S. epidermidis* RM1 possessed both AHL acylase and bile salt hydrolase activities, its possible superiority over available probiotic strains was tremendous (*Appl. Biochem. Biotech.* **2015**, *176*, 140).

## Advanced Materials

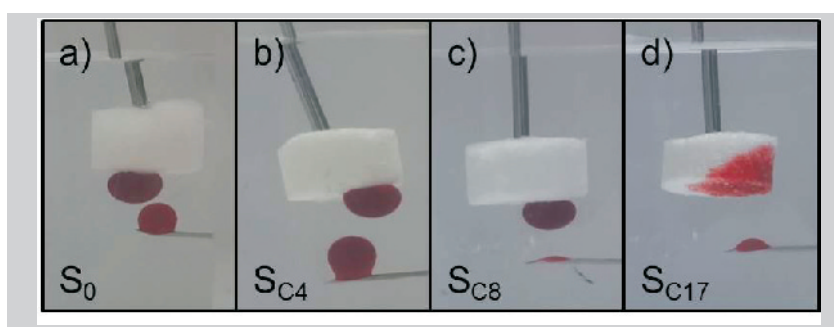
### Functional materials

Guruswamy Kumaraswamy | g.kumaraswamy@ncl.res.in

#### Omniphilic sponges for absorption of solvent spills:

Sponges that absorb a wide variety of solvents are used as universal absorbents for laboratory and industrial spills. While there are several materials available for selectively absorbing oils, such materials are inappropriate for cleaning up spills where the solvent polarity might vary or in cases the oils are emulsified with surfactant. The

porous polymeric sponges were prepared using the same cross linked polymer matrix which can be optimized to be hydrophilic or omniphilic or oleophilic underwater. These sponges are mechanically stable to compression and can be repeatedly compressed hundreds of times. This offers a simple way to recover the absorbed solvent (*Chem. Mater.* **2016**, *28*, 1823).



P.A. Joy | pa.joy@ncl.res.in

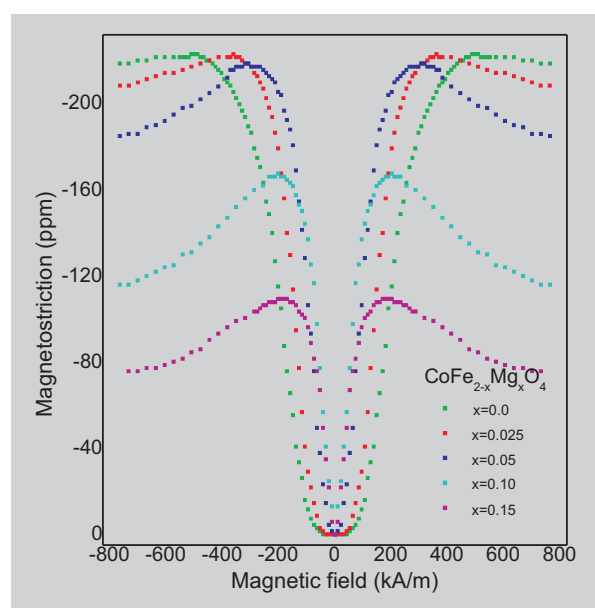
#### Enhancing magnetostriction parameters of sintered cobalt ferrite:

Attaining high magnetostrictive strain sensitivity with high magnetostriction coefficient was desirable for sintered polycrystalline cobalt ferrite for various applications. It was shown that replacing small amounts of Fe by Mg in cobalt ferrite gives a comparable maximum magnetostriction coefficient to that of the unsubstituted counterpart, with large improvement in the strain sensitivity at relatively low magnetic fields. A large increase in the magnetostriction coefficient was obtained at low magnetic fields for the substituted compositions. The magnetostriction parameters were further enhanced by magnetic field annealing of the sintered products (*Phys. Chem. Chem. Phys.* **2016**, *18*, 10516).

#### Structure-property correlation of lead-free dielectrics:

Solid solutions of the lead-free ferroelectric oxides  $\text{Bi}_{0.5}\text{Na}_{0.5}\text{TiO}_3$  and  $\text{Bi}_{0.5}\text{K}_{0.5}\text{TiO}_3$  were studied to understand the correlation between structure and the properties. A close relationship was obtained between the structure,

microstructure and properties of the different compositions. It was shown that best performance was obtained in the morphotropic phase boundary region between monoclinic and tetragonal phases (*J. Adv. Dielect.* **2015**, *5*, 1550028).



## Advanced Materials

### Functional materials

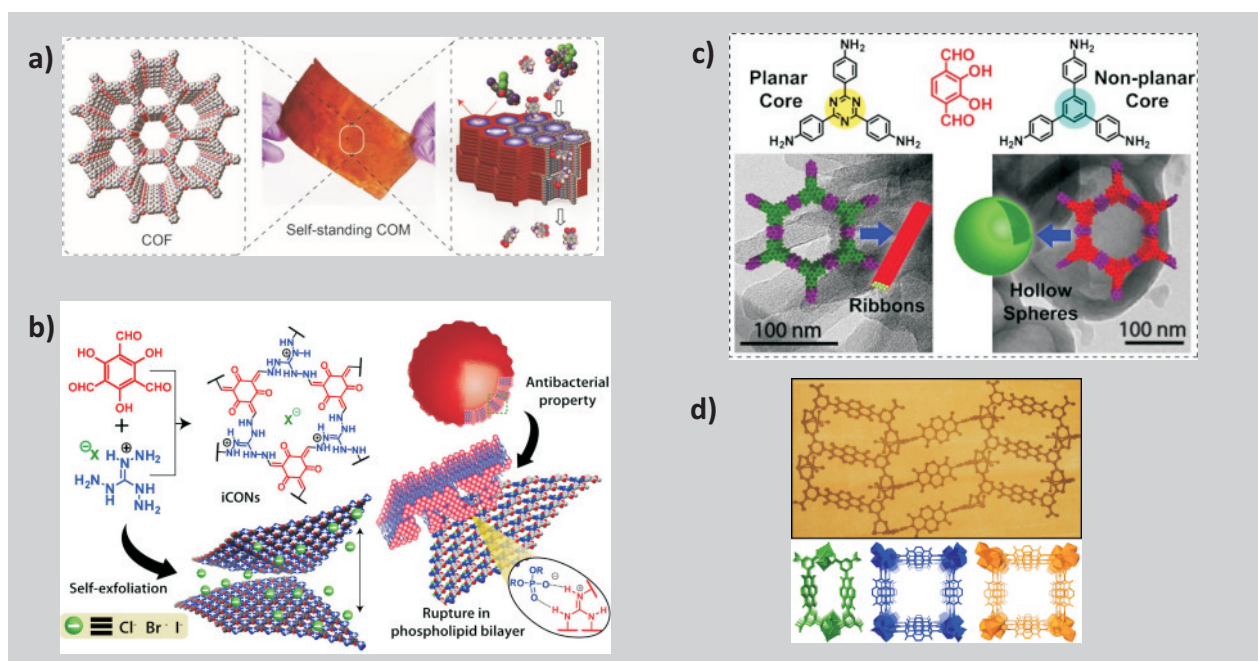
Rahul Banerjee | r.banerjee@ncl.res.in

**Selective molecular sieving in self-standing porous covalent organic framework membranes:** A novel methodology was developed for synthesis and fabrication of covalent organic framework membrane (COMs) into a self-standing form. The synthetic methodology adopted is simple, scalable and highly cost effective. These self-standing COMs are flexible, continuous, devoid of any internal defects or cracks. Further, COMs also showed long-term durability and recyclability; while maintaining the structural integrity of water, organic solvents and even in mineral acid (3 N HCl). These COMs were utilized for evaluating challenging separation applications such as waste water treatment and recovery of valuable active pharmaceutical ingredients [APIs] from organic solvents (*Adv. Mater.* **2016**, doi: 10.1002/adma.201603945).

**Self-exfoliated guanidinium-based ionic covalent organic nanosheets (iCONs):** It was anticipated that rational designing of an intrinsic ionic linker could be the solution to produce self-exfoliated CONs. Three self-exfoliated guanidinium halide based ionic CONs with antimicrobial property were synthesized. Self-exfoliation phenomenon has also been supported by MD simulation. Charged guanidinium unit played the pivotal role for both self-exfoliation and antibacterial property against both gram (+ve/-ve) bacteria. A membrane was devised by using iCONs that could be useful for antimicrobial coatings benefits (*J. Am. Chem. Soc.* **2016**, 138, 2823).

**Morphological diversity in 2D crystalline porous polymers:** Two new chemically stable triazine- and phenyl-core-based crystalline porous polymers (CPPs) were synthesized using a single-step template-free solvothermal route. Unique morphological diversities were observed for these CPPs [2,3-DhaTta (ribbon) and 2,3-DhaTab (hollow sphere)] by simply altering the linker planarity. A detailed time-dependent study established a significant correlation between the molecular level structures of building blocks with the morphology of CPPs. A DFT study was done for calculating the interlayer stacking energy, which revealed that the extent of stacking efficiency is responsible for governing the morphological diversity in these CPPs (*Angew. Chem. Int. Ed.* **2016**, 55, 7806)

**Photochromic metal-organic frameworks for inkless and erasable printing:** Inkless and erasable printing is the key solution towards a more sustainable paper industry, in terms of paper wastages and environmental hazards. The photochromic MOFs were used and tested for their capability as inkless and erasable printing media. The printing was performed using sunlight on MOF-coated papers. The resulting printing had good resolution and stability, and was capable of being read both by the human eye and electronic devices. The paper could be reused for several cycles without significant loss in intensity. Different coloured printing was also achieved by varying the MOF structure (*Chem. Sci.* **2016**, 7, 2195)



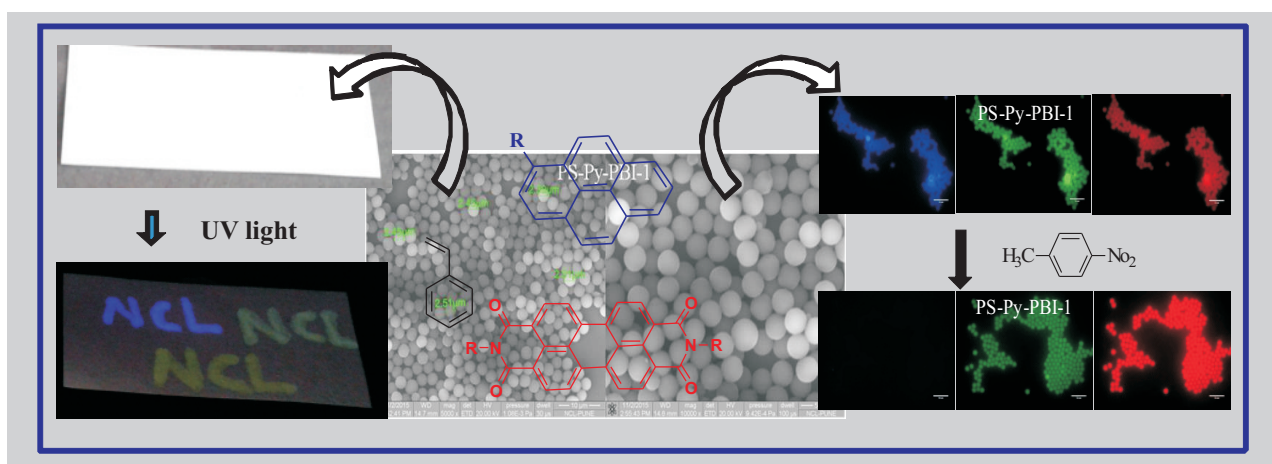
## Advanced Materials

### Functional materials

Asha Shyama | sk.asha@ncl.res.in

**Fluorescent polystyrene microbeads as invisible security ink and optical vapor sensor:** The color-tunable solid state emitting polystyrene (PS) microbeads have been developed successfully in the lab which showed excellent fluorescent security ink characteristics along with sensitive detection of vapors of nitro aromatics like 4-nitro toluene (4-NT). The fluorophores pyrene and perylenebisimide were incorporated into the PS backbone, that showed solid state quantum yields of 94 % and 20 % for the pyrene and perylenebisimide emission,

respectively. The ethanol dispersion of the polymer could be used as a fluorescent security 'invisible' ink which became visible only under ultraviolet light. The color of the ink could be tuned from blue and orange-green as well as various shades in between including pure white for beads incorporating both the fluorophores. More than 80 % quenching of pyrene emission was observed upon exposure of the polymer in the form of powder or as spin coated films to the vapors of 4-NT, with a detection limit of  $10^{-5}$  moles (2.7 ppm) of 4-NT vapors (*ACS Appl. Mater. Inter.* **2016**, *8*, 10590).



Kadhiravan Shanmuganathan | k.shanmuganathan@ncl.res.in

**Solution processed cellulose/melanin fibres with enhanced antibacterial properties:** An approach was developed to prepare antibacterial fibres comprising melanin and cellulose. Melanins exhibit a unique range of physical and chemical properties, their intractable nature precluded their dissolution in common solvents and further processing into functional materials. Commercially available 40 wt% tetrabutyl ammonium hydroxide solution (TBAH) as a potential solvent for

melanins was explored. It was found that TBAH could yield stable solutions of synthetic and natural melanins at ambient conditions and the dissolution rate could be accelerated by microwave radiation. The research group was able to successfully process cellulose/ synthetic melanin composite fibres using TBAH as a common solvent. These fibres demonstrated significant antibacterial activity (98-99.9% reduction) against both gram positive and gram negative bacteria.





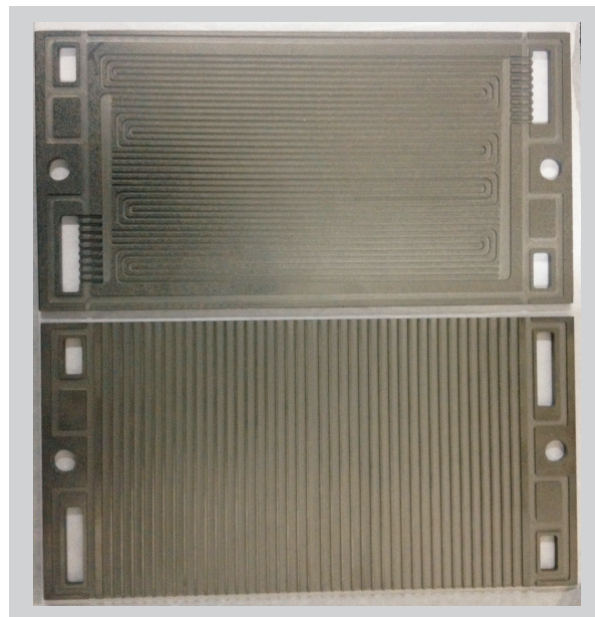
## Advanced Materials

### Materials for energy

Harshawardhan V. Pol | hv.pol@ncl.res.in

**Indigenous graphite-resin composite bipolar plates for PEM based fuel cells:** PEM based fuel cell technology offers a clean and green alternative to conventional fossil fuel based energy cycle. Graphite-resin composite bipolar plates constitute over 80% of the weight, about 30% of the cost and almost the entire volume of a typical PEM based fuel cell stack.

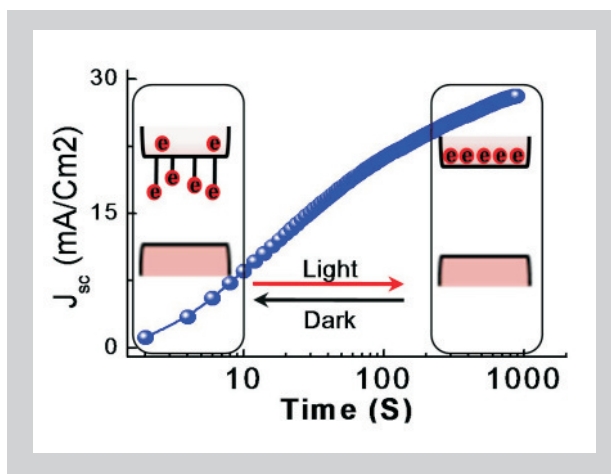
CSIR-NCL has contributed extensively over the last 2-3 years in developing indigenous bipolar plate technology through a rigorous in-house R&D as well as vendor development. The work done so far has resulted in development of indigenous bipolar plates that meet or sometimes even exceed the properties of benchmark foreign-make bipolar plates (which are used exclusively in commercial stacks). A patent disclosure on process and formulation development of indigenous bipolar plates has been filed (Patent: Ref. No. 0146-NF-2015: 1978-DEL-2015).



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

**Low temperature processed titanium oxide and niobium doped titanium oxide for photovoltaic applications:** Anatase titanium oxide ( $\text{TiO}_2$ ) was widely studied n-type window layer for the collection of photogenerated electrons in QD solar cells. Requirement of high temperature ( $\sim 500^\circ\text{C}$ ) processing steps proved to be disadvantageous for its applications in flexible solar cells, roll to roll processing and also show adverse commercial implications.

It was shown that solar light exposure to low temperature processed ( $80^\circ\text{C}$  -  $150^\circ\text{C}$ )  $\text{TiO}_2$  and niobium doped  $\text{TiO}_2$  films led to unprecedented enhancement in their electron densities and electron mobilities which enabled them to be used as efficient n-type layer in quantum dot solar cell. Photovoltaic devices based on low temperature processed  $\text{TiO}_2$  films showed improved performance over high temperature processed  $\text{TiO}_2$  film.



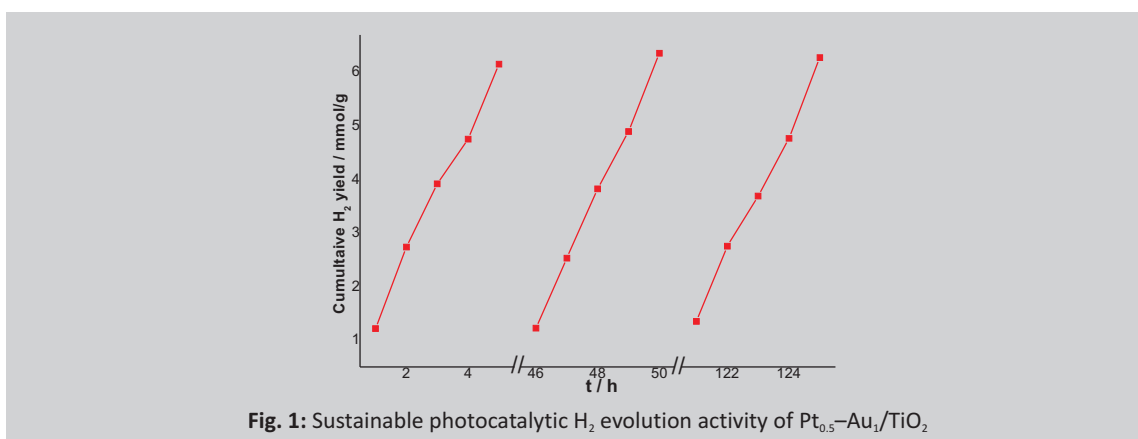
## Advanced Materials

### Materials for energy

C.S. Gopinath | cs.gopinath@ncl.res.in

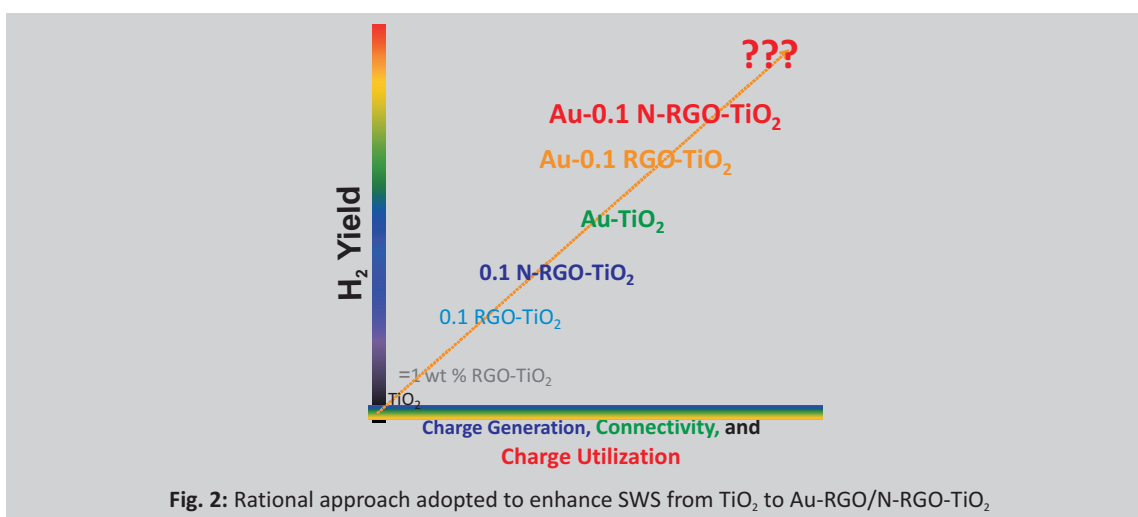
**Solar water splitting:** Photocatalytic production of hydrogen was demonstrated using a semiconductor bimetal nanocomposite. Au/TiO<sub>2</sub> was used as the base composite, on which a second metal (Ag, Pt and Pd) was deposited to validate the significance of any second metal. Metal-metal and metal-semiconductor junction property is essential for high water splitting activity. High

and sustainable hydrogen generation activity (Fig. 1) associated with Pt–Au/TiO<sub>2</sub> was investigated. Sustainable photocatalytic H<sub>2</sub> evolution activity of Pt<sub>0.5</sub>–Au<sub>1</sub>/TiO<sub>2</sub> under onesun conditions with aqueous methanol solution reported. After every five hours the gaseous products were evacuated and the results were reported (*Nanoscale* **2015**, *7*, 13477).



**Rational approach to solar water splitting:** The genesis of solar water splitting (SWS) activity has rarely been investigated thoroughly. A systematic and rational approach was reported to address a few critical issues of SWS and its genesis. A semiconductor (TiO<sub>2</sub>) for redox reactions, a component (nanogold) for sunlight

absorption and charge generation, a component for instant charge conduction (reduced graphene oxide), and the electronic integration of all components were achieved in Au-RGO-TiO<sub>2</sub>. Fig. 2 shows a linear increase in hydrogen generation activity (*Nanoscale* **2015**, *7*, 11206).





## Advanced Materials

### Materials for energy

Sreekumar Kurungot | k.sreekumar@ncl.res.in

#### Advanced materials for energy conversion and storage:

The group has focused on the development of cost-effective and environmental friendly energy conversion and storage devices. The key areas of the current research focus involved development of activity modulated electrode materials for polymer electrolyte membrane fuel cells (PEMFCs), flexible solid-state supercapacitors, metal oxide based cathode catalysts for metal-air batteries and MOF based proton conducting materials and electrocatalysts for various energy devices. A significant progress was made on developing various nanostructured low-Pt and Pt-free catalysts for facilitating the oxygen reduction reaction (ORR) in PEMFCs. The application of the electrocatalysts was demonstrated in the system level by developing prototypes of PEMFCs, flexible solid-state supercapacitors and metal-air batteries. Demonstration of single cells of anion exchange membrane fuel cells (AEMFCs) operating with totally Pt-free cathodes, paper-like solid-state supercapacitor devices and thin metal-air battery units were the key highlights of the group's recent research outputs. Electrocatalysts for water splitting for generating oxygen and hydrogen were also developed that can be used as the feed gases in fuel cells.

#### Pt-free and noble metal-free electro-catalysts for fuel cells:

A nitrogen-sulphur co-doped crumpled graphene sheet catalyst was prepared by simple oxidative polymerization of ethylenedioxythiophene followed by annealing at different temperatures. The derived catalyst exhibited high performance with just 100 mV shift in the onset potential from the state-of-art Pt/C catalyst. Application of the material as a catalyst in PEMFC delivered a power density of 193 mW cm<sup>-2</sup>, a value which is comparable to many of the metal-free electrocatalysts reported in the literature. An efficient graphene nanotube-based ORR electrocatalyst was developed from single walled nanohorns, comprising a thin layer of graphene nanotubes possessing encapsulated iron oxide nanoparticles at the tip. A PEMFC derived from this catalyst in the cathode displayed good activity with a power output of 200 mW cm<sup>-2</sup> at 60°C. Transition metal layered chalcogenides were demonstrated for the ORR activity. Layer separated MoS<sub>2</sub> mediated by Co(OH)<sub>2</sub> was prepared, which performed very well for ORR. This strategy helped to overcome some of the inherent limitations of the chalcogenides like low electrical conductivity and restricted mass transfer caused by the layer stacking (*ACS Appl. Mater. Inter.* **2015**, *7*, 24256; *J. Mater. Chem. A* **2016**, *4*, 6014; *Nanoscale* **2015**, *7*, 16729).

**Zinc-air battery and OER catalysts:** A high performing zinc-air battery was developed by using Cu-Pt nanocage inter-metallic structures as the cathode catalyst. The catalyst was prepared by galvanic exchange method. The unique nanocage structure possessed large surface area and improved electrochemical activity. At 1.0 V, the battery showed 1.30 fold improvements in the power density compared to the standard Pt catalyst. A cobalt ferrite catalyst was also demonstrated as an ORR catalyst for efficient zinc-air battery application. High-quality fine dispersion of very small ferrite particles was attained on nitrogen doped reduced graphene oxide. The zinc-air battery based on this catalyst was discharged for 15 h at a discharge current density of 20 mA cm<sup>-2</sup>. In another development, covalent organic framework (COF) containing bipyridine was used as an oxygen evolution catalyst by engineering Co(II) active sites into COF. The catalyst performed well with overpotential of 400 mV showing remarkable stability even after 1000 cycles. Similarly, spinel cobalt oxide supported over N-doped graphene was also synthesized, which performed with a reduced overpotential for OER (280 mV@10mA cm<sup>-2</sup>). The OER activity of the catalyst was further improved by supporting the NiCo bimetallic alloy oxide nanoparticles over N-doped porous graphene, which displayed excellent performance (260 mV@10 mA cm<sup>-2</sup>) (*ACS Catal.* **2015**, *5*, 1445; *ACS Appl. Mater. Inter.* **2016**, *8*, 20730; *Chem. Mater.* **2016**, *28*, 4375; *Adv. Mat. Interfaces* **2016**, *3*, 532).

**Solid-state flexible supercapacitors:** A high performing flexible supercapacitor was developed by employing entangled network of carbon nanotubes as a scaffold for the deposition of a conducting polymer, poly-(ethylenedioxythiophene). The device resulted in a high areal capacitance of 354 mF cm<sup>-2</sup> along with a low ESR of 0.9 Ω, which helped the system to capture a high power density of 8.85 Wcm<sup>-3</sup>. The electrolyte in a supercapacitor forms an integral and important part. A high performing gel electrolyte was devised with high acid loading capacity through in-situ polymerization of the monomer on the active material itself. The electrolyte-electrode interface was enhanced which showed a behavior matching with that of the liquid electrolytes. The basic matrix of the gel polymer network showed excellent thermal stability in acid, and the polymer further interacted with the acid moiety through the CO functional groups of the polymer chain. It helped the system to hold more acid moieties, an ability that was found to be superior to that of the conventionally used PVA- acid gel (*ACS Appl. Mater. Inter.* **2016**, *8*, 1233).

## Advanced Materials

### Materials for energy

#### Dye-sensitized solar cells

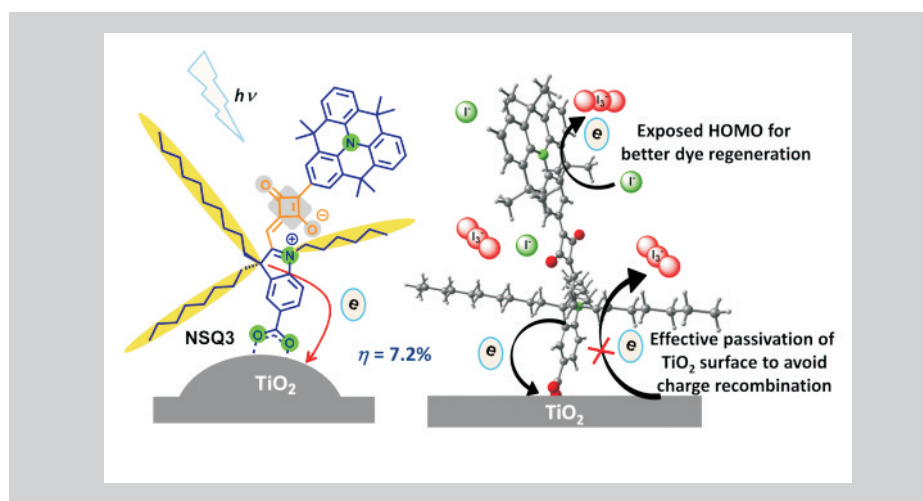
J.Nithyanandhan | j.nithyanandhan@ncl.res.in

#### Heterotriangulene-based unsymmetrical squaraine dyes: Synergistic effects of donor moiety and out-of-plane branched alkyl chains on the dye cell performance:

Unsymmetrical squaraine sensitizers with two different donor moieties, triphenylamine (NSQR) and heterotriangulene (NSQ1-3), for dye-sensitized solar cell (DSSC) were designed and synthesized. These dyes utilized the indolium moiety to control charge recombination dynamics at  $\text{TiO}_2$ -dye-electrolyte interface by connecting linear and branched alkyl functionalities. An efficient heterotriangulene (HT) donor and branched alkyl group at  $\text{sp}^3$ -C atom were strategically incorporated to increase the power conversion efficiency (PCE) of zwitterionic dyes by improving photo-current density ( $J_{sc}$ ) and open-circuit potential ( $V_{oc}$ ) of the cell. Among these four dyes, NSQ3 exhibited the highest efficiency of 6.73% with a  $J_{sc}$  of 18.74  $\text{mA}/\text{cm}^2$ ,  $V_{oc}$  of 0.53 V, and fill factor ( $ff$ ) of 68.3%, without any co-adsorbent under irradiance of 100  $\text{mW}/\text{cm}^2$  (simulated AM 1.5G sunlight). In presence of  $3\alpha,7\alpha$ -dihydroxy-5 $\beta$ -cholanic acid (CDCA), NSQ1, NSQ2 and NSQ3 showed efficiency of 7.07%, 7.38% and 7.17%, respectively. Despite the low  $V_{oc}$ , far red light harvesting efficiency, reduced dye aggregation, long lifetime of injected electron and high quantum efficiency of NSQ1-3 played constructive role to achieve high PCE efficiency. Deceleration of charge recombination for NSQ dye cells were further studied by electrochemical impedance spectroscopy (EIS) and open-circuit photo-voltage decay (OCVD) measurements (*J. Mater. Chem. A* **2016**, 4, 18910).

#### Effect of out-of-plane alkyl group's position in dye sensitized solar cell efficiency: A structure-property relationship utilizing indoline based unsymmetrical squaraine dyes:

A series of indoline based unsymmetrical squaraine (SQ) dyes that contain alkyl chains at N- and  $\text{sp}^3$ -C-atoms of indoline moieties with a carboxylic acid anchoring group were synthesized. The optical and electrochemical properties of the SQ dyes in solution were nearly identical as there was no change in the D-A-D SQ framework. Remarkable changes in respect to the power conversion efficiencies (PCE) were observed depending upon the position of alkyl groups in the dye. Introduction of alkyl groups to the indoline unit that was away from anchoring unit were helped in more dye loading with controlled organization of dyes on surface, increased charge transfer resistance, long electron lifetime. Hence it exhibited high PCE than the corresponding isomer in which the alkyl groups functionalized indoline unit contained the carboxylic acid anchoring group. Careful analysis of incident photon-to-current conversion efficiency (IPCE) profiles indicated the presence of aggregated structure on the  $\text{TiO}_2$  surface that contributed to the charge injection in presence of a co-adsorbent. A dye-sensitized solar cell (DSSC) device made out of SQ5 achieved an efficiency of 9.0 %, with an open-circuit potential ( $V_{oc}$ ) of 660 mV and short-circuit current of ( $J_{sc}$ ) of 19.82  $\text{mA}/\text{cm}^2$ , under simulated AM 1.5G illumination (100  $\text{mW}/\text{cm}^2$ ). The IPCE profile of SQ5 showed an onset near to 750 nm with a good quantum efficiency (> 80%) in the range of 550-700 nm indicated the importance of self organization of dyes on the  $\text{TiO}_2$  surface for an efficient charge injection. This present investigation revealed the importance of position of alkyl groups in the squaraine based dyes for the better PCE.



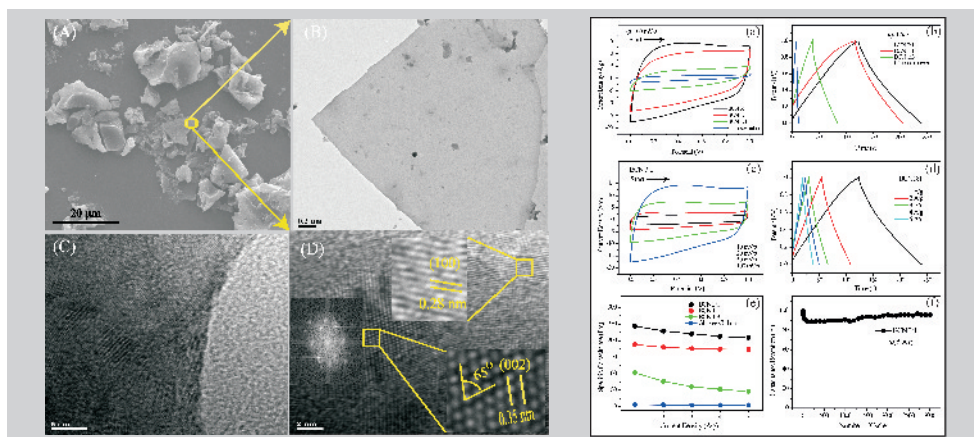
## Advanced Materials

### Materials for energy

Manjusha Shelke | mv.shelke@ncl.res.in

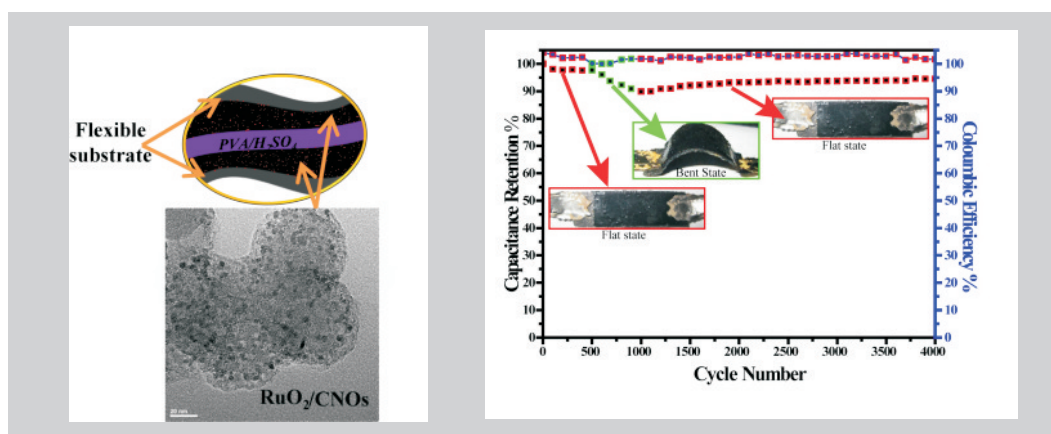
**Facile green synthesis of BCN nanosheets as high-performance electrode material for electrochemical energy storage:** Two-dimensional hexagonal BCN nanosheets were synthesized by a new approach in which a mixture of glucose and adduct of boric acid and urea was heated at 900°C. The method is green, scalable and gives a high yield of BCN NSs with average size of about 1 μm and thickness of about 13 nm. Structural characterization of

the as-synthesized material was carried out by several techniques. Its energy storage properties were evaluated electrochemically. The material showed excellent capacitive behaviour with a specific capacitance as high as 244 Fg<sup>-1</sup> at a current density of 1 Ag<sup>-1</sup>. The material retained up to 96% of its initial capacity after 3000 cycles at a current density of 5 Ag<sup>-1</sup> (*Chem. Eur. J.* **2016**, *22*, 7134).



**RuO<sub>2</sub>nH<sub>2</sub>O Nanoparticles anchored on carbon nano-onions: An efficient electrode for solid state flexible electrochemical supercapacitor:** The group has developed a flexible solid state electrochemical capacitor based on hydrous RuO<sub>2</sub> nanoparticles, supported onto the nanoporous and highly accessible ion adsorptive carbon nano-onions (CNOs) was fabricated in a novel process of modifying a conducting carbon paper to a flexible conducting substrate, separated with a poly(vinyl alcohol)/H<sub>2</sub>SO<sub>4</sub>gel electrolyte. The sol-gel technique tends to form homogeneously dispersed RuO<sub>2</sub> nanoparticles

with the average size of ~2.3 nm on the positive surface curvatures of multilayer fullerene (CNOs), which helped the high diffusivity of ions in both the aqueous and solid state gel electrolytes. The flexible substrate worked excellently as an electrical conductor as well as a stable mechanical support. This solid state flexible energy storage device showed a maximum energy density of 10.62 Whkg<sup>-1</sup> and a maximum power density of 4.456 kWkg<sup>-1</sup> for the hydrous RuO<sub>2</sub>/ CNOs nanocomposite with 94.47% cycling stability even after 4000 cycles (*ACS Sustain. Chem. Eng.* **2016**, *4*, 2528).





## Advanced Materials

### Materials for energy

Manjusha Shelke | mv.shelke@ncl.res.in

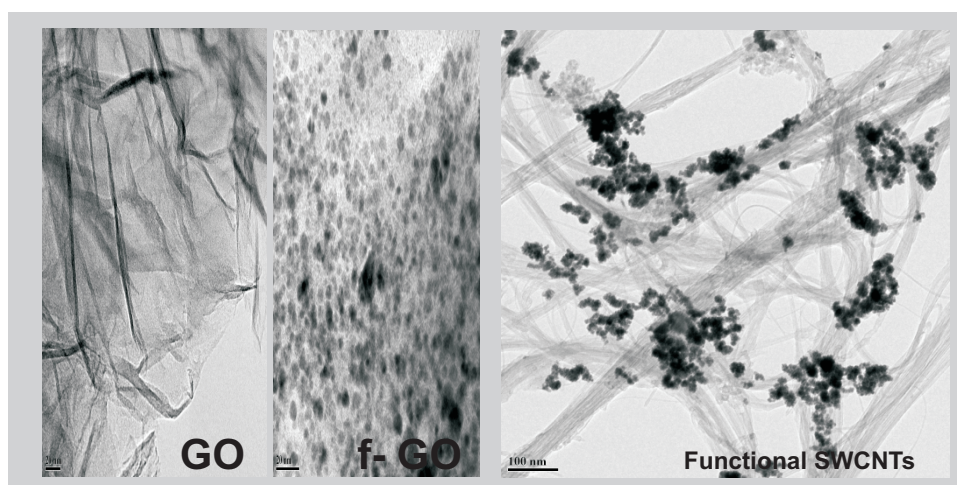
**Synthesis of novel Cu<sub>2</sub>S nanohusks as high performance counter electrode for CdS/CdSe sensitized solar cell:** Unique Cu<sub>2</sub>S nanohusks were synthesized directly on FTO coated glass substrates by electrodeposition and used as a counter electrode in QDSSC. When these electrodes are used for the reduction of polysulfide electrolyte in QDSSC,

it exhibited higher catalytic activity and photovoltaic performance as compared to the platinum counter electrode. The power conversion efficiency of about 4.68% was achieved by optimizing the deposition time of Cu<sub>2</sub>S (*J. Power Sources* **2016**, 315, 277).

Suresh Gokhale | sp.gokhale@ncl.res.in

**Modified SWCNTs for hydrogen storage:** Single-walled carbon nanotubes were explored for efficient hydrogen storage. The hydrogen storage capacity of single-walled carbon nanotubes was improved by effective surface modification, and met the US-DOE technical target value of gravimetric hydrogen storage capacity set for 2015.

**High quality GO and rGO:** Graphitic carbon is mostly oxidized to produce graphene oxide, which is further chemically processed to obtain reduced graphene oxide. Both the processes were improved to produce high quality graphene oxide and reduced graphene oxide. The graphene oxide so produced can be effectively metal functionalized for various potential applications.



## Advanced Materials

### Materials for energy

K. Krishnamoorthy | k.krishnamoorthy@ncl.res.in

**Polymeric coatings to enhance the efficiency of dye sensitized solar cells:** Recombination of charges residing in the titanium dioxide and redox electrolyte is one of the factors affecting the efficiency of DSSCs. Conducting polymers with different band edges used to suppress the charge recombination. Amongst the four polymers that are used as barrier layers, a polymer with a HOMO energy

at - 5.8 eV and LUMO at - 3.1 eV was found to increase the electron life time at titanium dioxide and decrease the charge recombination. DSSCs fabricated with a polymer as barrier layer exhibited an efficiency of 9.2%, which was 22% higher than that of DSSCs without polymer barrier layer (*Adv. Energy Mater.* **2016**, 6, 1502334).

Kaliaperumal Selvaraj | k.selvaraj@ncl.res.in

**Novel non-templated ambient nanoporation of graphene for energy and environmental applications:** Current options for nano-perforation of graphene involved industrially undesirable steps viz., usage of expensive metal or silica nanoparticle templates and hazardous chemicals. It hamper its scope for large scale production and further exploitation.

A scalable non-templated route to produce hG at ambient conditions was invented for the first time. Nano-perforation was achieved with tunable pore size via simple few layer co-assembly of silicate-surfactant

admicelles along the surface of graphene oxide. A gentle alkali treatment and a reduction at optimized conditions readily yielded holey graphene with a remarkable capacitance (~250 F g<sup>-1</sup>) and interesting adsorption abilities for pollutants. Density functional theory based computational studies revealed interesting insights on the template free nano-perforation at a molecular level. This simple rapid process not only excluded the need for expensive templates and harmful chemicals to yield hG at attractively ambient, chemically placid and industrially safer conditions, but also created no hurdles in terms of scaling up (*Nanoscale*, **2015**, 7, 19705).

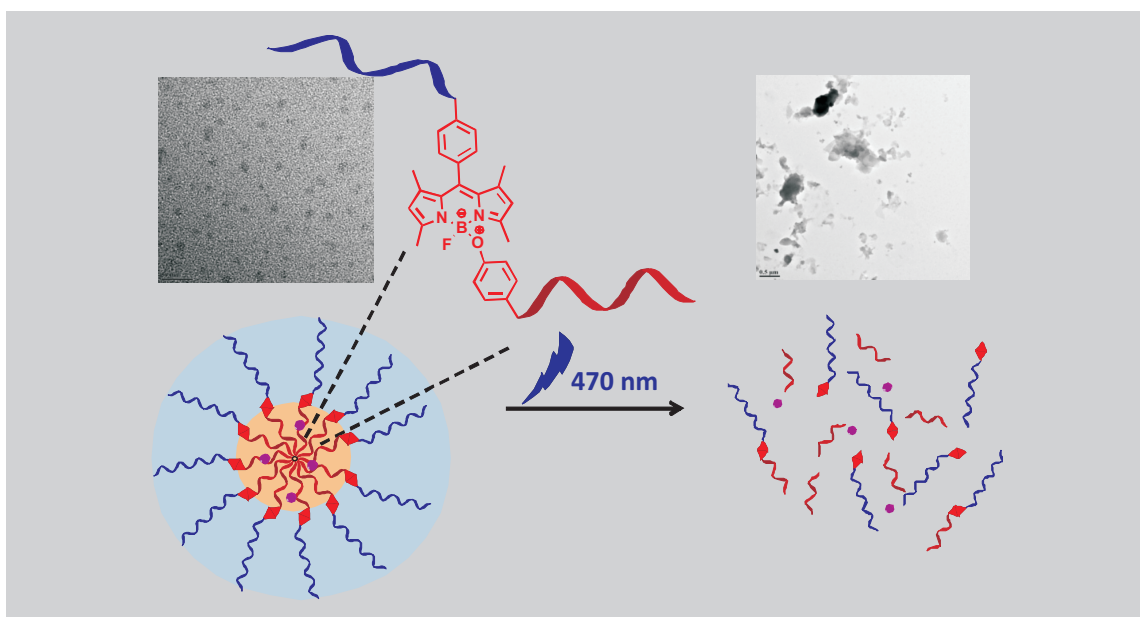
## Advanced Materials

### Materials for environmental and healthcare applications

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

**Visible light-cleavable polymeric micelles:** The visible light-cleavable polymer was developed to overcome the limitations of UV-sensitive polymers in drug delivery applications. Visible light-cleavable BODIPY molecule was incorporated at the junction of an amphiphilic block

copolymer by conducting the coupling reaction and polymerization simultaneously. Micellar assembly of the polymer was disintegrated under visible light irradiation with release of cargo (*Chem. Commun.* **2015**, *51*, 17708).



### Bioresponsive carbon nano-gated multifunctional theranostics

Kaliaperumal Selvaraj | k.selvaraj@ncl.res.in

Designing bioresponsive nanocarriers for controlled and efficient intracellular drug release for cancer therapy is a major thrust area in nanomedicine. Mesoporous silica nanoparticles (MSNPs) are being extensively explored as promising theranostic agents as it has recognized recently by US FDA. Green fluorescent carbon quantum dots (CQDs), though known as possible alternates for their more toxic and relatively less efficient predecessors, are less known as gate keepers for drug release control.

An efficient bioresponse of CQDs was reported while preparing a design using glutathione cleavable (redox responsive) disulphide bonds. When anticancer drug, doxorubicin loaded MSNPs were capped with these CQDs, they displayed promising drug release control on exposure to mimicked intracellular cancer environment.

Their dual functionality was well established with good control on preventing the premature release and exceptional bio-imaging of HeLa cancer cells. Fluorescence images proved selective targeting of HeLa cells by over expression of folate receptors from the surface functionalized folic acid ligand. Extensive characterization using XRD, TEM, BET analysis, drug loading tests, drug release kinetics, MTT assay and fluorescence cell imaging helped in understanding the multifunctionalities of the successful design, extending its scope with exciting prospects towards noninvasive targeted drug delivery and bio-imaging for effective cancer diagnosis and treatment [*Nanoscale*, **2015**, *7*, 19705].



## Advanced Materials

### Materials for environmental and healthcare applications

Rajesh G. Gonnade | rg.gonnade@ncl.res.in

**Pharmaceutical cocrystals of an anticancer drug gefitinib:** Pharmaceutical co-crystals apart from offering potential improvements in solubility, dissolution rate, bioavailability and physical stability, it can enhance other essential properties of the APIs such as flowability, chemical stability, compressibility and hygroscopicity. Gefitinib, an anticancer drug suffers from poor aqueous solubility. The technique was developed to obtain its novel polymorphs and was also successful in getting several cocrystals with FDA approved cocrystal formers. The resultant cocrystals showed significant improvement in solubility and dissolution rate (*J. Pharm. Sci.* **2015**, *104*, 4207; Patent: WO2015170345 A1).

**Novel metal coordination complex for multi-action naked eye colorimetric anion sensor:** The novel multi-action copper complex was successfully synthesized consisting dinitratebis (N- Phenethylisonicotinamide) copper(II) of formula and tetraaquabis(N-phenethylisonicotinamide)copper(II)nitrate. It has proved to be useful for reversible vapochromic detection of polar solvents and for anion sensing in both aqueous and non-aqueous media. The complex changes colour in the solid state after absorbing the anion from the aqueous/non-aqueous media within a minute. The anions were selected from the group consisting of chloride, bromide, nitro, thiocyanate, formate and acetate (Patent: WO 2016056027 A1).

**Acid responsive turn-on fluorescence of benzophenone quinoline conjugates in solution and solid state:** A novel heterocyclic probe based on benzophenone-quinoline scaffold was successfully designed and synthesized that showed remarkable changes in the absorption and emission bands under acidic conditions. The sensor device was also fabricated for acid leakage detection comprising a novel benzophenone-quinoline scaffold.

**Acyl group migration and intramolecular cyclization reaction in crystalline state:** The solvent free thermally induced intramolecular cyclization reaction of myo-inositols in the solid state was reported. The thermal cyclization also occurs in the solution and molten states, but less efficiently, suggesting that these cyclization reactions are aided by molecular pre-organization. Crystal structures of these derivatives revealed that the relative orientation of the electrophile (C=O) and the nucleophile (-OH) in the crystal lattice facilitates the intramolecular cyclization reaction. The correlation observed between the chemical reactivity and the intermolecular interactions in the crystal of the reactants provide a way to estimate the chemical stability of analogous molecules in the solid state (*Chem. Eur. J.* **2015**, *21*, 13676).

## Advanced Materials

### Nanostructured materials

Dattatray J. Late | dj.late@ncl.res.in

**2D Materials for sensors:** One step synthesis method was developed for wafer scale size highly crystalline 2D nanomaterials such as MoS<sub>2</sub>, WS<sub>2</sub> etc. thin film by using hot wire chemical vapor deposition (HW-CVD) technique. The average thickness of film was measured to be ~25 nm over an entire 4 inch wafer of quartz substrates. This method was also utilized to grow films on 4 inch SiO<sub>2</sub>/Si wafer for industrial applications. The XRD data of WS<sub>2</sub> nanoparticle showed highly crystalline nature with orientation (002) direction. Raman spectroscopy showed two prominent phonon vibration modes of E<sub>2g</sub><sup>1</sup> and A<sub>1g</sub> at ~356 cm<sup>-1</sup> and ~420 cm<sup>-1</sup> respectively indicating few atomic layer thicknesses. The TEM analysis showed a good crystalline quality of sample. The synthesized WS<sub>2</sub> nanoparticle thin film based device showed good response to humidity and photo sensitivity along with good long-term stability of the device. It was found that the resistance of the films decreased with increasing relative humidity (RH). The maximum humidity sensitivity of 469% along with response time of ~12 sec and recovery time of ~13 sec were observed for the WS<sub>2</sub> thin film humidity sensor device. In case of photo detection the response time of ~51 sec and recovery time of ~88 sec were observed with sensitivity ~137% under white light illumination. These results opened up several avenues to grow other TMDCs nanoparticle thin film for large area nanoelectronics as well as industrial applications (*ACS Appl. Mater. Inter.* **2016**, *8*, 3359; *Nanoscale* **2016**, *8*, 3008; *Appl. Phys. Lett.* **2016**, *109*, 142101; *Chem. Select.* **2016**, *1*, 5380; *Mater. Res. Express* **2016**, *3*, 105038; *Appl. Mater. Today* **2016**, *5*, 98; *Appl. Phys. A- Mater.* **2016**, *122*, 899; *Adv. Device Mater.* **2016**, *2*, 8; 15; *ACS Appl. Mater. Interfaces* **2016**, *8*, 11548; *Appl. Phys. A.* **2016**, *122*, 560; *RSC Adv.* **2016**, *6*, 29734; 41261; 48843; 76551; *Chem. Phys. Lett.* **2016**, *651*, 148; *J. Vac. Sci. Technol. B* **2016**, *34*, 41803).

**Liquid exfoliation of 2D materials:** The bulk crystal of black phosphorus was exfoliated by liquid exfoliation method for duration of 8 hours using N-Methyl-2-Pyrrolidone as the solvent. The exfoliated sample was centrifuged at different rpm such as 3000, 5000 and 10,000 to separate out the 2D black phosphorus nanosheets with different thickness and length. The synthesized black phosphorus nanosheets collected at these rpm values were characterized with TEM, AFM, Raman spectroscopy and Vis-NIR spectroscopy. The humidity sensing behaviour of the devices fabricated by using these samples was investigated. The results obtained showed that the device fabricated with black

phosphorus nanosheets and nanoparticles obtained by filtration of the sample collected after 10,000 rpm exhibited better performance as compared to the nanosheets collected at 3000 and 5000 rpm. The response and recovery times of devices were found promising and better than those of the black phosphorus gas sensor reported earlier. The present investigations open up a new avenue for further studies in improving the performance of black phosphorus nanosheets based gas sensing devices (*Micropor. Mesopor. Mat.* **2016**, *225*, 494).

**Materials for vacuum nanoelectronics:** One step facile chemical vapour deposition method for synthesis of single-layer MoSe<sub>2</sub> nanosheets with average lateral dimension ~60 μm on 300 nm SiO<sub>2</sub>/Si and n-type silicon substrates was reported. The field emission investigation of MoSe<sub>2</sub>/Si was at the base pressure of ~1×10<sup>-8</sup> mbar. The morphological and structural analyses of the deposited single-layer MoSe<sub>2</sub> nanosheets were carried out using an optical microscopy, Raman spectroscopy and atomic force microscopy. The values of turn-on and threshold electric fields required to extract an emission current densities of 1 and 10 A/cm<sup>2</sup>, were found ~1.9 and ~2.3 V/m, respectively. The MoSe<sub>2</sub> nanosheet emitter delivered maximum field emission current density of ~1.5 mA/cm<sup>2</sup> at a relatively lower applied electric field of ~3.9 V/m. The long term operational current stability recorded at the preset values of 35 A over the entire duration was found stable. The observed results demonstrated that the layered MoSe<sub>2</sub> nanosheet based field emitter can open up many opportunities for their potential application as an electron source in flat panel display, transmission electron microscope, X-ray generation. The facile one step synthesis approach and robust emitter nature of single-layer MoSe<sub>2</sub> nanosheets can provide prospects for the future development of practical electron sources based on this layered material (*J. Mater. Chem. C* **2016**, *4*, 1096; *RSC Adv.* **2016**, *6*, 95092; 9932; *Chem. Select* **2016**, *1*, 3723; *Chem. Phys. Lett.* **2016**, *667*, 167; *Micropor. Mesopor. Mater.* **2016**, *225*, 573; *Mater. Res. Express* **2016**, *3*, 35003).

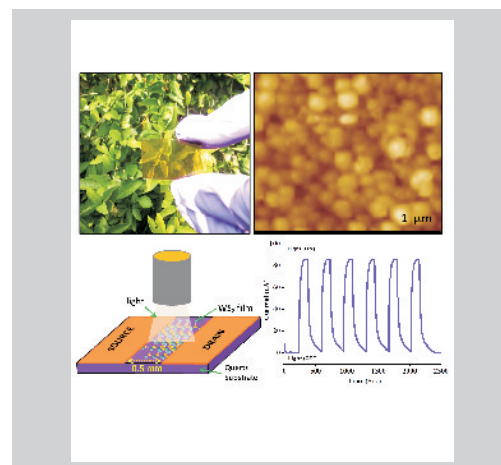
**Materials for energy storage and generations:** The growth of nickel cobalt sulfide (NCS) ultrathin nanosheets directly on Ni foam substrate by a facile and novel electrodeposition method was reported. The prepared NCS sample was used as an electrode material for supercapacitor application due to their large electrochemically active surface area and interconnected nanosheet channels for the facilitation of ion

## Advanced Materials

### Nanostructured materials

Dattatray J. Late | dj.late@ncl.res.in

transportation. The NCS nanosheets possessed enhanced electrochemical performance in terms of fast and high reversible faradaic reactions characterized by prominent oxidation and reduction peaks. NCS nanosheets showed an ultrahigh specific capacitance of 1712 Fg<sup>-1</sup> at a current density of 1 Ag<sup>-1</sup> with excellent cyclic stability. The excellent supercapacitor performance of NCS nanosheets can be attributed to its rich redox reactions as well as high transport rate for both electrolyte ions and electrons.



P.A. Joy | pa.joy@ncl.res.in

**Thermal conductivity of magnetite nanofluids:** Magnetic nanofluids are surfactant coated superparamagnetic nanoparticles dispersed in liquid carriers, having tunable thermophysical properties. The research was focused on understanding the various factors that affect the thermal conductivity of magnetite based nanofluids, such as the role of surfactant, base fluid, nanoparticles, interface, etc. It was shown that the thermal conductivity of the lauric acid coated magnetite nanofluids depended on the amount and nature of the primary and secondary

surfactants on the dispersed nanoparticles. The different surfactant layers determined the interaction between the base fluid and the surfactant and therefore the dispersibility and stability of the nanofluids. Stable fluids showed relatively lower enhancement in the thermal conductivity due to the highly dispersive nature of the nanoparticles, but these fluids showed larger enhancement in the thermal conductivity in a magnetic field (*J. Phys. Chem. C* **2016**, *120*, 11640).

## Advanced Materials

### Nanostructured materials

#### Scaling up the shape: Novel growth pattern of gallium clusters

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

#### Detection of water in dry solvents

Spherical  $\text{SrF}_2:\text{Eu}^{3+}$ @TTA nanoparticles were used for the detection of water in dry solvents. The nanoparticles upon 343 nm excitation gave enhanced sensitised luminescence in THF, DCM *etc.* due to efficient energy transfer from TTA molecule to  $\text{Eu}^{3+}$ . The Vibronic coupling of Eu (III) ion excited states with the -OH oscillators also contributed to the quenching phenomenon. Limit of detection of water by this method was  $1 \times 10^{-4}$  % by weight (RSC Adv. **2015**, 5, 47131)

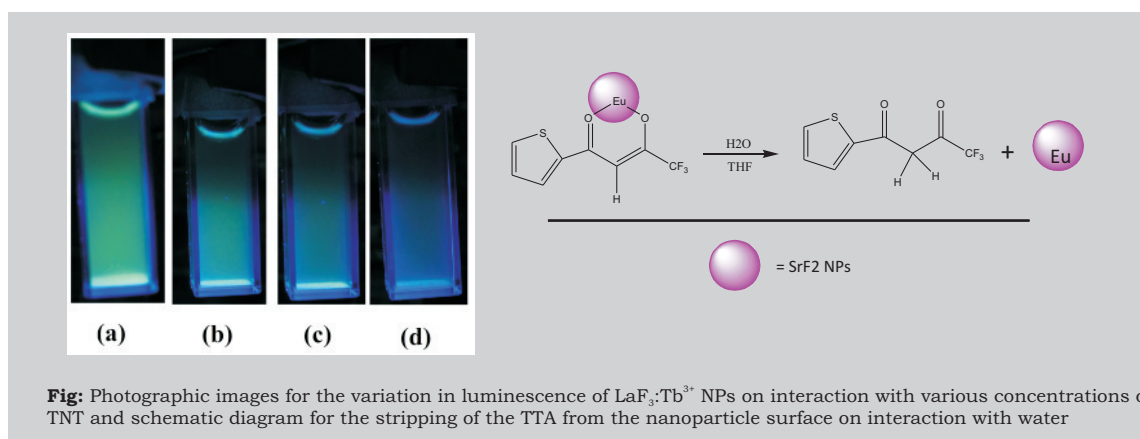
#### Highly explosive aromatic nitro compounds: Detection

A novel approach was reported for the detection of highly explosive aromatic nitro compounds utilizing  $\text{LaF}_3:\text{Tb}^{3+}$ @pABA nano particles. Functionalised particles give 100 times stronger emission than  $\text{LaF}_3:\text{Tb}^{3+}$ . Luminescence intensity was decreased exponentially upon addition of nitro compounds. Both energy transfer and electron transfer were occurred. Low lying stable LUMOs of nitroexplosives were responsible for the

electron transfer quenching, which is thermodynamically favored. The detection at ppm level was quite easily achieved for all the compounds (PA, 2,4-DNT, 2,4-DNP, NP, 2,6-DNT) but the nanoparticles showed very high sensitivity up to 50 ppb level for TNT (RSC Adv. **2015**, 5, 10468; WO 2016/020939 A1).

#### Detection of heavy metals in water sources

$\text{Gd}_2\text{O}_3:\text{Eu}^{3+}$  nanoparticles were utilized for the selective detection of heavy metal ions in water. Detection limit for  $\text{Fe}^{3+}$ ,  $\text{Cr}^{3+}$  and  $\text{Cu}^{2+}$  are 2, 4 and 4 ppm, respectively. Ferric ion was detected in presence of  $\text{Cr}^{3+}$  and  $\text{Cu}^{2+}$  without much interference. The particles were used to analyze environmental water samples (Pashan lake and Khadakwasla Dam). Luminescence of the particles was not remarkably quenched by the environmental samples indicating very low concentration of metal ions of interest in the samples, which was further supported by ICP-AES (*J. Lumin.* **2016**, 171, 1).



**Fig:** Photographic images for the variation in luminescence of  $\text{LaF}_3:\text{Tb}^{3+}$  NPs on interaction with various concentrations of TNT and schematic diagram for the stripping of the TTA from the nanoparticle surface on interaction with water

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

**Modified digestive ripening for ultra small nanoparticle synthesis:** The group worked extensively in the area of bottom up synthesis of nanoparticle dispersions and their catalytic applications. The preparation of ultra small transition metal nanoparticles (<3nm) was reported by

using a process called “modified digestive ripening” that are mediated by bromide ion. The resultant nanoparticles exhibited an enhanced catalytic activity than those prepared by the conventional digestive ripening process (*Nano Res.* **2016**, 9, 2007).

## Energy and Environment

### Emission and effluent control including water and soil management

Vinay M. Bhandari | vm.bhandari@ncl.res.in

**Industrial wastewater treatment and environmental pollution control:** Cleaner environment is not just priority goal for developed countries, but is an essential and priority agenda for developing country like India which houses numerous chemical industries. The group tried to address the issues pertaining to pollution control through development of newer materials and methods for effective industrial wastewater treatment for removal of refractory pollutants and also for deep desulfurization of transportation fuels. The focus was on development of newer separation processes and process integration of adsorption, coagulation and cavitation (*Ind. Eng. Chem. Res.* **2015**, *54*, 11844; *ACS Sustain. Chem. Eng.* **2016**, *4*, 2495; *Desalin. Water Treat.* **2016**, *57*, 27934).

**Development of newer separation processes and process integration of adsorption, coagulation and cavitation:** The coagulation processes have potential for removing COD levels significantly at low cost of operation. Recent developments include coagulant formulations, biocoagulants that can dramatically enhance the performance with reduced sludge formation. Similarly, newer adsorbents have potential for treating variety of effluents e.g. dyes, fertilizer, pharmaceutical etc. CSIR-NCL is working on the development, modifications and application of novel materials that can further improve the existing methods of industrial wastewater treatment processes. CSIR-NCL developed a cavitation process using vortex flow (newer device-vortex diode) and is shown to be effective for industrial wastewater treatment. This technology can be used for removal of COD, ammoniacal nitrogen and color. It can be implemented alone or in combination with other processes.

Ravi Kumar | v.ravikumar@ncl.res.in

**Degradation studies of brominated compounds:** Use of persistent organobromines for industrial applications led to their accumulation in environment. *Yarrowia lipolytica* NCIM 3589, a tropical marine yeast, was found to degrade and detoxify bromo compounds. By optimizing culture conditions with 1-bromodecane as reference compound, the dehalogenase involved was remarkably enhanced 13-

fold (384.13 U/ml) by a hybrid statistical design of experiments. Studies brought out in a novel way the role of aliasing and other masked interactions in growth media factors. The enzyme acted on C3-C16 bromoalkanes and bromoaromatics, thereby generalizing this 'green chemistry' approach (*J. Ind. Eng. Chem.* **2016**, *41*, 114).



## Energy and Environment

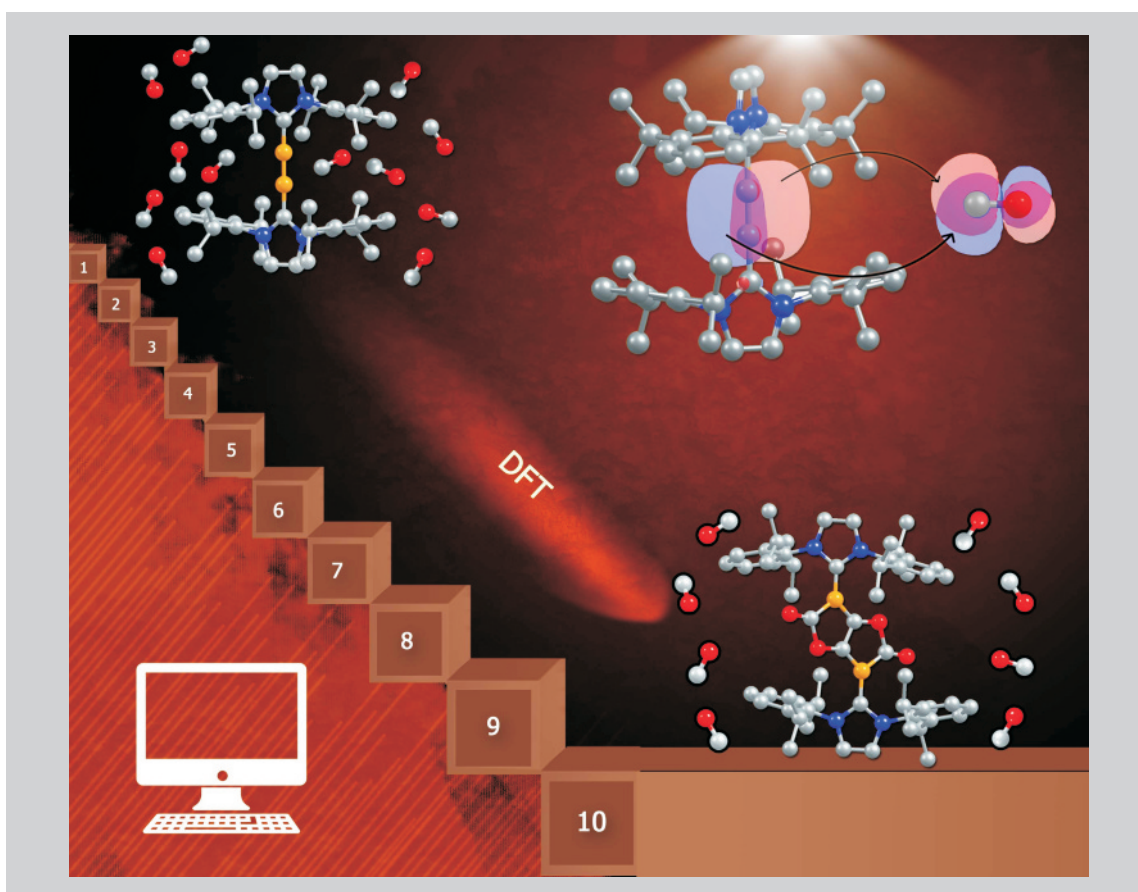
### Renewable and alternative energy technologies

#### Small molecule activation by main group compounds

Kumar Vanka | k.vanka@ncl.res.in

**Constrained phosphorus compounds for dehydrogenating ammonia borane:** An exciting new development in main group chemistry has been the use of a constrained, “flat”, phosphorus based complex to mediate in reactions such as the dehydrogenation of ammonia borane (AB), and the activation of the N-H bond in primary amines. It showed that main group compounds, when properly designed, can be as effective as transition metal complexes for doing significant chemical transformations. This computational study, employing density functional theory (DFT), revealed the correct mechanism to account for the behavior of the flat phosphorus compound in the different reactions that have been experimentally reported to date. The significance of the work lies in the fact that the insights gained can be utilized to design new constrained phosphorus based compounds in the future. Given the immense importance of small molecule activation by main group compounds in the world today (*Inorg. Chem.* **2016**, *55*, 558).

**Exploring the reducing role of boron: Added insights from theory:** Carbon-carbon coupling in CO molecules is a challenging proposition, and very few main group complexes were shown to affect this process. A recently reported triply bonded diboryne system is notable for coupling four CO molecules to produce a (bis)boralactone species. The current full quantum chemical computational calculations with density functional theory (DFT) provided important insights into the nature of the CO coupling process by triply bonded diboryne systems. The complete reaction pathway leading to the formation of the (bis)boralactone was determined. Factors that make this system so successful in coupling CO groups were elucidated. The pertinent issues such as why the coupling process stops after four CO additions were explored. The insights were gained through the natural bond order (NBO) analysis into how the back-donation from diboryne activates CO (*Dalton T.* **2016**, *45*, 5978).





## Energy and Environment

### Renewable and alternative energy technologies

#### Utilization of dairy-waste whey for production of biodiesel

Ravi Kumar | v.ravikumar@ncl.res.in

**Statistical process optimization studies:** Optimization studies for the in-situ transesterification step were carried out to obtain improved yields from dried biomass of an oleaginous fungus *Aspergillus candida* grown on abundantly available agro-dairy waste, whey etc. Statistical screening for varying process conditions and variables showed biomass to be the predominant factor in

conversion to fatty acid methyl esters, i.e., biodiesel, with higher conversion or process efficiency obtained on employing lower biomass loadings. Properties of the biodiesel obtained met national and international norms. This work was carried out in collaboration with Savitribai Phule Pune University (*Bioresource Technol.* **2015**, *197*, 502).

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Debashree Ghosh | debashree.ghosh@ncl.res.in

**Computational and theoretical understanding of alternative energy technologies:** The nature of excited states involved in singlet fission in promising molecules like polyacenes was studied. It was found that it is a delicate balance of static and dynamic correlation that gave rise to the low singlet triplet gap and required the use of multi reference electronic structure methods for the proper understanding of these processes (*Phys. Chem. Chem. Phys.* **2015**, *17*, 9849).

**Computational and theoretical understanding of photo-processes in biology:** The photodamage mechanism of melanin was proposed via ionization mediated processes. Photodamage mechanism via excited state proton transfer in DNA bases was studied and ionization was

found to be a major factor in it. Absorption and fluorescence in GFP chromophore was studied in various environment and the competing factors were noticed (*J. Phys. Chem. B*, **2015**, *119*, 13288; **2016**, *120*, 4410; *J. Phys. Chem. A* **2014**, *118*, 5323; *Phys. Chem. Chem. Phys.* **2016**, *18*, 6526; *J. Mater. Chem. C* **2016**, *4*, 2793)

**Development of hybrid QM/MM techniques for excited state processes in condensed phase:** Hybrid QM/MM techniques for excited state processes in condensed phase such as biological systems were developed and implemented. It is available in the quantum chemistry software Q-Chem as well as online for free usage (*Mol. Phys.* **2015**, *113*, 184; *J. Phys. Chem. B* **2016**, *120*, 6562).

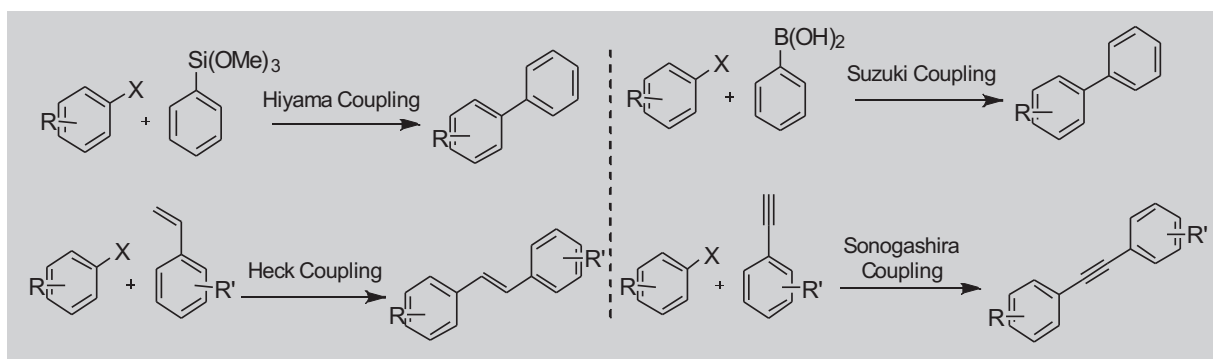
## Healthcare

### Natural products and methodology

**Asymmetric total synthesis of biologically active compounds and development of synthetic methodologies** Pradeep Kumar | pk.tripathi@ncl.res.in

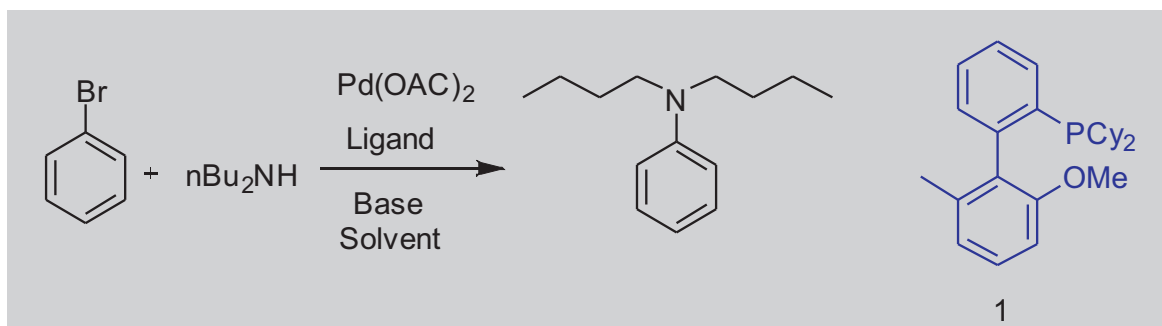
**Carbon-carbon bond forming reactions:** A highly active SBA-15-TAT-Pd(II) catalyst was synthesized. The catalyst was employed in carrying out Heck, Sonogashira, Suzuki and Hiyama cross coupling reactions. Under the optimized conditions the catalyst displayed excellent catalytic

activity in delivering the desired products in good to excellent yields. The catalyst also exhibited ease of recovery from reaction mixture and was used for several times without any appreciable loss of catalytic activity (*Catal. Commun.* **2015**, 69, 11).



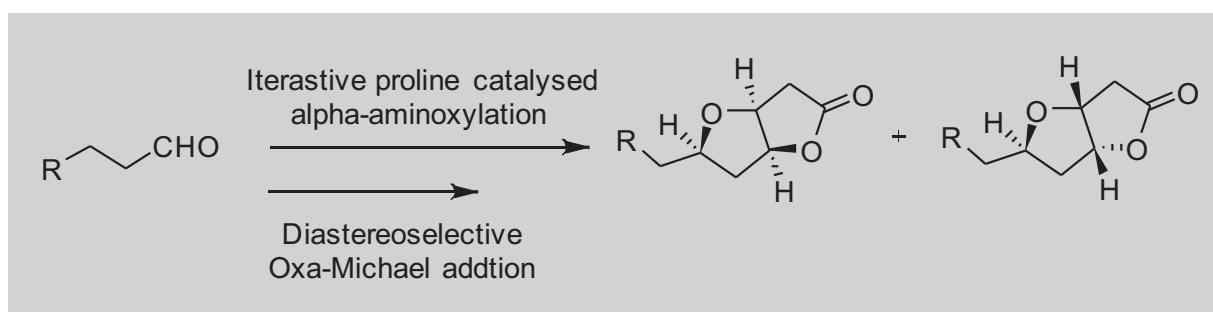
**Modular synthesis of biaryl-substituted phosphine ligands: Application in microwave-assisted palladium-catalyzed C–N cross-coupling reactions:** The C-1 symmetric biaryl monophosphine based ligands were synthesised by aryne cross-coupling of aryllithium with

functionalized 1,3-dibromobenzene or substituted bromobenzodioxole derivative. These ligands were employed in the palladium catalyzed C-N bond forming reactions (*Eur. J. Org. Chem.* **2015**, 6515).



**A stereo-controlled synthesis of Hagen's gland lactones via iterative proline catalyzed  $\alpha$ -aminoxylation and oxamichael addition reactions:** A simple and efficient synthesis of Hagen's gland lactones was achieved using a sequential  $\alpha$ -aminoxylation/oxa-Michael approach in a

highly diastereoselective manner with assignment of relative configurations. This method was found to be applicable for the synthesis of various other isomers of Hagen's gland lactones (*RSC Adv.* **2015**, 5, 61000).

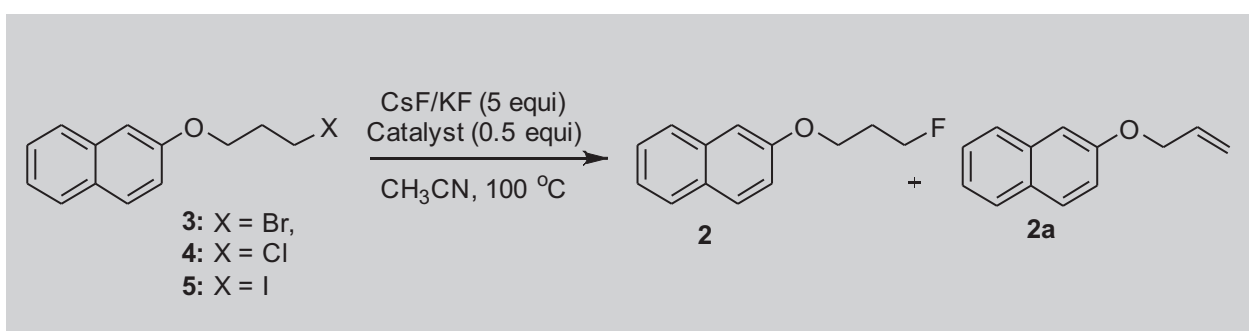


## Healthcare

### Natural products and methodology

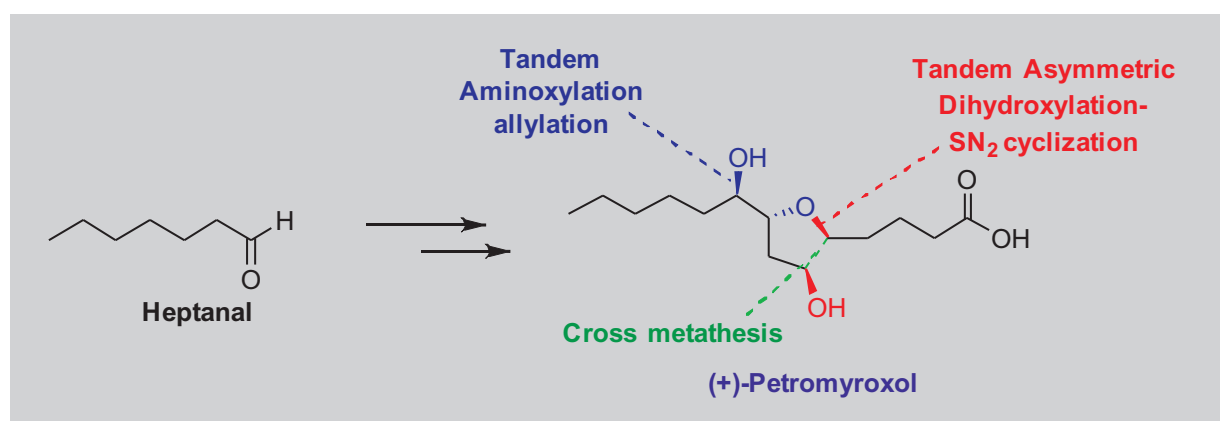
**Nucleophilic fluorination using imidazolium based ionic liquid bearing tert-alcohol moiety:** The ionic liquid bearing *tert*-butanol moiety ([mim-<sup>t</sup>OH][OMs]) was employed as an organocatalyst in nucleophilic

fluorination of a variety of substrates containing halogen/sulfonate as a leaving group. The low reactive metal fluorides including KF were used as a fluoride source in the reaction (*New J. Chem.* **2015**, *39*, 4368).



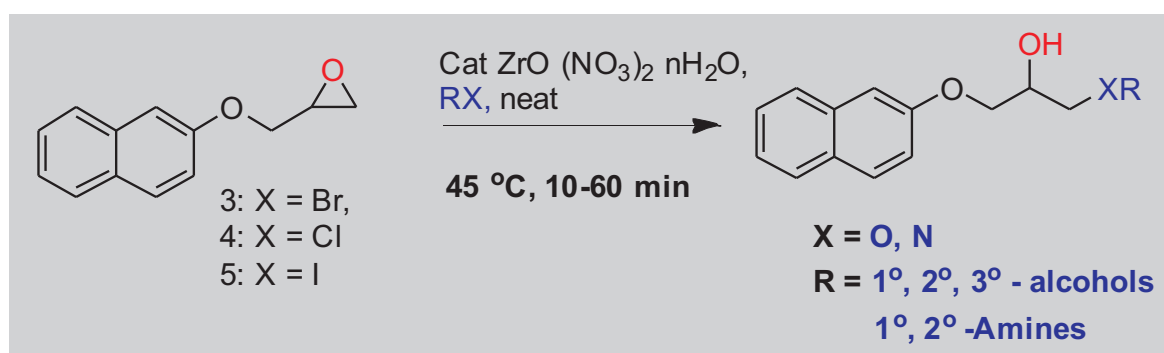
**Total synthesis of (+)-petromyroxol via tandem  $\alpha$ -aminoxylation-allylation and asymmetric dihydroxylation-SN<sup>2</sup> cyclization approach:** A non-racemic mixture of petromyroxol (2.9 mg) was isolated from >100 000 L of water conditioned with the larvae of *Petromyzon marinus*. The (+)-enantiomer was found to be

just 0.9 mg (36%) of the isolated mixture was found to trigger a better olfactory response among the lamprey fish than its (-)-antipode. The present synthesis employed a tandem  $\alpha$ -aminoxylation-allylation, cross metathesis and tandem asymmetric dihydroxylation-SN<sup>2</sup> cyclization as key steps (*RSC Adv.* **2015**, *5*, 63311).



**Mild regioselective alcoholysis and aminolysis of epoxides catalyzed by zirconium(IV) oxynitrate:** Mild regioselective method was developed for ring-opening of epoxides with

various general alcohols and amines using zirconium (IV) oxynitrate as catalyst under solvent-free condition (*Tetrahedron Lett.* **2015**, *56*, 5916).

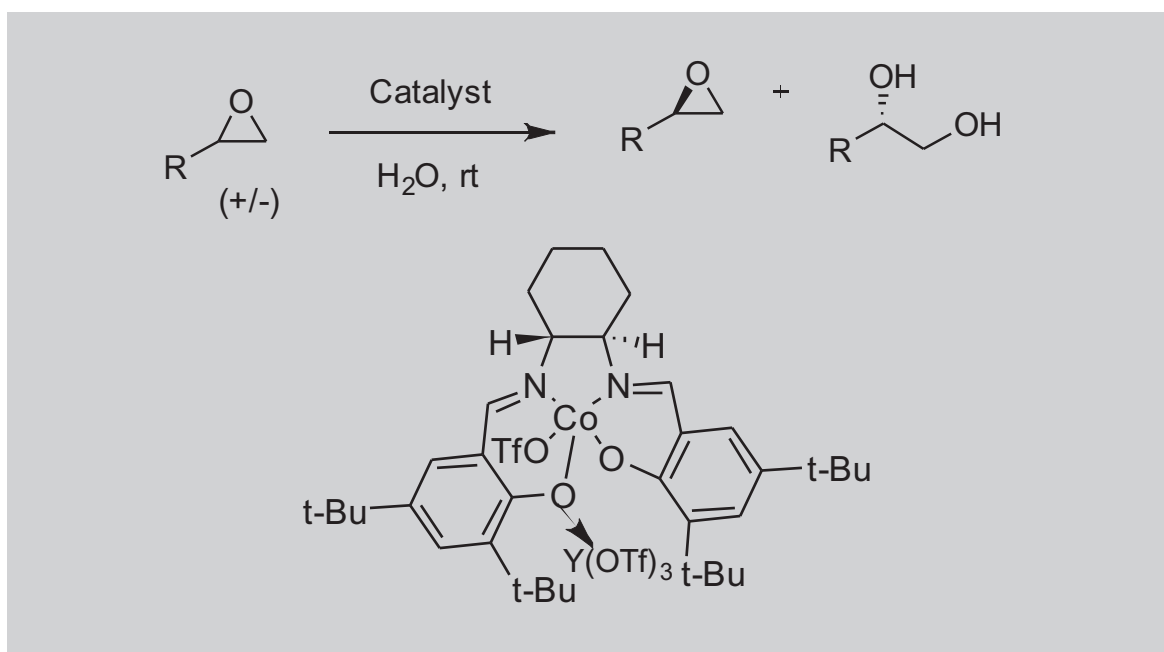


## Healthcare

### Natural products and methodology

**Dinuclear salen cobalt complex incorporating Y(OTf)<sub>3</sub>: Enhanced enantioselectivity in the hydrolytic kinetic resolution of epoxides:** The activation of inactive Jacobsen chiral salen Co(II) (salen = *N,N'*-bis(3,5-di-*tert*-butylsalicylidene)-1,2-cyclohexane-diamine) compound is attained by dinuclear chiral salen Co(III)-OTf complex

formation with yttrium triflate. We found that the binuclear Co-complex significantly enhanced reactivity and enantioselectivity in the hydrolytic kinetic resolution of terminal epoxides compared to its monomer analogous and kinetic data is also consistent with these results (*RSC Adv.* **2015**, *5*, 82699).



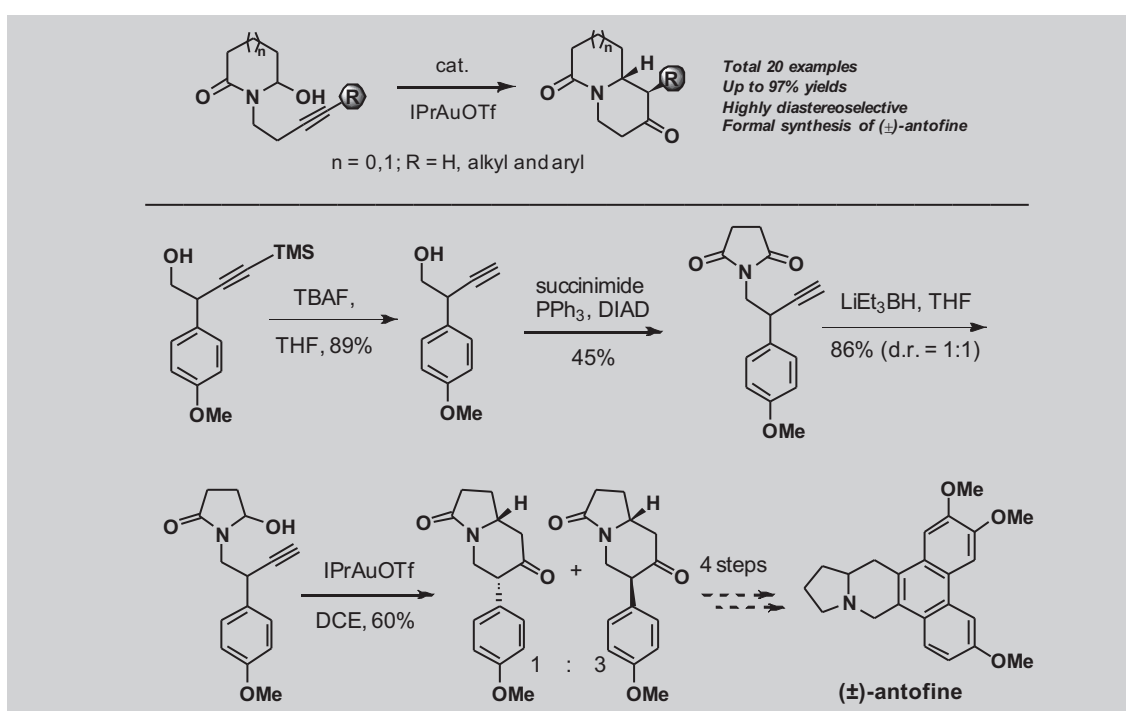
## Healthcare

### Natural products and methodology

Nitin T. Patil | n.patil@ncl.res.in

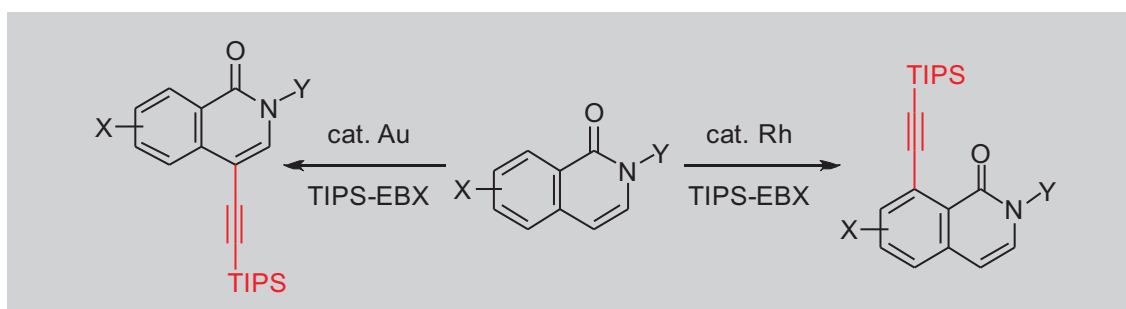
**Gold (I)-catalyzed hydroaminaloxylation and petasis-ferrier rearrangement cascade of aminated alkynes:** The indolizidines and quinolizidines are an important structural motif found in numerous natural products and pharmaceutically important compounds. Hence, the development of novel strategies for the stereoselective synthesis of these "izidine"-type alkaloids is also

important. An efficient method was developed to generate a diverse array of indolizidines and quinolizidines from readily available aminated alkynes via gold(I)-catalyzed hydroaminaloxylation and Petasis-Ferrier rearrangement cascade. The method enabled a formal synthesis of (±)-antofine (*Org. Lett.* **2016**, *18*, 1844).



**Gold vs. rhodium catalysis: Tuning reactivity through catalyst control in the C-H alkylation of isoquinolones:** Efforts have been devoted to the effective synthesis and functionalization of isoquinolones. It was found that site-selective C-4/C-8 alkylation of isoquinolones was possible by the use of either gold or rhodium complexes. A

broad range of synthetically useful functional groups (-F, -Cl, -Br, -CF<sub>3</sub>, -OMe, alkyl etc.) were tolerated, providing an efficient and robust protocol for the synthesis of either C-4 or C-8 alkynylated isoquinolones (*Org. Lett.* **2016**, *18*, 1056).



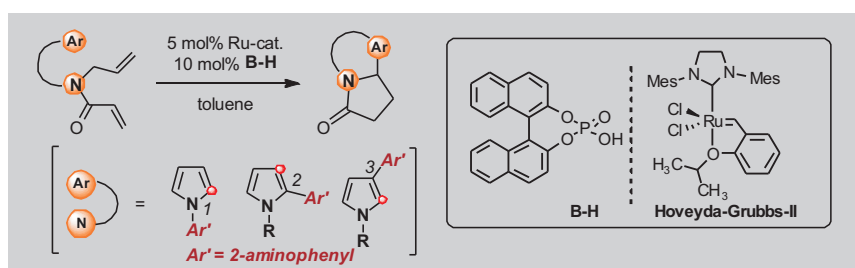
## Healthcare

### Natural products and methodology

Nitin T. Patil | n.patil@ncl.res.in

**A unified approach to pyrrole-embedded aza-heterocyclic scaffolds based on RCM/ isomerization/ cyclization cascade catalyzed by Ru/BH binary catalyst system:** An easy and straightforward preparation of pyrrole-embedded aza-heterocyclic scaffolds employing Ru/B-H binary catalyst system was developed. The strategy generated a diverse array of privileged scaffolds from 2-aminophenyl group appended pyrroles that was

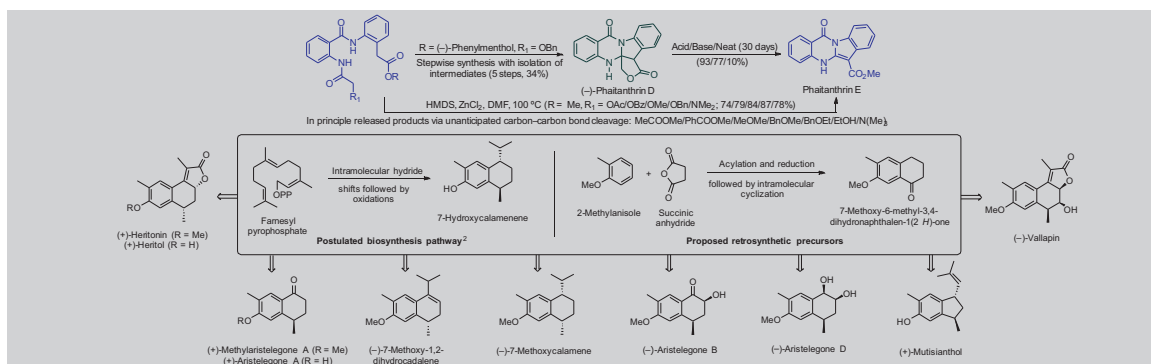
prepared by a two-step process from corresponding aminoaryl-substituted pyrroles. The technique of incorporating 2-aminoaromatic groups in the heterocycles and their subsequent ring-closing-metathesis (RCM), isomerization followed by subsequent Pictet-Spengler type reaction was also applicable to other heterocycles for generating a library of multi-ring compounds in an efficient manner (*RSC Adv.* **2016**, *6*, 34428).



Narshinha P. Argade | np.argade@ncl.res.in

**Total synthesis of recently isolated bioactive natural products:** The group has done the total synthesis of several desired, complex bioactive natural and unnatural products, pseudo natural products and natural product hybrids using cyclic anhydrides as potential precursors, employing variety of new synthetic strategies. The real challenge was in designing these molecules with highly efficient practical routes. A collective total synthesis of bioactive natural products is of contemporary interest from the strategic flexibility and dedicated SAR studies point of view. Biogenetic type total synthesis of alkaloids ( $\pm$ )/(-)-phaitanthrin D and phaitanthrin E was accomplished. The Csp<sup>3</sup>-Csp<sup>3</sup> bond cleavage with the release of several heteroatom bearing unexpected leaving groups in intramolecular substitution reactions on an iminium double bond in the quinazolinones was demonstrated using HMDS/ZnCl<sub>2</sub> or NaHMDS.

The mechanistic aspects were supported by isolation and characterization of appropriate intermediates. Starting from succinic anhydride and 2-methylanisole chemoenzymatic collective formal/ total synthesis of several optically active tetrahydronaphthalene based bioactive natural products was completed via advanced level common precursors; the natural product and antipode (-)/(+)-aristelegone B. Regioselective benzylic oxidations, stereoselective introduction of hydroxyl groups at the  $\alpha$ -position of ketone moiety in *syn*-orientation, efficient enzymatic resolutions with high enantiomeric purity, stereoselective reductions, samarium iodide induced deoxygenations and tandem acylation-Wittig reactions; without racemization and/or eliminative aromatization were the key features (*Org. Lett.* **2015**, *17*, 6218; *Org. Biomol. Chem.* **2015**, *13*, 11331).





## Healthcare

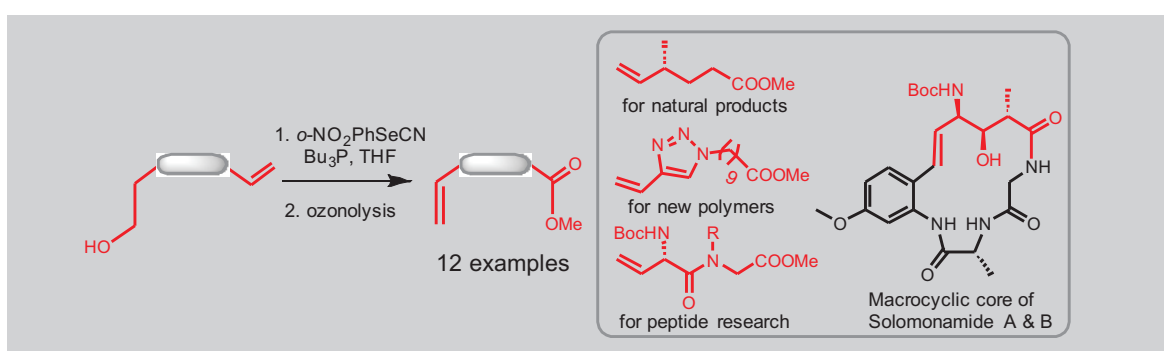
### Natural products and methodology

D. Srinivasa Reddy | ds.reddy@ncl.res.in

#### Breaking and making of olefins simultaneously using ozonolysis: Application to the synthesis of useful building blocks and macrocyclic core of solomonamides:

Solomonamide A showed potent anti-inflammatory activity in mouse model at a very low concentration of 100 µg/kg and solomonamide B could not be tested due to scarcity of the material. The potent biological activity and challenging macrocyclic skeleton prompted us to take up

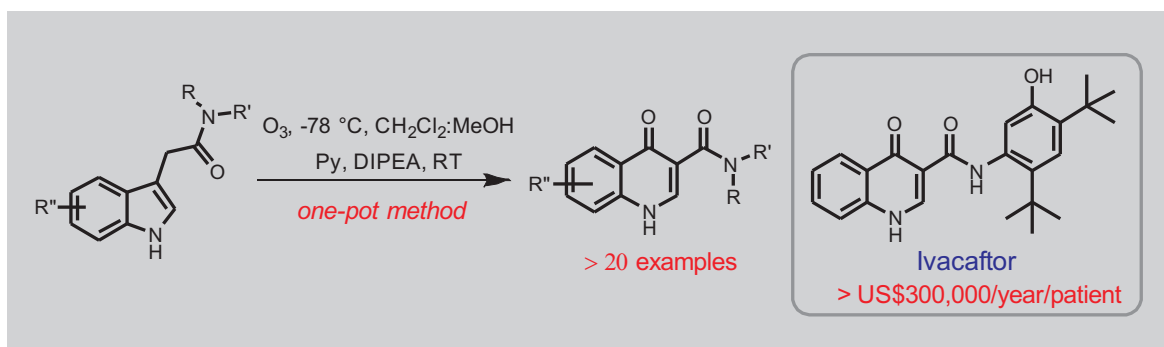
this molecule for total synthesis. A simple and practical one-pot, two-directional approach was developed to access olefinic esters through simultaneous breaking and making of olefins using ozonolysis of alkenyl aryl selenides. The scope of the method was generalized with several examples. The end products obtained using developed method can serve as useful building blocks (*Org. Lett.* **2015**, *17*, 2090).



#### Breaking and making of rings: A method for the preparation of 4-quinolone-3-carboxylic acid amides and the most expensive drug Ivacaftor:

A simple and convenient method was developed to access 4-quinolone-3-carboxylic acid amides from indole-3-acetic acid amides using one-pot oxidative cleavage of indole ring followed by condensation (Witkop-Winterfeldt type

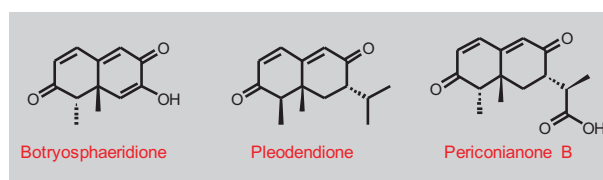
oxidation). The 4-quinolone-3-carboxylic acid motif regarded as a privileged structure in medicinal chemistry and is present in many biologically active compounds. Scope of the method was confirmed with more than 20 examples and successfully applied to the synthesis of ivacaftor drug, the most expensive drug in the market (*Eur.J. Org. Chem.* **2015**, *34*, 7433).



#### Total syntheses and biological evaluation of (±)-botryosphaeridione, (±)-pleodendione, 4-epi-periconianone B, and analogues:

The first syntheses of several compounds based on dihydro-, tetrahydro-naphthalene-2,6-dione skeleton, in particular, botryosphaeridione, pleodendione, 4-epi-periconianone B and hoansieremodione were accomplished. All the synthesized target compounds were screened in neural anti-inflammatory assays using LPS induced microglia cells (N9). Based on potency, selectivity index and modulation of inflammatory markers, two compounds

were identified as potential leads for further optimization. All these compounds with new chemotype are being explored in other biological assays (*ACS Med. Chem. Lett.* **2015**, *6*, 1117).

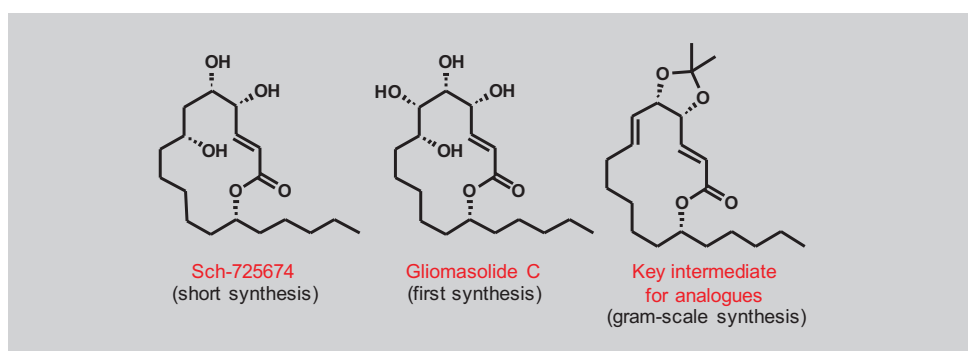


## Healthcare

### Natural products and methodology

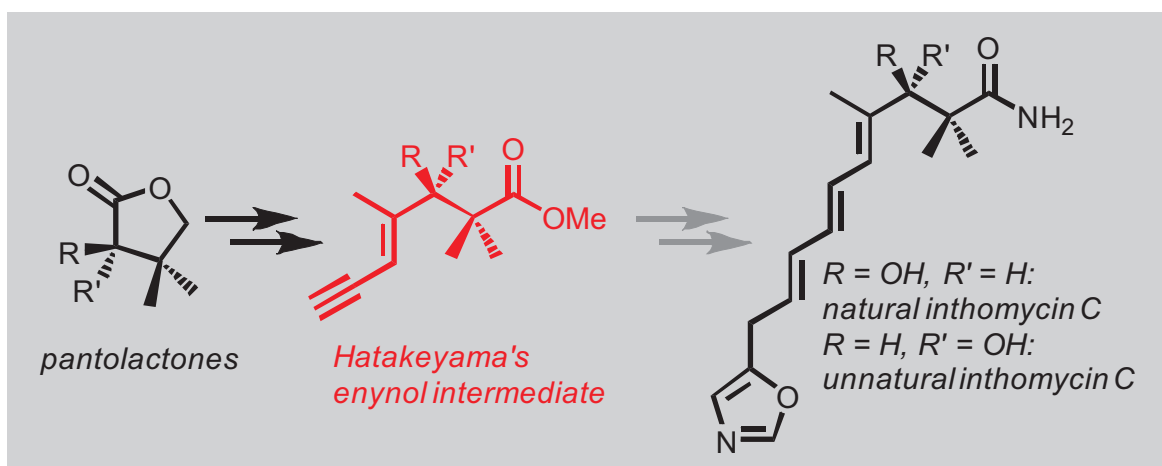
**First total synthesis of gliomasolide C and formal synthesis of Sch-725674:** The first total synthesis of gliomasolide C and a short synthesis of Sch-725674 were achieved in our group. Regioselective Wacker oxidation of

internal olefin and the gram scale synthesis of a key macrocycle with orthogonal functionalities are the highlights of this work (*J. Org. Chem.* **2016**, *81*, 290).



**Enantiospecific formal synthesis of inthomycin C:** An enantiospecific synthesis of Hatakeyama's intermediate enynol was reported in both enantiomeric forms. For this purpose, pantolactone was chosen as a starting material because of its availability in both enantiopure forms and also our continued interest in using pantolactone as chiral

pool in total synthesis. This synthesis highlighted the use of pantolactone chiral pool and thus reconfirmed the previously assigned absolute stereochemistry as 3R to the natural product inthomycin C (*Chemistry Select.* **2016**, *3*, 495).



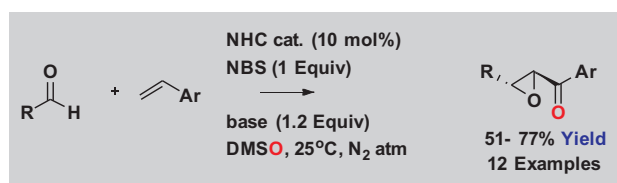
## Healthcare

### Natural products and methodology

A. Sudalai | a.sudalai@ncl.res.in

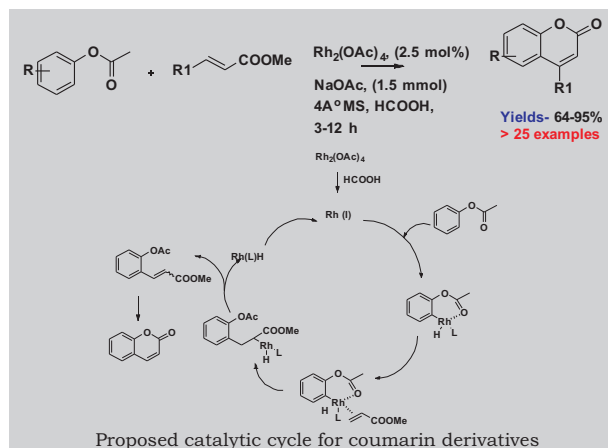
#### N-heterocyclic carbene catalyzed oxidative coupling of alkenes/ $\alpha$ -bromoacetophenones with aldehydes:

Novel, N-heterocyclic carbene (NHC) catalyzed direct oxidative coupling of styrenes with aldehydes was reported for the synthesis of  $\alpha, \beta$ -epoxy ketones in good yields. This unprecedented Regioselective oxidative coupling employed NBS/DBU/DMSO (DBU=1,8-diazabicyclo [5.4.0] undec-7-ene, DMSO=dimethylsulfoxide, NBS=N-bromosuccinimide) as an oxidative system at ambient conditions. First NHC-catalyzed Darzens reaction of  $\alpha$ -bromoketones and aldehydes under mild reaction conditions was also reported. The mechanistic studies have revealed the preferred reactivity of NHC with alkene/ $\alpha$ -bromoketone rather than aldehydes, thus proceeding via the ketodeoxy Breslow intermediate (*Angew. Chem. Int. Ed.* **2015**, *54*,14150).



#### Rh-catalyzed synthesis of coumarin derivatives from phenolic acetates and acrylates via C-H bond activation:

An efficient annulation strategy was developed which involved the reaction of phenolic acetates with acrylates in the presence of  $[Rh_2(OAc)_4]$  as catalyst and formic acid as reducing agent. It led to the high yield synthesis of coumarin derivatives. The addition of NaOAc as a base increased the yield of the products. The reaction is quite successful for both electron-rich as well as electron-deficient phenolic acetates, affording coumarins with excellent regioselectivity, and proceeds via C-H bond activation proven by deuterium incorporation studies (*J. Org. Chem.* **2015**, *80*, 11544).

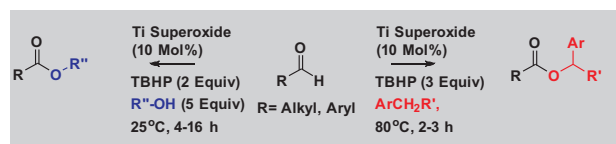


#### Organocatalytic [4+1]-annulation approach for the synthesis of densely functionalized pyrazolidine carboxylates:

A novel one-pot [4+1]-annulation process for the asymmetric synthesis of densely functionalized pyrazolidine carboxylates was reported. The *in situ* generated  $\gamma$ -hydrazino- $\alpha, \beta$ -unsaturated ester obtained *via* proline catalysis acted as a four-atom component, and Corey's sulfur ylide or ethyl bromoacetate acted as a one-atom carbon source to construct pyrazolidine carboxylate units in a highly enantio- and diastereoselective fashion (*RSC Adv.* **2015**, *5*, 65554).

#### Titanium superoxide a stable recyclable heterogeneous catalyst for oxidative esterification of aldehydes:

Titanium superoxide efficiently catalysed the oxidative esterification of aldehydes with alkyl arenes or alcohols, under truly heterogeneous conditions, to afford the corresponding benzyl and alkyl esters in excellent yields. Mechanistic studies have established that this "one pot" direct oxidative esterification process proceeded through a radical pathway, proven by a FTIR spectral study of a titanium superoxide aldehyde complex as well as spin trapping experiments with TEMPO. The intramolecular version of this protocol was successfully demonstrated in the concise synthesis of 3-butylphthalide, an anti-convulsant drug (*Org. Biomol. Chem.* **2015**, *13*, 10631).



## Healthcare

### Natural products and methodology

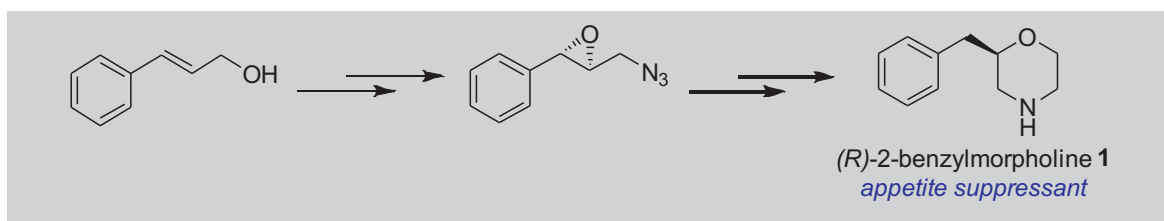
#### Asymmetric synthesis of biologically important compounds

M. Muthukrishnan | m.muthukrishnan@ncl.res.in

The research work involved the asymmetric synthesis of biologically important compounds, especially chiral drugs employing newly developed enantioselective strategies.

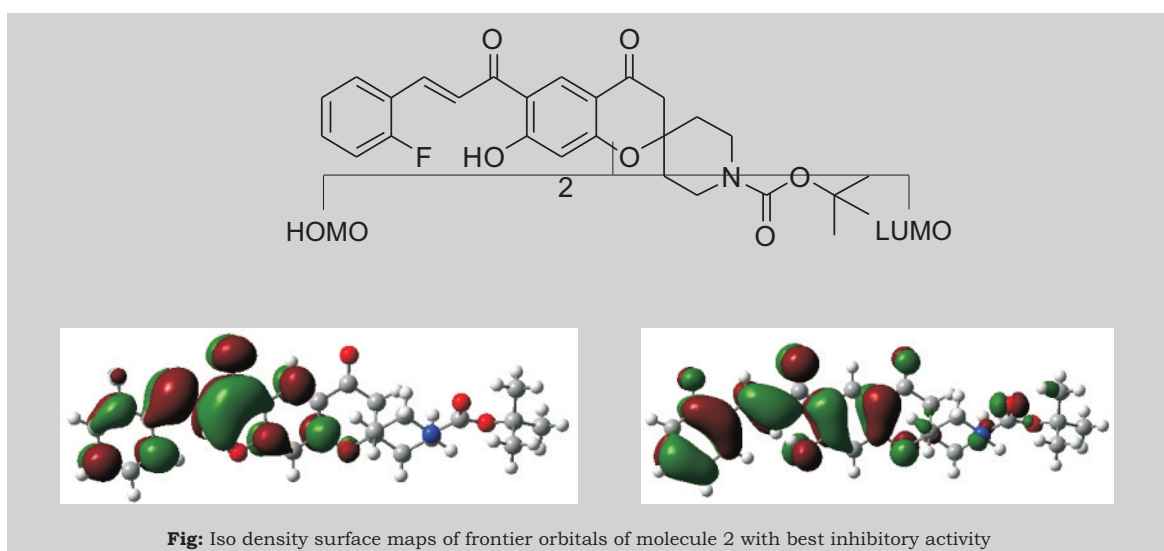
**Synthesis of appetite suppressant (R)-2-benzylmorpholine employing sharpless asymmetric epoxidation (SAE) strategy:** C-Substituted morpholine analogues are potential therapeutic agents for wide variety of medical disorders such as depression (Reboxetine, Viloxesine), anorectic (Phenmetrazine, Phendimetrazine), chemotherapy induced nausea and vomiting (Aprepitant) etc. In that series, (R)-2-benzylmorpholine is a classical example of chiral 2-morpholine

analogues, known to be a potent appetite suppressant. It was widely studied for its pharmacological properties. Further, its potential utility in treating diabetes mellitus and certain CNS disorders are also under investigation. A new and alternative synthesis of (R)-2-benzylmorpholine 1 was developed employing SAE as a key step. Simple procedures, ready availability of the starting materials and high enantiopurity are some of the salient features of this approach (*Tetrahedron Lett.* **2016**, *57*, 861).



**Spirochromone-chalcone conjugates as antitubercular agents: synthesis, bio evaluation and molecular modeling studies:** A series of spirochromone annulated chalcone conjugates was synthesized for the first time using a synthetic procedure beginning from resorcinol. The *in vitro* antimycobacterial evaluation of all the synthesized compounds showed that five compounds possessed moderate to good antimycobacterial activity. Importantly, compound 2 is most potent compound

*in vitro* with a MIC value of 3.13  $\mu\text{g}/\text{mL}$ , against MTB. Molecular docking studies were utilized to explore the putative targets among the known chalcone specific protein receptors. The compounds showed greater affinity towards the *Mycobacterium phosphatase* Ptp B enzyme. QSAR modeling established the correlation between frontier molecular orbital energies and biological activities of the compounds (*RSC Adv.* **2015**, *5*, 106448).



## Healthcare

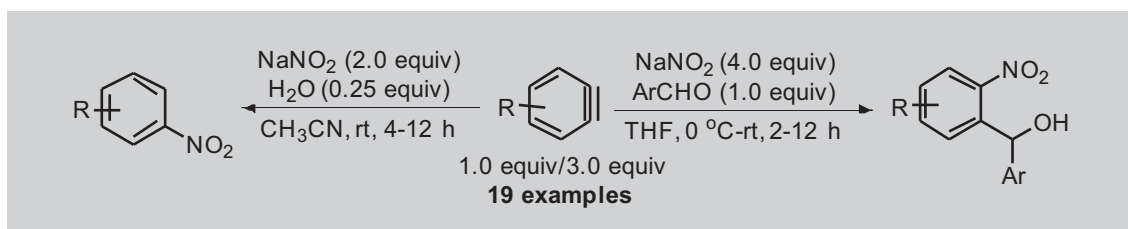
### Natural products and methodology

Santosh B. Mhaske | sb.mhaske@ncl.res.in

**New synthetic methodologies and their application in natural products and drugs:** The group has focused on development of novel methodologies and their application in the total synthesis of drugs and bioactive natural products as well as known drugs.

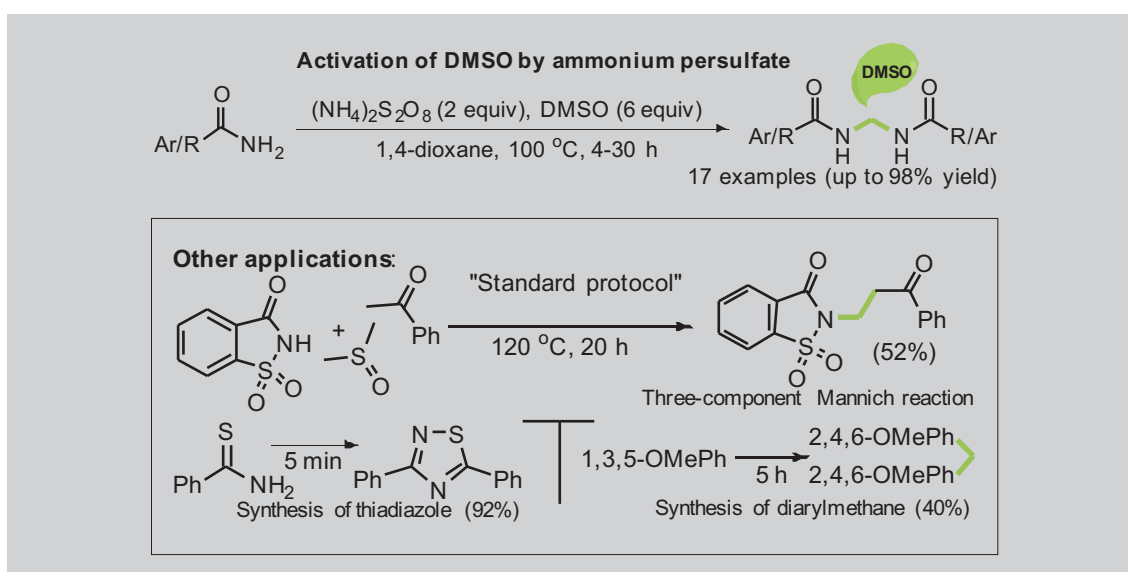
**Nucleophilic nitration of arynes by sodium nitrite and its multicomponent reaction leading to double-functionalized arenes:** An unusual nucleophilic nitration of arynes by  $\text{NaNO}_2$  in the presence of water was developed, and the concept was further demonstrated to accomplish a double functionalization of arynes using a

multi-component reaction (MCR) protocol to synthesize pharmaceutically important (2-nitrophenyl) methanol derivatives. Such substitution ortho to  $-\text{NO}_2$  is difficult by other means. The reaction conditions were mild and it avoided the use of strong acids, expensive transition metal catalysts and additives (*Org. Lett.* **2016**, *18*, 3010).



**Ammonium persulfate activated DMSO as the one-carbon synthon for the synthesis of methylenebisamides and other applications:** Activation of DMSO to work as an economical and environmentally benign one-carbon synthon was achieved by using a bench-top reagent ammonium persulfate for a general and efficient access to symmetrical methylenebisamides from primary amides. This methodology was used to achieve a three-

component Mannich reaction using acetophenone, saccharin and DMSO to furnish  $\beta$ -amino ketone. It also provided a metal-free synthesis of thiadiazole and bis(phenyl)methane. Effectively, this method used DMSO as a safer surrogate to formaldehyde. A mechanism for methylenebisamide formation involving radical intermediates was proposed based on mechanistic studies (*RSC Adv.* **2015**, *5*, 101641).



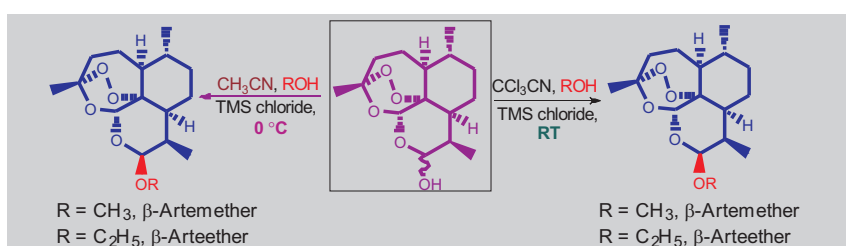
## Healthcare

### Natural products and methodology

Asish K. Bhattacharyal ak.bhattacharya@ncl.res.in

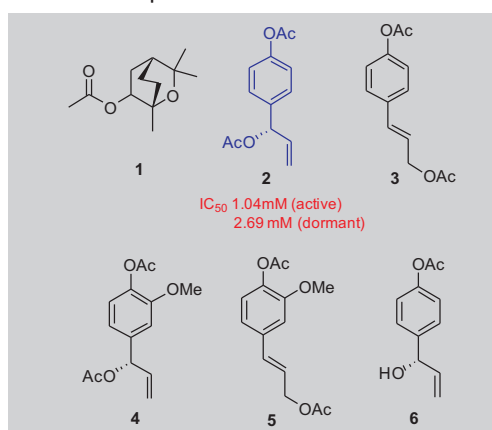
**Diastereoselective synthesis of  $\beta$ -ether derivatives of artemisinin, an antimalarial drug: The effect of nitrile on stereoselectivity:** Artemisinin isolated from *Artemisia annua* and its oil and water-soluble derivatives along with other existing antimalarials are being recommended as artemisinin combination therapy (ACT) by WHO. A method was established for the stereoselective synthesis of  $\beta$ -ether derivatives of dihydroartemisinin in high yield

well as high diastereoselectivity. The reaction either in acetonitrile or dichloromethane-trichloroacetonitrile (6:1) combinations at 0°C or room temperature, respectively furnished the antimalarial drug, artemether or arteether in high yield with a very high diastereomeric ratio. The role of nitrile on the yield as well as stereoselectivity was mechanistically explained (*Asian J. Org. Chem.* **2016**, 5, 201; Patent: IN 2014DE03079).



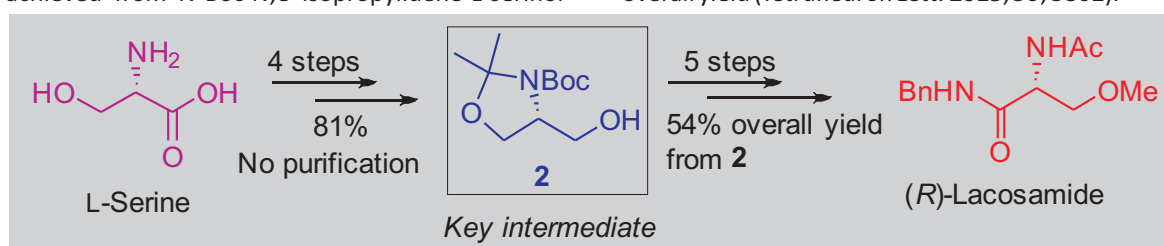
**Naturally occurring anti-TB agents: Isolation and *in vitro* antitubercular activities of secondary metabolites of rhizomes of *Alpinia galanga*:** Bioactivity-guided chemical examination of acetone extract of rhizomes of *Alpinia galanga* led to the isolation of six secondary metabolites, eucalyptol derivative (1) and phenylpropanoids (2-6). The structures of all the isolated compounds were elucidated on the basis of their spectral

data. The isolated compounds were *in vitro* assayed against active and dormant phenotypes of *M. tuberculosis* H37Ra, respectively. Interestingly, 1'S-1'-acetoxychavicol acetate (2) showed good antitubercular activities against both active and dormant phenotypes of *M. tuberculosis* with 1.04 M and 2.69 M, respectively (*Planta Medica Int. Open* **2016**, 3, e55).



**Chiral pool approach for the synthesis of functionalized amino acids: Synthesis of antiepileptic drug (R)-lacosamide:** An efficient total synthesis of (R)-lacosamide was achieved from *N*-Boc-*N*,*O*-isopropylidene-L-serinol

which could easily be obtained from natural L-serine. The synthesis of (R)-lacosamide starting from the key intermediate 2 using chiral pool strategy resulted in 54% overall yield (*Tetrahedron Lett.* **2015**, 56, 5802).





## Healthcare

### Natural products and methodology

J.M. Gajbhiye | jm.gajbhiye@ncl.res.in

**Computational strategies to explore antimalarial thiazine alkaloid lead compounds based on an Australian marine sponge *Plakortis Lita*:** New lead based natural scaffold thiaplakortone-A was proposed which is active against malaria. The 2D QSAR studies suggested that three descriptors were correlated with the anti-malarial activity with an R(2) value of 0.814. Robustness, reliability, and predictive power of the model were tested by internal validation, external validation, Y-scrambling, and applicability domain analysis. HQSAR studies were carried out as an additional tool to find the sub-structural fingerprints. The CoMFA and CoMSIA models gave Q(2) values of 0.813 and 0.647, and values of 0.994 and 0.984, respectively. Using the 2D-QSAR equation, the activity values of the seven modified compounds were calculated and it was found that three molecules showed good anti-malarial activity. Molecular docking of the 42 Thiaplakortone-A derivatives with *Plasmodium falciparum* calcium-dependent protein kinase 1 (PfCDPK1) was carried out to find out protein-ligand interactions. Data mining of the bioassay data-set AID: 504850 suggested that all of the eight molecules selected and three out of the seven virtual molecules were active anti-malarial. Both the virtual molecules and drug molecules were docked with CYP3A4, indicating that the virtual molecules could metabolize easily. Toxicity studies using Osiris showed that three molecules showed no toxic characteristics (*J. Biomol. Struct. Dyn.* **2016**, 1).

**Virtual screening techniques to probe the antimalarial activity of some traditionally used phytochemicals:** A new approach was reported by which virtual screening of 292 unique phytochemicals present in 72 traditionally important herbs was used for finding out inhibitors of plasmepsin-2 and falcipain-2 for antimalarial activity against *P. falciparum*. Initial screenings of the selected molecules by Random Forest algorithm model of Weka using the bioassay datasets AID 504850 and AID 2302 screened 120 out of the total 292 phytochemicals were active against the targets. Toxtree scan cautioned 21 compounds to be either carcinogenic or mutagenic that

were removed for further analysis. Out of the remaining 99 compounds, only 46 compounds offered drug-likeness as per the 'rule of five' criteria. Out of ten antimalarial drug targets, only two target proteins such as 3BPF and 3PNR of falcipain-2 and 1PFZ and 2BJU of plasmepsin-2 were selected as targets. The potential binding of the selected 46 compounds to the active sites of these four targets were analyzed using MOE software. The docked conformations and the interactions with the binding pocket residues of the target proteins were understood by 'Ligplot' analysis. It was found that 8 compounds were dual inhibitors of falcipain-2 and plasmepsin-2, with the best binding energies. Compound 117 (6aR, 12aS)-12a-hydroxy-9-methoxy-2,3-dimethylenedioxy-8-prenylrotenone (Usaratenoid C) present in the plant *Millettia usaramensis* showed maximum molecular docking score (Comb. Chem. High Throughput Screen. **2016**, 19, 572).

**Molecular docking and QSAR analyses for understanding the antimalarial activity of some 7-substituted-4-aminoquinoline derivatives:** A series of 7-substituted-4-aminoquinoline derivatives were selected to understand their antimalarial properties computationally by molecular modeling techniques including 2D QSAR, comparative molecular field analysis (CoMFA), comparative molecular similarity indices analysis (CoMSIA) and molecular docking. The 2D-QSAR model built with four descriptors selected by genetic algorithm technique and CoMFA model showed satisfactory statistical results (Q(2)=0.540, R(2) ncv=0.881, F value=157.09). A reliable CoMSIA model out of the fourteen different combinations has a Q(2) value of 0.638. The molecular docking studies of the compounds for 1CET as the protein target revealed that ten compounds showed maximum interactions with the binding site of the protein. The present study highlighted the unique binding signatures of the ligands within the active site groove of the target and it explained the subtle differences in their EC<sub>50</sub> values and their mechanism of inhibition (*Eur. J. Pharm. Sci.* **2015**, 77, 9).

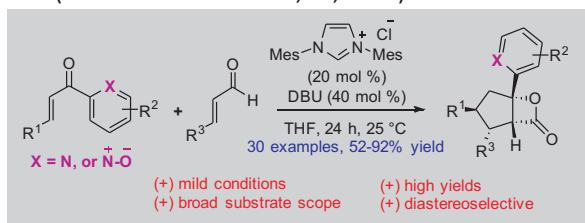
## Healthcare

### Natural products and methodology

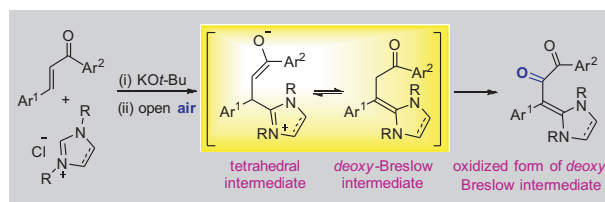
Akkattu T. Biju | at.biju@ncl.res.in

**Transition-metal-free carbon-carbon bond-forming reactions using aryne chemistry and N-heterocyclic carbene organocatalysis:** The transition-metal-free carbon-carbon bond-forming reactions using arynes resulted in the one-pot construction of molecular complexity, which was applied to the synthesis of various heterocyclic scaffolds and 1,2-disubstituted arenes. The application of arynes in transition-metal-free multicomponent coupling reactions initiated by aziridines was examined. The NHC-organocatalyzed umpolung of aldehydes was carried out, which led to the formation of nucleophilic acyl anion intermediates, homoenolate intermediates, and enolate intermediates depending on the reaction conditions. It resulted in the construction of various carbocycles and heterocycles via unique carbon-carbon and carbon-heteroatom bond-forming reactions.

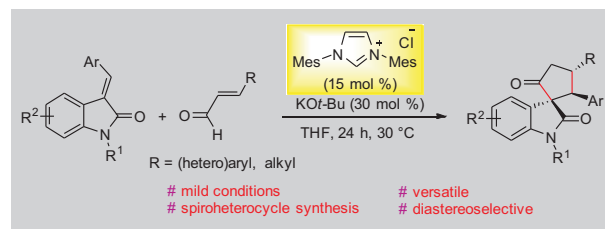
**N-Heterocyclic carbene-catalyzed diastereoselective synthesis of  $\beta$ -lactone-fused cyclopentanes using homoenolate annulations reaction:** The group has developed the NHC-catalyzed homoenolate annulation with 2-enoylpyridines or 2-enoylpyridine *N*-oxides leading to the diastereoselective synthesis of  $\beta$ -lactone-fused cyclopentanes in moderate to good yields. The pyridine moiety in the enone played a vital role in stabilizing the  $\beta$ -lactone intermediate. Mild reaction conditions, broad substrate scope and good yield of products were the notable features of the reaction. Moreover, treatment of enone with enal in the presence of chiral NHC resulted in the enantioselective synthesis of the  $\beta$ -lactone-fused cyclopentane in 56% yield, and in excellent diastereoselectivity of >20:1, and enantiomeric excess of 99% (*Chem. Commun.* **2015**, 51, 9559).



**Umpolung of Michael acceptors by N-heterocyclic carbenes: Synthesis of deoxy-Breslow intermediates in their oxidized form from chalcones:** The group has reported the umpolung of chalcones, which are widely used Michael acceptors in NHC-catalysis. The resultant deoxy-Breslow intermediate was isolated in the oxidized form and well-characterized. Moreover, the initial tetrahedral adduct formed from the 1,4-addition of NHCs to chalcones was also isolated (*Chem. Commun.* **2015**, 51, 13690).



**Diastereoselective synthesis of cyclopentanone-fused spirooxindoles by N-heterocyclic carbene-catalyzed homoenolate annulations with isatilidenes:** The NHC-catalyzed formal [3+2] annulation of  $\alpha,\beta$ -unsaturated aldehydes with *N*-substituted isatilidenes resulting in the diastereo-selective synthesis of cyclopentanone-fused spirooxindoles was demonstrated. Mechanistically, the reaction proceeded via the generation of homoenolate equivalent intermediates from NHC and enals, which on interception with isatilidenes afforded spiro-heterocyclic compound bearing an all-carbon quaternary spiro-center in moderate to good yield with high diastereoselectivity. The functionalization of the spirooxindoles as well as the initial studies on the enantioselective version of this reaction was reported (*Org. Chem. Front.* **2015**, 2, 1584).

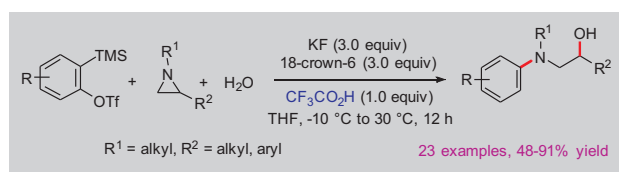


**Enantioselective synthesis of spirocyclohexadienones by NHC-catalyzed formal [3+3] annulation reactions of enals:** The enantioselective synthesis of pyrazolone-fused spirocyclohexadienones was reported by the reaction of  $\alpha,\beta$ -unsaturated aldehydes with  $\alpha$ -arylidene pyrazolinones under oxidative NHC-catalysis. This atom-economic and formal [3+3] annulation reaction proceeded via a vinylogous Michael addition/spiroannulation/dehydrogenation cascade affording the spirocyclic compounds having an all-carbon quaternary stereocentre in moderate to good yields and excellent ee values. Key to success for the present reaction was the cooperative NHC catalyzed generation of chiral  $\alpha,\beta$ -unsaturated acyl azoliums from enals, and base-mediated tandem generation of dienolate/enolate intermediates from pyrazolinones (*Angew. Chem. Int. Ed.* **2015**, 55, 268).

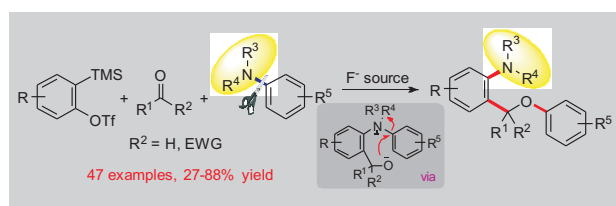
## Healthcare

### Natural products and methodology

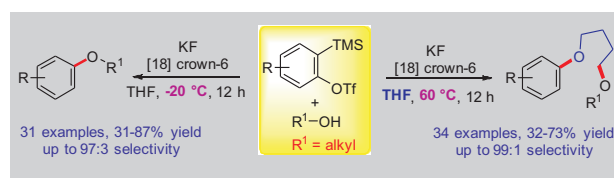
**Synthesis of *N*-aryl  $\beta$ -amino alcohols by trifluoroacetic acid-promoted multicomponent coupling of aziridines, arynes and water:** The group has uncovered a transition-metal-free, three-component coupling involving *N*-substituted aziridines, arynes and water promoted by trifluoroacetic acid (TFA) was reported. The reaction furnished medicinally important *N*-aryl  $\beta$ -amino alcohol derivatives in moderate to good yields. In addition, the use of azetidines in this reaction afforded *N*-aryl  $\gamma$ -amino alcohol derivatives (*J. Org. Chem.* **2015**, *80*, 11131).



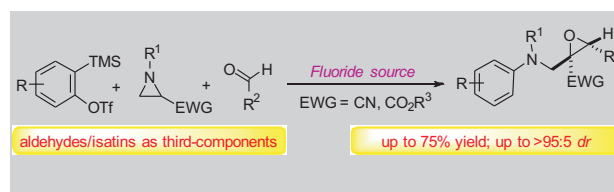
**Three-component coupling involving arynes, aromatic tertiary amines and aldehydes via aryl-aryl amino group migration:** The transition-metal-free multicomponent coupling of arynes, aromatic tertiary amines and aldehydes proceeding via the aryl to aryl amino group migration was demonstrated. This protocol allowed the rapid access to *ortho*-functionalized tertiary amines in moderate to good yields. The preliminary studies showed that activated ketones can also be used as the aldehyde component in the present reaction. The similarity of the aryl-aryl tertiary amino group migration proposed in the present reaction with the Smiles rearrangement is striking (*Org. Lett.* **2015**, *17*, 6270).



**From insertion to multicomponent coupling: Temperature dependent reactions of arynes with aliphatic alcohols:** The reaction of arynes with aliphatic alcohols in THF was demonstrated; the product formation depended on the temperature employed. At  $-20^\circ\text{C}$ , arynes smoothly insert into the O-H bond of alcohols to form alkyl aryl ethers. Interestingly, at  $60^\circ\text{C}$ , highly selective multicomponent coupling occurs with solvent THF acting as the nucleophilic trigger affording (4-(alkoxy) butoxy) arenes. Both reactions tolerated a broad range of functional groups, and the desired products were formed in moderate to good yields and high selectivities (*Chem. Commun.* **2016**, *52*, 1665).



**Synthesis of functionalized amino epoxides by a three-component coupling involving aziridines, arynes and aldehydes:** A transition-metal-free three-component coupling involving *N*-substituted aziridines, arynes and aldehydes resulting in the formation of trisubstituted *N*-aryl  $\alpha$ -amino epoxides was demonstrated. The reaction likely proceeded via the highly strained cyclic nitrogen ylide intermediates generated from aziridines and arynes (*Chem. Commun.* **2016**, *52*, 9044).



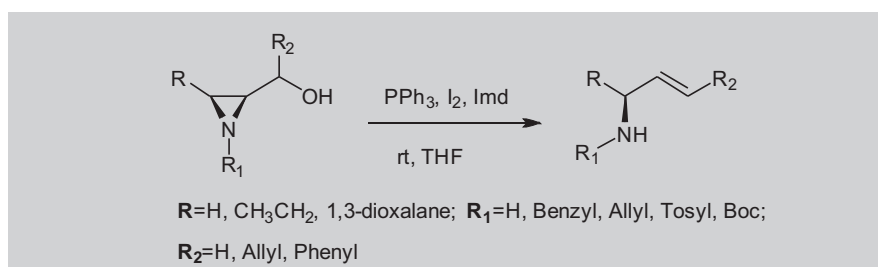
## Healthcare

### Chemical biology

Subhash P. Chavan | sp.chavan@ncl.res.in

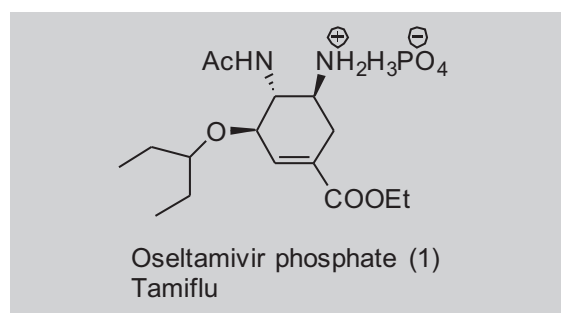
**Reparation of allylic amines from aziridine-2-alcohols using Ph<sub>3</sub>I<sub>2</sub>/imidazole:** Chiral aziridine-2-alcohols represent attractive tool for the synthesis of chiral allyl amines because of their increasing accessibility in chiral form and their obvious disposition towards selective ring opening due to ring strain. An efficient, practical method

for the direct conversion of aziridine alcohols to chiral allyl amines in a straightforward manner from chiral aziridine-2-alcohols under mild conditions was developed using PPh<sub>3</sub>/I<sub>2</sub>/imidazole in good to excellent yields. The present methodology worked efficiently with unactivated as well as activated aziridines (*Tetrahedron Lett.* **2014**, *55*, 5905).



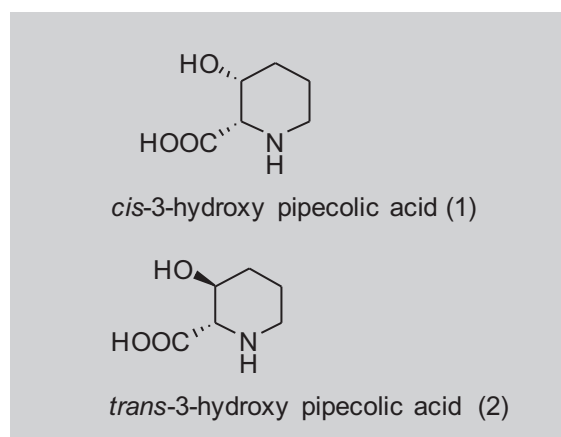
**Synthesis of tamiflu employing stereospecific amidoalkylation protocol and ramberg-backlund reaction:** The formal synthesis of tamiflu was achieved from inexpensive, abundant and easily available L-cysteine as the renewable resource. an azide and aziridine free route was developed utilising a novel stereospecific amidoalkylation, Ramberg-Backlund reaction, azide free protocol in an efficient manner for synthesis of neuraminidase inhibitor drug tamiflu. The strategy involved stereoselective epoxidation, Sharpless-Reich protocol for the transformation of epoxide to access allylic alcohol. Ramberg-Backlund reaction was for the first time utilised for the synthesis of tamiflu as a key step to

construct the cyclohexene intermediate which furnished desired vicinal *trans* diamine (*RSC Advances.* **2014**, *4*, 62281).



**Syntheses of (2R, 3R)-3-hydroxy pipercolic acid and (2R, 3S)-3-hydroxy pipercolic acid from L-ascorbic acid:** Formal syntheses of both *cis* and *trans* 3-hydroxy pipercolic acids was achieved from L-ascorbic acid. Present synthesis described the use of chiral pool approach in which epimerization, Staudinger reaction and cyclization reactions were employed as the key steps. L-ascorbic acid was converted in to key synthon required for the synthesis of three hydroxy pipercolic acid. This was carried out by transforming this key synthon into alcohol which on oxidation and 2-carbon homologation provided unsaturated ester. This ester on hydrogenation gave an inseparable mixture of diastereomers. It was used as such in the next transformation. The reduction of ester to alcohol followed by its transformation into azide provided a key azide synthon as the diastereomeric mixture. This azide was cyclized under Staudinger reaction conditions

and the diastereomers were separated to achieve formal synthesis of their respective 3-hydroxy pipercolic acid (*Tetrahedron Lett.* **2014**, *56*, 805).

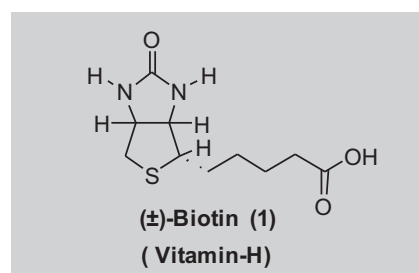


## Healthcare

### Chemical biology

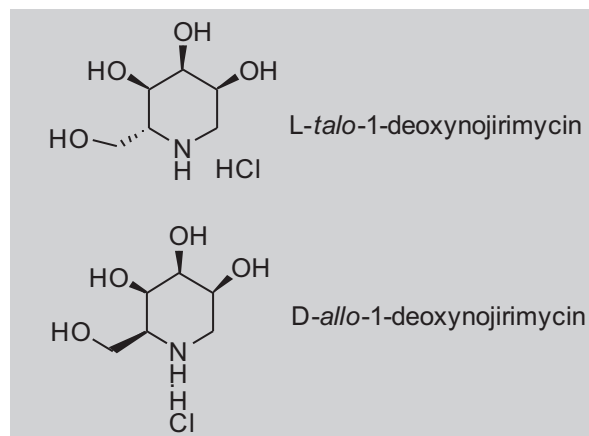
**Synthesis of (±)-biotin via MgCl<sub>2</sub>/Et<sub>3</sub>N-mediated C-C coupling and Mitsunobu reaction:** The interest in the synthesis of biologically important molecule led to explore a practical route for biotin. This strategy described a facile and convenient synthesis for total synthesis of biotin which involved notable features like MgCl<sub>2</sub>/Et<sub>3</sub>N mediated C-C coupling reaction, Mitsunobu inversion, ozonolysis, Staudinger reduction, novel urea formation and subsequent dibenylation as the key organic reactions. Synthesis of biotin was accomplished in 13 purification steps with 13.7% overall yield. This method showed great value in terms of its simplicity in the construction of urea, tetrahydrothiophene ring and also

elaboration of the pentanoic acid side chain of biotin skeleton. Enzymatic and catalytic asymmetric reduction procedures to accomplish the asymmetric total synthesis of (+)-biotin are being studied (*Synlett* **2014**, 25, 2879).



**Total syntheses of D-allo-1-deoxynojirimycin and L-talo-1-deoxynojirimycin via reductive cyclisation:** Synthesis of polyhydroxypiperidine framework for L-talo-1-deoxynojirimycin and D-allo-1-deoxynojirimycin was achieved from L-tartaric acid by employing flash dihydroxylation and reductive lactamisation as the key steps. The syntheses of D-allo-1-deoxynojirimycin and L-talo-1-DNJ were undergone by a chiral pool strategy using L-tartaric acid as the renewable starting material. For the L-talo-1-DNJ and D-allo-1-DNJ syntheses, the main synthetic challenge was the construction of piperidine moiety and installation of hydroxy groups in a stereoselective manner. The total syntheses of D-allo-1-DNJ and L-talo-1-DNJ were accomplished by employing flash dihydroxylation and reductive lactamisation as key

steps from readily available L-tartaric acid (*RSC Adv.* **2014**, 4, 40852).



Durba Sengupta | d.sengupta@ncl.res.in

**Structural insights and functional implications of inter-individual variability in β<sub>2</sub>-adrenergic receptor:** The human β<sub>2</sub>-adrenergic receptor is a membrane receptor that plays a central role in bronchodilation and is an important drug target. The inter-individual variability in the receptor was implicated in disease susceptibility and differential drug response. Nine potentially deleterious single nucleotide polymorphisms (SNPs) were identified using a computational approach and characterized their functional dynamics. The variants were classified as ranging from activating to damaging; prioritizing them for experimental and clinical studies (*Sci. Rep.* **2016**, 6, 24379).

**Designing novel antimicrobial peptides:** Three antimicrobial peptides were designed based on computational search and design. The peptides were demonstrated to exhibit inhibitory activity by exhibiting antifungal mechanisms such as membrane damage and reactive oxygen species generation. In particular, the peptides inhibited the activity of pathogenic microorganisms, such as *S. aureus*, *P. aeruginosa*, *S. enterica* and fungal pathogens such as *C. albicans*, *C. neoformans*, *F. oxysporum* and *N. crassa* (Patents: 2320/DEL/2014; WO/2016/024296).



## Healthcare

### Chemical biology

Moneesha Fernandes/Vaijayanti Kumar | m.dcosta/va.kumar@ncl.res.in

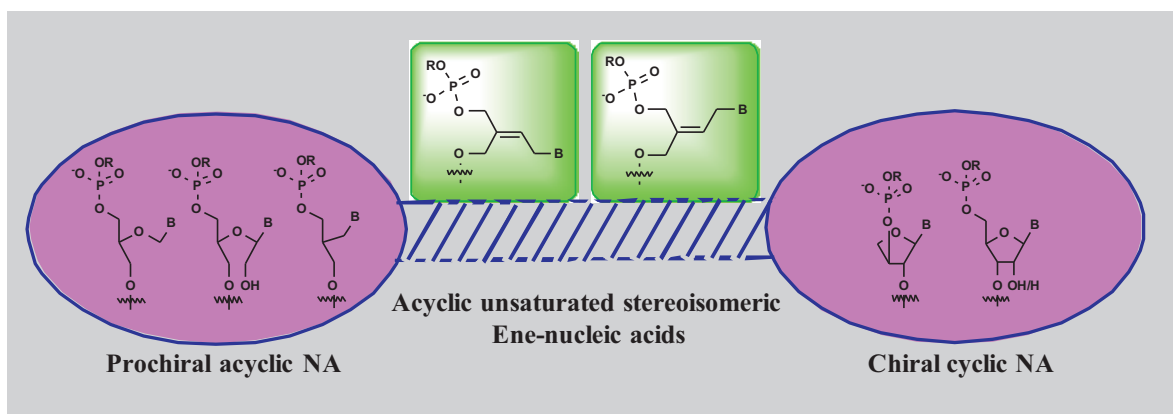
**Nucleic Acid Analogues:** The overall objectives of the project were to achieve nuclease resistance together with improved binding affinity to target nucleic acid sequences in the designed, synthetic analogues in order to make them more applicable in biological systems.

**2'-5'-Phosphodiester-linked thrombin binding aptamers:** A 2'-5'-linked isoTBA 15-mer sequence with (232) loop composition formed stable antiparallel quadruplex structures similar to the SELEX derived 15-mer 3'-5'-linked

**Ene-nucleic acids:** Ene-nucleic acids derived from an isoprenoid skeleton possess requisite flexibility and rigidity while forming stable duplex structures with complementary DNA and RNA. It could be the missing link

TBA sequence with (232) loop composition. The parallel vs. antiparallel topology of 3'-5'-linked G-quadruplexes is largely dictated by the loop length, and it is known that shorter loops favour parallel quadruplexes. In contrast to TBA, systematic reduction of the loop length in isoTBA from (232) to (222), (131) or even (111) did not alter the antiparallel topology of the resulting 14-mer, 13-mer and 11-mer G-rich modified isoTBA-like sequences (*Org. Biomol. Chem.* **2015**, *13*, 11696).

between acyclic prochiral nucleic acids such as FNA, UNA, GNA and cyclic chiral TNA that are all considered as precursors of DNA and RNA in the chemical etiology of nucleic acids (*RSC Adv.* **2015**, *5*, 97824).



Moneesha Fernandes/Mahesh Kulkarni | m.dcosta/mj.kulkarni@ncl.res.in

**Anti-glycation agents:** A new series of non-natural N-(3-aminoalkyl)proline derivatives were reported as a novel class of antiglycating agents (AGE). The *in vitro* antiglycation activity was studied by circular dichroism and fluorescence spectrometry. They were found to act by inhibition of Amadori product formation. The inhibition of AGE formation was further confirmed by western blot and

LC-MS/MS analyses. The compounds were additionally found to possess good anti-oxidant properties, which could lead to further reduction in AGE formation. Moreover, the title compounds were found to have low cytotoxicity in mammalian cells, another important attribute (*RSC Adv.* **2015**, *5*, 77332).



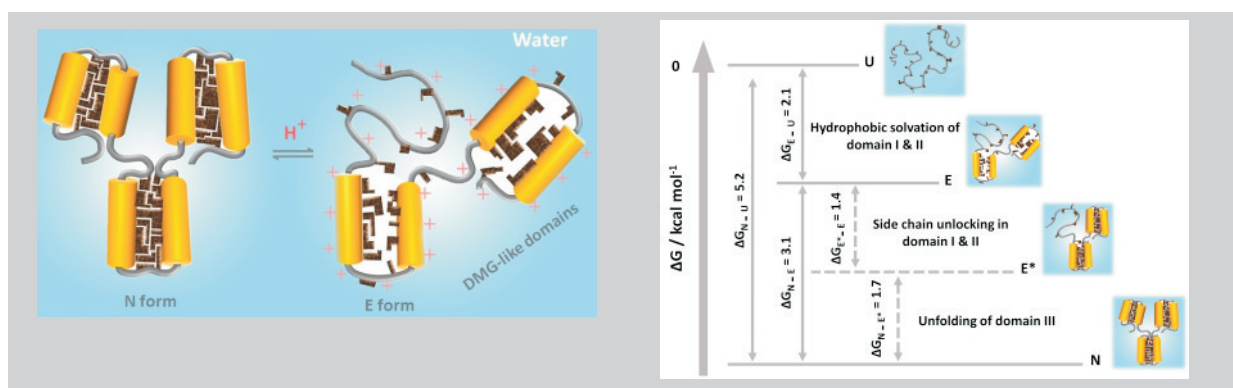
## Healthcare

### Chemical biology

Santosh Kumar Jha | sk.jha@ncl.res.in

**Protein stability and folding:** It was showed that the pH-induced structural perturbation of a multi-domain protein led to the formation of a state in which two out of the three domains have characteristics of dry molten globules, i.e. the domains are expanded compared to the native protein with disrupted packing interactions, but have dry cores. The fluorescence resonance energy transfer, dynamic fluorescence quenching, red-edge excitation shift, and near- and far-UV circular dichroism

were used. The group quantitatively estimated the energetic contribution of vdW interactions and showed that they played an important role in the stability of the native state and cooperativity of its structural transition, in addition to the hydrophobic effect. The results also indicated that during the pH-induced unfolding, side-chain unlocking and hydrophobic solvation occurred in two distinct steps and not in a concerted manner, as commonly believed (*J. Phys. Chem. Lett.* **2016**, 7, 173).



Archana Pundle | av.pundle@ncl.res.in

**A highly active penicillin V acylase from *Pectobacterium atrosepticum*:** Penicillin V acylases (PVAs) belong to Ntn hydrolase family of enzymes that catalyze the deacylation of phenoxymethyl penicillin (Pen V). PVA from gram-negative bacterium *P. atrosepticum* was cloned and expressed in *E. coli*, attaining high enzyme yield (250 mg/l) and maximum Pen V hydrolysis activity (434 IU/mg). The enzyme showed unique kinetic behaviour, exhibiting positive cooperativity and substrate inhibition. A PaPVA-based system was developed for efficient industrial 6-APA production (*Int. J. Biol. Macromol.* **2015**, 79, 1).

**Structural interactions in PaPVA effecting enhanced activity:** The three-dimensional structure of PaPVA was determined at 2.5 Å resolution using X-ray crystallography and molecular replacement techniques. Structural comparison with PVAs from Gram-positive bacteria revealed that PaPVA had a distinctive oligomeric interaction and active site organization. In addition, the importance of residue Trp23 and Trp87 side chains in Pen V binding and enhanced activity of PVAs was confirmed through characterization of site-directed mutants and substrate docking with a 15 ns molecular dynamics simulation. (*J. Struct. Biol.* **2016**, 193, 85).

### Identification of lead molecules

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

**Dual role of eugenol in inhibiting advanced glycation:** Identified molecule from Ocimum plants viz., eugenol having dual mode of action in combating diabetes; it lowered blood glucose by inhibiting α-glucosidase and

prevented the AGE formation by binding to ε-amine group on lysine, protecting it from glycation, offering potential use in diabetes management (*Sci. Rep.* **2016**, 6, 18798).

## Healthcare

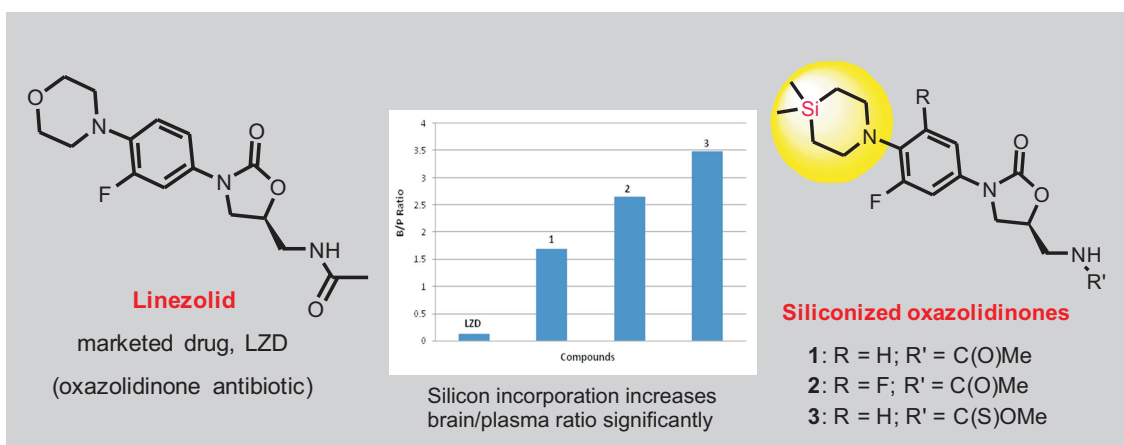
### Medicinal chemistry

D. Srinivasa Reddy | ds.reddy@ncl.res.in

Silicon analogues are more lipophilic than their carbon counterparts. Hence this strategy would be beneficial in CNS drug discovery wherein siliconized compounds could potentially display better blood-brain barrier (BBB) penetration.

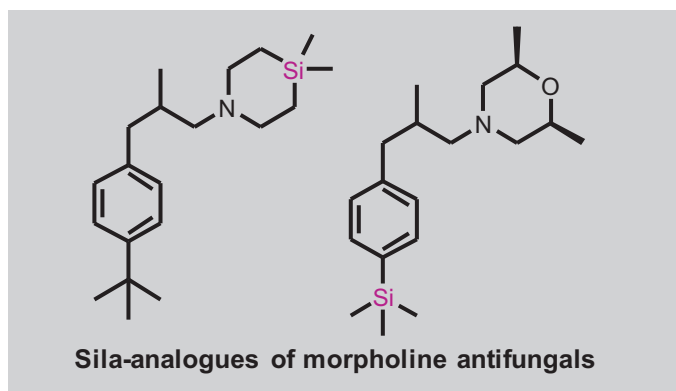
**Identification of brain penetrant linezolid analogues and potent anti-TB agents:** Recent reports on the potential use of linezolid in treating brain infections prompted

researchers to design novel compounds around this scaffold. Three compounds were identified as potential lead compounds, demonstrating up to 30-fold higher brain to plasma ratio as compared to the marketed oxazolidinone antibiotic drug, linezolid in animal models. These results can be considered as a step towards the development of brain penetrant oxazolidinone antibiotics (*ACS Med. Chem. Lett.* **2015**, *6*, 1105).



**Design, synthesis, and biological evaluation of sila morpholine antifungals with:** Silicon was incorporated in morpholine class antifungals, fenpropidin and fenpropimorph. Twelve sila-morpholines exhibited potent antifungal activity against different human fungal pathogens such as *Candida albicans*, *Candida glabrata*, *Candida tropicalis*, *Cryptococcus neoformans* and

*Aspergillus niger*. The mode of action of sila-morpholines was similar to morpholines i.e. inhibition of sterol reductase and sterol isomerase enzymes of ergosterol synthesis pathway. The synthesized compounds were non-hemolytic, non-toxic and lead obtained needs to be further explored for development as antifungal drug (*ACS Med. Chem. Lett.* **2015**, *6*, 1111).



## Healthcare

### Screening methods and bioassays

Mahesh Dharne | ms.dharne@ncl.res.in

**Antibiofilm potential of ionic liquids:** A series of varying alkyl chain length substituted tert-BuOH-functionalized-imidazoliummesylate salts[alkyl-tOHim][OMs] were synthesized and evaluated for antimicrobial activity and antibiofilm potential on selected pathogenic microorganisms including bacteria, yeast, and fungi. The dodecyl substituted ionic liquid [C12-tOHim][OMs] significantly prevented the bio-film formation of *S. epidermidis* at 100 mM concentration as well as showed noteworthy antimicrobial activity. It was concluded that the ionic liquids (ILs) bearing chain lengths lower than the dodecyl length were found to be less effective (*RSC Adv.* **2015**, *5*, 68136).

**Detection of *Clostridium tetani* in clinical samples:** The successful detection of *Clostridium tetani* was reported using tetX specific primers targeting the *Cl. tetani* neurotoxin. The sample was obtained from an ear discharge of a case of otogenic tetanus in a 2-year-old male child. Based on the culture results of the ear discharge, Gram staining and virulence testing by genotyping, a diagnosis of tetanus was confirmed. A neurotoxin based PCR for detection of *Cl. tetani* in a human clinical sample was reported (*J. Infect. Public Health* **2016**, *9*, 105).

**Microbial metagenomics of geothermal environment:** Microbial diversity in geothermal waters of the Unkeshwar hot springs in Maharashtra was studied using 16S rRNA amplicon metagenomic sequencing and whole metagenome sequencing. Taxonomic analysis revealed the presence of various phyla. Metabolic function prediction analysis indicated a battery of biological information systems indicating rich and novel microbial diversity. The Unkeshwar hot springs offer rich phylogenetic diversity and metabolic potential for biotechnological applications (*Genome Announc.* **2016**, *4*, e01766, *Genomics Data* **2016**, *7*, 140).

**Graphenes in antimicrobial resistance:** The antibacterial activities of nanosheets of the graphene analogue tungsten disulphide (WS<sub>2</sub>) and a composite of reduced graphene oxide-tungsten disulphide (rGO-WS<sub>2</sub>) were studied and compared them with reduced graphene oxide (rGO) by a time and concentration dependent viability assay and growth curve studies against four bacterial strains. The antimicrobial mechanism is due to the combined effect of initial cell deposition on the rGO-WS<sub>2</sub> materials, the membrane stress due to direct contact with the nanosheets, and the produced super oxide anion-independent oxidation mechanisms (*RSC Adv.* **2015**, *5*, 74726).

Syed G. Dastager | sg.dastager@ncl.res.in

**Systematics, polyphasic, biotechnological applications:** Classification of microorganisms on the basis of traditional microbiological methods (morphological, physiological and biochemical) created a blurred image about their taxonomic status and thus needed further clarification. Hence, the methods employed for bacterial systematics included, the complete 16S rRNA gene sequencing and its comparative analysis by phylogenetic trees, DNA-DNA hybridization studies with related organisms, analyses of molecular markers and signature pattern(s), biochemical assays, physiological and morphological tests. Collectively these genotypic, chemotaxonomic and phenotypic methods were applied to determine taxonomic position of bacteria. With this approach, many novel bacterial species, i.e. *Bacillus encimensis*, *Streptomyces lonarensis* and *Bacillus cellulasensis* were proposed (*Int. J. Syst. Evol. Microbiol.* **2015**, *65*, 1421; *Antonie van Leeuwenhoek* **2016**, *109*, 225; *Arch. Microbiol.* **2016**, *198*, 83).

**Draft genome of *arthrobacterenclensis* NCIM 5488T for secondary metabolism:** The draft genome sequence of *Arthrobacterenclensis* NCIM 5488T, an Actinobacteria isolated from a marine sediment sample from Choroa Island, India. This draft genome sequence consisted of 4,226,231 bp with a G+C content of 67.08%, 3,888 protein-coding genes, 50 tRNAs, and 10 rRNAs. Analysis of the genome using the bioinformatics tools like, anti SMASH, NaPDoS showed the presence of many unique natural product biosynthetic gene clusters. These clusters were reported for the first time for any *Arthrobacter* species reported till date, and the results highlighted the genome mining potential of novel strain *Arthrobacterenclensis* NCIM 5488 for natural products discovery research (*Genome Announc.* **2016**, *4*, e00497).

## Sustainable Chemical Industry

### Biochemical processes and engineering

Mugdha Gadgil | mc.gadgil@ncl.res.in

**Delivery of DNA:Liposome complexes to animal cells in the presence of shear stress:** Animal cells in suspension experience shear stress in different situations such as *in vivo* due to hemodynamics, or *in vitro* due to agitation in large-scale bioreactors. Shear stress is known to affect cell physiology, including binding and uptake of extracellular cargo. The effect of shear stress on transfection of suspension adapted CHO-S cells was evaluated using Lipofectamine 2000 in a simple flow apparatus. The results showed decreased cell growth and transfection efficiency upon lipoplex assisted transfection of CHO-S while being subjected to shear stress. This effect was not

seen to the same extent when cells were exposed to shear stress in absence of the lipoplex complex and subsequently transfected, or if the lipoplex is subjected to shear stress and subsequently used to transfect the cells. It is also not seen to the same extent when cells are exposed to shear stress in presence of liposome alone, suggesting that the observed effect is dependent on interaction of the lipoplex with cells in the presence of shear stress. These results suggest that studies for end goal applications involving liposomal DNA delivery in presence of shear stress should account for the effect of shear on lipoplex performance (*Cytotechnology* **2016**, *68*, 2529).

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### Biodegradable polymers

Samir Chikkali | s.chikkali@ncl.res.in

**Synthesis of renewable copolyacetals with tunable degradation:** Crude oil reserves are constantly depleting, whereas use of crude oil in polymers and plastics is consistently increasing. Therefore, the future of the “new-to-the-world” material will heavily rely on two decisive parameters such as renewable origin and degradability of the resultant plastics. It is necessary to make materials that can be grown every year like an agricultural crop and that can degrade in the environment without affecting the

surroundings. A plant oil and sugar derived monomers were polymerized to corresponding polymers called copolyacetals. These materials are stable in open air for weeks but slowly degrade in acidic media. The degradability can be controlled by choosing the right combination of sugar derived water loving fragment and plant oil derived water repelling fragment (*Macromol. Chem. Phys.* **2016**, *217*, 1396).

## Sustainable Chemical Industry

### Catalysis

C.V. Rode | cv.rode@ncl.res.in

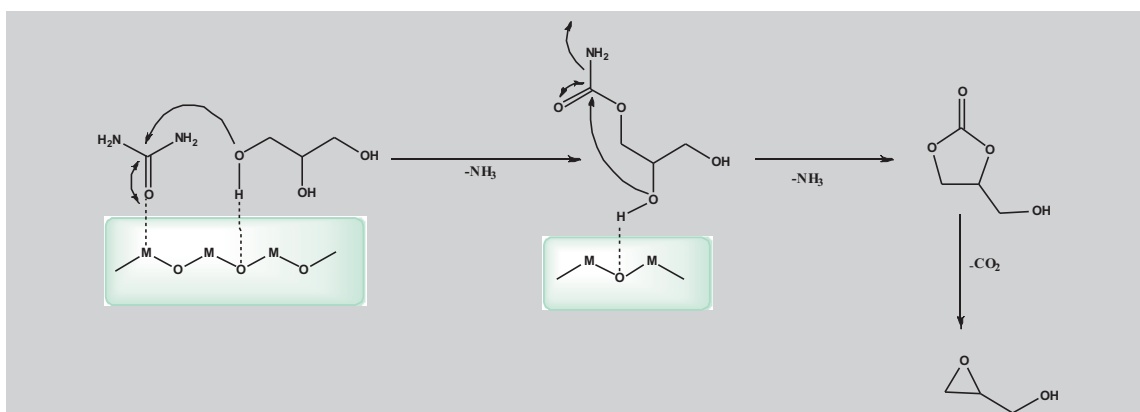
**Solvent-free carbonylation of glycerol with urea:** Among several transition metal catalysts, Zn/MCM-41 (im) prepared by wet impregnation proved to be the most active catalyst for glycerol carbonate synthesis with 75% conversion of bioglycerol and 98% selectivity to GC. The higher activity of the catalyst was explained by well dispersion of ZnO phase over the mesoporous framework of MCM-41 support. The balanced acid (0.020 mmole/g) and basic site (1.61 mmole/g) present in the catalyst responsible for the excellent multifunctional performance of the catalyst. HRTEM images clearly showed presence of amphoteric ZnO phase, which is important for the activation of glycerol molecule. Easy separation, excellent activity and recyclability of the catalyst make it candidate for the application in industrial synthesis of GC (*RSC Adv.* **2015**, 5, 16452).

**Liquid phase oxidation of *p*-cresol using molecular oxygen:** Highly selective mixed oxide (MnCo) catalyst on graphene oxide was prepared by solvothermal method showed 71% product yield with almost complete selectivity to the *p*-hydroxybenzaldehyde in 1 h. Cyclic voltammetry (CV) study revealed the increase of redox

potential of mixed oxide after supporting on to the GO, which led to the higher activity of the catalyst for oxidation reaction. The stability of the catalyst under the reaction condition was studied by its successful three recycles.

**Triphenyl (3-sulfopropyl) phosphonium functionalized phosphotungstic acid on silica as a solid acid catalyst:**

Silica supported phosphotungstic acid functionalized with triphenyl (3-sulfopropyl) phosphonium (PW-Si/TPSP) was developed as a solid acid catalyst for C-C bond formation via Hosomi-Sakurai allylation of acetals. Functionalization of PW as well as its binding to silica was confirmed by solid state <sup>31</sup>P-NMR and <sup>29</sup>Si-NMR, respectively. 30% PW loaded (30PW-Si/TPSP) catalyst gave an excellent yield of homoallylethers (HAEs) via selective mono allylation of acetals with allyltrimethylsilane. A plausible reaction pathway was proposed in which the strong Brønsted acid sites of 30PW-Si/TPSP play an important role in activating the acetal to form the corresponding oxonium cation. The versatility of our catalyst was demonstrated for the allylation of a wide variety of acetals while, its stability was established by five successful recycle runs (*Catal. Sci. Technol.* **2015**, 5, 4039).



### Redox nature of ceria

C.S. Gopinath | cs.gopinath@ncl.res.in

**Gas-Solid Interaction:** Direct interaction between reduction medium (H<sub>2</sub>) and porous Ce<sub>0.95</sub>Zr<sub>0.05</sub>O<sub>2</sub> (CZ) solid surface was explored through ambient pressure photoelectron spectroscopy (APPEs) to understand its redox nature. An unprecedented decrease in the valence band (VB) energy up to 1.4 eV was observed on reduction along with a narrowing of VB. Ce 4f band shifts very close

to EF. This study showed the dynamic changes in the nature of the surface due to gas (H<sub>2</sub>) - solid (CZ) interaction and ensuing electronic structure changes that influenced heterogeneous catalysis. It also underscores the necessity to study the catalytic materials under *in-situ* conditions or closer to that and the elaborate results were reported (*Catal. Sci. Technol.* **2016**, 6, 1746)

## Sustainable Chemical Industry

### Mathematical and computational modeling

Sanjeev S. Tambe | ss.tambe@ncl.res.in

**Genetic programming based quantitative structure: Retention relationships for the prediction of Kovats retention indices:** An artificial intelligence based data-driven modeling formalism, namely, genetic programming (GP) was introduced for the development of quantitative structure based models predicting Kovats retention indices (KRI). The novelty of the GP formalism was that given an example dataset, it searched and optimized both the form (structure) and the parameters of an appropriate linear/nonlinear data-fitting model. It was not necessary to pre-specify the form of the data-fitting model in the GP-based modeling. These models were less complex, simple to understand, and easy to deploy. The effectiveness of GP in constructing QSRRs was demonstrated by developing models predicting KRIs of light hydrocarbons (case study-I) and adamantane derivatives (case study-II). In each case study, two-, three- and four-descriptor models were developed using the KRI data available in the literature. The results of these studies clearly indicated that the GP-based models possessed an excellent KRI prediction accuracy and generalization capability. Specifically, the best performing four-descriptor models in both the case studies yielded high (>0.9) values of the coefficient of determination (R<sup>2</sup>) and low values of root mean squared error (RMSE), and mean absolute percent error (MAPE) for training, test and validation set data. The characteristic feature of this study is that it introduces a practical and an effective GP-based method for developing QSRRs in gas chromatography that can be gainfully utilized for developing other types of data-driven models in chromatography science (*J. Chromatogr. A* **2015**, 1420, 98).

**High ash char gasification in thermogravimetric analyzer and prediction of gasification performance parameters using computational intelligence formalisms:** Extensive gasification experiments were conducted using char samples derived from the high ash Indian coals in the CO<sub>2</sub> atmosphere in a thermogravimetric analyzer. Next, the gasification data were fitted using shrinking unreacted core model to obtain the values of char gasification rate constants. Finally, generalized data-driven models were developed using three computational intelligence (CI) formalisms, namely, genetic programming (GP), multilayer perceptron (MLP) and support vector regression (SVR) for the prediction of two gasification performance variables, namely, char gasification rate constant and reactivity index. The inputs of CI-based models consist of seven parameters representing gasification reaction conditions and, coal and char

properties. It was observed that all CI-based models possessed an excellent prediction and generalization ability. Thus, these models were used for predicting the magnitudes of important kinetic parameters in the high-ash coal gasification and thereby in the design and operation of fixed and fluidised bed coal gasifiers (*Chem. Eng. Commun.* **2016**, 203, 1029).

**Genetic programming based high performing correlations for prediction of higher heating value of coals of different ranks and from diverse geographies:** Three proximate and ultimate analysis based nonlinear correlations were developed for the prediction of HHV of coals by utilizing the computational intelligence (CI) based *genetic programming* (GP) formalism. Each of these correlations possessed following noteworthy characteristics: (i) the highest HHV prediction accuracy and generalization capability as compared to the existing models, (ii) wider applicability for coals of different ranks and from diverse geographies, and (iii) structurally lower complex than other CI-based existing HHV models. The GP technique was used for the first time for developing the coal-specific HHV models. Owing to the above-stated attractive features, the GP-based models proposed here possessed a significant potential to replace the existing models for predicting the HHV of coals (*J. Energy Inst. DOI: 10.1016/j.joei.2016.03.002*).

**Role of chemical reactivity and transition state modeling for virtual screening:** Every drug discovery research program involves synthesis of a novel and potential drug molecule utilizing atom efficient, economical and environment friendly synthetic strategies. The current work focuses on the role of the reactivity based fingerprints of compounds as filters for virtual screening using a tool ChemScore. A reactant-like (RLS) and a product-like (PLS) score can be predicted for a given compound using the binary fingerprints derived from the numerous known organic reactions which capture the molecule-molecule interactions in the form of addition, substitution, rearrangement, elimination and isomerization reactions. The reaction fingerprints were applied to large databases in biology and chemistry, namely ChEMBL, KEGG, HMDB, DSSTox, and the Drug Bank database. A large network of 1113 synthetic reactions was constructed to visualize and ascertain the reactant product mappings in the chemical reaction space. The cumulative reaction fingerprints were computed for 4000 molecules belonging to 29 therapeutic classes of compounds, and these were found capable of



# Sustainable Chemical Industry

## Mathematical and computational modeling

Sanjeev S. Tambe | ss.tambe@ncl.res.in

discriminating between the cognition disorders related and anti-allergy compounds with reasonable accuracy of 75% and AUC 0.8. The transition state based fingerprints were also developed and used effectively for virtual screening in drug related databases. The methodology presented here provided an efficient handle for the rapid scoring of molecular libraries for virtual screening (*Comb. Chem. High T. Scr.* **2015**, *18*, 638).

### A study of applications of machine learning based classification methods for virtual screening of lead molecules:

A number of classification models were built using three types of inputs namely structure based descriptors, molecular fingerprints and therapeutic category for performing virtual screening. The activity and affinity descriptors of a set of inhibitors of four target classes DHFR, COX, LOX and NMDA were utilized to train a total of six classifiers viz. Artificial Neural Network (ANN), k nearest neighbor (k- NN), Support Vector Machine

(SVM), Naïve Bayes (NB), Decision Tree - (DT) and Random Forest - (RF). Among these classifiers, the ANN was found as the best classifier with an AUC of 0.9 irrespective of the target. New molecular fingerprints based on pharmacophore, toxicophore and chemophore (PTC), were used to build the ANN models for each dataset. A good accuracy of 87.27% was obtained using 296 chemophoric binary fingerprints for the COX-LOX inhibitors compared to pharmacophoric (67.82 %) and toxicophoric (70.64 %). The methodology was validated on the classical Ames mutagenicity dataset of 4337 molecules. Selectivity and promiscuity of molecules from five drug classes viz. anti-anginal, anti-convulsant, anti-depressant, anti-arrhythmic and anti-diabetic were studied to evaluate it further. The TPC fingerprints computed for each category were able to capture the drug-class specific features using the k-NN classifier. These models can be useful for selecting optimal molecules for drug design (*Comb. Chem. High T. Scr.* **2015**, *7*, 658).

Suman Chakrabarty | s.chakrabarty@ncl.res.in

## Molecular modeling of complex biophysical processes and self-assembly

### Structure and dynamics of interfacial and confined water:

Structural and dynamical properties of interfacial and confined water can drastically deviate from bulk characteristics with potential applications. A demonstration was done for a flexible (bio)polymer the water structure and dynamics in hydration layer is strongly coupled to the local curvature, topographical and chemical heterogeneity, and flexibility of the molecule. Moreover, properties of water under nano-confinement of reverse micelles and water-in-oil nanodroplets showed that various structural properties can be perturbed to different extent depending on the nature of the confinement and interface (*J. Phys. Chem. B* **2015**, *119*, 11346; *Phys. Chem. Chem. Phys.* **2016**, *18*, 21767).

### Structural instability and misfolding pathways in Prion protein:

Misfolding and aggregation of Prions were implicated in a wide variety of neurodegenerative disorders. The conformational free energy landscape for human Prion monomer and dimer was evaluated by using extensive replica exchange molecular dynamics simulations. The study highlighted that there existed multiple intermediate partially disordered states stabilized by non-native hydrogen bonds leading to the propensity towards misfolding. The weak spots for structural instability were identified that might be quenched upon dimerization (*J. Phys. Chem. B* **2016**, *120*, 7332).

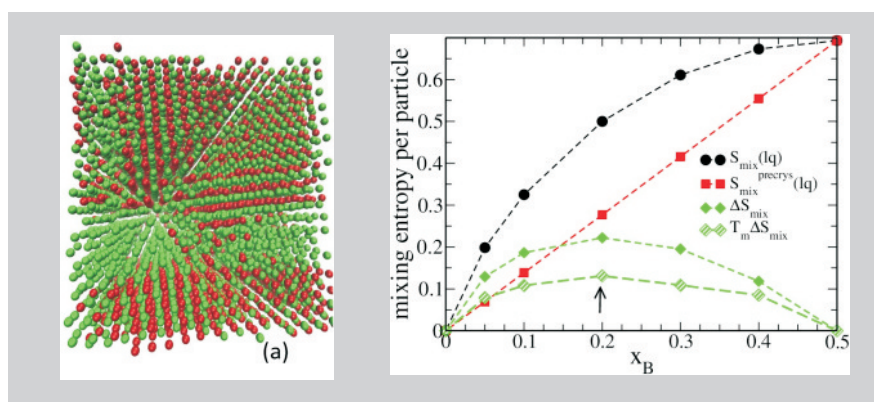
## Sustainable Chemical Industry

### Mathematical and computational modeling

Sarika M. Bhattacharyya | mb.sarika@ncl.res.in

**Composition dependence of glass forming ability of binary mixture:** A comparative study of the glass forming ability of binary systems with varying composition was presented where the systems have similar global crystalline structure (CsCl+fcc). Biased Monte Carlo simulations using umbrella sampling technique showed that the free energy cost to create a CsCl nucleus increases as the composition of the smaller particles are decreased. It was found that systems with comparatively lower free energy cost to form CsCl nucleus exhibited more pronounced pre-crystalline demixing near the liquid/crystal interface. The structural frustration between the CsCl and fcc crystal demands this demixing. It was shown that closer to the equimolar mixture the entropic penalty for demixing is lower and a glass forming system may crystallize when seeded with a nucleus. This entropic penalty as a function of composition showed a non-monotonic behavior with a maximum at a composition

similar to the well known Kob-Anderson (KA) model. Although the KA model showed the maximum entropic penalty and thus maximum frustration against CsCl formation, it also showed a strong tendency towards crystallization into fcc lattice of the larger "A" particles which can be explained from the study of the energetics. Thus for systems closer to the equimolar mixture although it is the requirement of demixing which provided their stability against crystallization, for KA model it is not demixing but slow dynamics and the presence of the "B" particles which makes it a good glass former. The locally favoured structure around "B" particles is quite similar to the CsCl structure and the incompatibility of CsCl and fcc hindered the fcc structure growth in the KA model. Although the glass forming binary systems studied here are quite similar, differing only in composition, it was found that their glass forming ability cannot be attributed to a single phenomenon (*J. Chem. Phys.* **2016**, *145*, 34503).



V. Ravi Kumar | v.ravikumr@ncl.res.in

### Optimization methodologies for inverse problems in complex dynamical systems

**Novel and powerful algorithm for process optimization problems (ETFGA):** The work led to the development of a highly efficient metaheuristic global-local optimization approach that solved inverse parameter and state estimation problems for applications in interdisciplinary fields. It employed the novel concept of embedding local training functions, viz., embedded multiple shooting, slope regression and ODE decomposition in a global search genetic algorithm.

**Applications of ETFGA:** From noisy dynamics, true dynamics of monitor edandun monitored process variables were recovered. ETFGA validated by studying the chaotic dynamics of a CSTR, glycolysis regulation in *I. lactis* for production of lactic acid, gene regulatory networks, circadian oscillations in *Drosophila* and cAMP oscillations in *Dictyostelium discoideum*. ETFGA can train generalized canonical S-system models for network/ structure identification and thus innovatively addressed the model identifiability issues in inverse problems (*Chem. Eng. Sci.* **2015**, *134*, 605; *Math. Biosci.* **2016**, *275*, 93).

# Sustainable Chemical Industry

## Mathematical and computational modeling

### Understanding relation between structure and properties of materials by employing ab initio DFT based techniques

Kavita Joshi | k.joshi@ncl.res.in

**Density functional theory calculations of cyano-benzaldehyde isomers, cyanobenzaldehyde molecular crystals:** A variety of physical phenomena ranging from atomic transitions to dynamics of biological molecules was studied using THz spectroscopy. It involved a wide range of disciplines including physics, chemistry, engineering, astronomy, biology, and medicine. To understand the origin of differences in the Terahertz spectra of 2,3,4-cyanobenzaldehyde molecules as well as their molecular crystals as a function of their crystal structure group has simulated their vibrational spectra as well as phonons using density functional perturbation theory. The resonances were highly sensitive to the relative position of atoms in a molecule as well as the crystal packing arrangement. The results showed that low frequency modes (<3 THz) were mediated through hydrogen bonds and were dominated by intermolecular vibrations (*J. Phys. Chem. A* **2015**, *119*, 7991).

**Pt-nanoparticle functionalized carbon nanoonions for ultra-high energy supercapacitors and enhanced field emission behavior:** The charge storage capacitive response and field emission behaviour of platinum (Pt) nanoparticles decorated on carbon nano onions (CNOs)

were investigated and compared with those of pristine carbon nano onions. The specific capacitance observed for Pt-CNOs was 342.5 F/g, about six times higher than that of pristine CNOs, at a scan rate of 100 mV/s. The Density Functional Theory (DFT) calculations of these systems revealed enhancement in the Density of States (DOS) near the Fermi energy (EF) on account of platinum decoration on the CNOs (*RSC Adv.* **2015**, *5*, 80990).

### Multifaceted thermodynamics of $Pb_n$ (n = 16- 24) clusters:

**A case study:** The thermodynamic behavior of small Pb clusters (size 16-24) was studied using Born-Oppenheimer molecular dynamics. A new ground state structure was reported for  $Pb_{20}$ . Except for  $Pb_{21}$ , all clusters fragment at temperatures above  $T_{m[bulk]}$  and showed no signs of melting. Characteristic behavior like restricted diffusion and solid-solid transition was discussed in detail. Variation in the isomerization temperature of these clusters was explained using the bond length analysis. Our investigations demonstrated that it is not possible to define 'liquid state' for these small clusters, in the conventional frame of understanding (*J. Phys. Chem. C* **2015**, *119*, 23698).

Kaliaperumal Selvaraj | k.selvaraj@ncl.res.in

**Tailor-made complexation properties for terpyridine ligand-metal:** The group was focused to understand the binding of different metals with TPy ligand and its modulation in different ways. TPy shows a large scope to be functionalized with electron exchanging groups to alter its electronic structure and consequently its binding with metal atoms.

It was demonstrated that a convenient modulation of TPy-M binding is possible through functionalization of TPy for M = Co, Ru, Fe, Mo and Au. Electron donating groups viz.,  $CH_3$ ,  $OCH_3$ ,  $C_6H_5$ ,  $NH_2$  and electron withdrawing groups viz.,  $CF_3$ ,  $COOH$ ,  $CN$  and  $NO_2$  were considered for functionalization of TPy ligand. The work was focused on the functionalization at 4 and 4' positions of TPy molecule.

The role of such functionalization in influencing the ligands structure-property correlation was missing in the literature. The present investigation quantified that by pertinent functionalization of TPy, TPy-M binding energies can be modified up to ~60 kcal/mol. The results revealed that functionalization led to a considerable charge redistribution within the TPy-M complex with carbon atoms in pyridine rings functioning as major electron sink/source with a corresponding red/blue shift of C = C stretching frequency. This modified the red-ox, optical and other chemical properties of TPy-M complexes. In brief, the report illustrated a way to design ligands such as TPy for diverse applications through tailor-made functionalization using electronic structure methodology (*Mol. Simulat.* **2015**, *42*, 618).

## Agriculture, Food and Nutrition

### Functional food and nutrition

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

**Understanding Alphonso mango flavor related metabolites and their biosynthesis during ripening:** The flavour of ripened Alphonso mango is invariably dominated by the de novo appearance of lactones and furanones during ripening. Of these, furanones comprising furaneol (4-hydroxy-2,5-dimethyl-3(2H)-furanone) and mesifuran (2,5-dimethyl-4-methoxy-3(2H)-furanone) are of particular importance due to their sweet, fruity caramel-like flavour characters and low

odour detection thresholds. The gene encoding S-adenosyl-L-methionine-dependent O-methyltransferase were isolated from Alphonso mango (MiOMTS). The recombinant MiOMTS showed substrate specificity towards furaneol and protocatechuic aldehyde synthesizing mesifuran and vanillin. These results helped to understand biosynthesis mango-flavour related metabolites (*Mol. Biotechnol.* **2016**, *58*, 340).

Narendra Kadoo | ny.kadoo@ncl.res.in

**Genetic dissection of dough rheology traits in hexaploid wheat:** Genetic dissection of dough rheology traits (DRT) in hexaploid wheat was conducted using nine mixograph characters. Composite interval mapping using a linkage map of 202 SSR markers identified 144 DRT QTLs. Sixteen QTL clusters located on ten chromosomes were

identified. For each trait, majority of the DRT QTLs detected in single- as well as multiple- environments showed location-specificity and suggested that breeding for wheat dough quality needed careful selection of QTLs targeted for individual agro-climatic zones (*J. Cereal. Sci.* **2015**, *64*, 82)

### Plant diversity and bio-prospecting

Narendra Kadoo | ny.kadoo@ncl.res.in

**Development of DNA barcodes for ten *Dalbergia* species:** DNA barcodes were developed for ten *Dalbergia* species that are economically important timber plants. The 10 species were selected from Western Ghats of India and evaluated using three plastid regions (matK, rbcL, trnH-psbA), a nuclear transcribed spacer (nrITS) and their combinations. Five stringent statistical criteria were

employed for species discrimination. Considering the overall performance, matK and matK +rbcL were recommended as the most suitable barcodes to unambiguously differentiate *Dalbergia* species (Fig). These findings helped to delineate various species of *Dalbergia* and other related genera (*PLoS One* **2015**, *10*, e0142965).

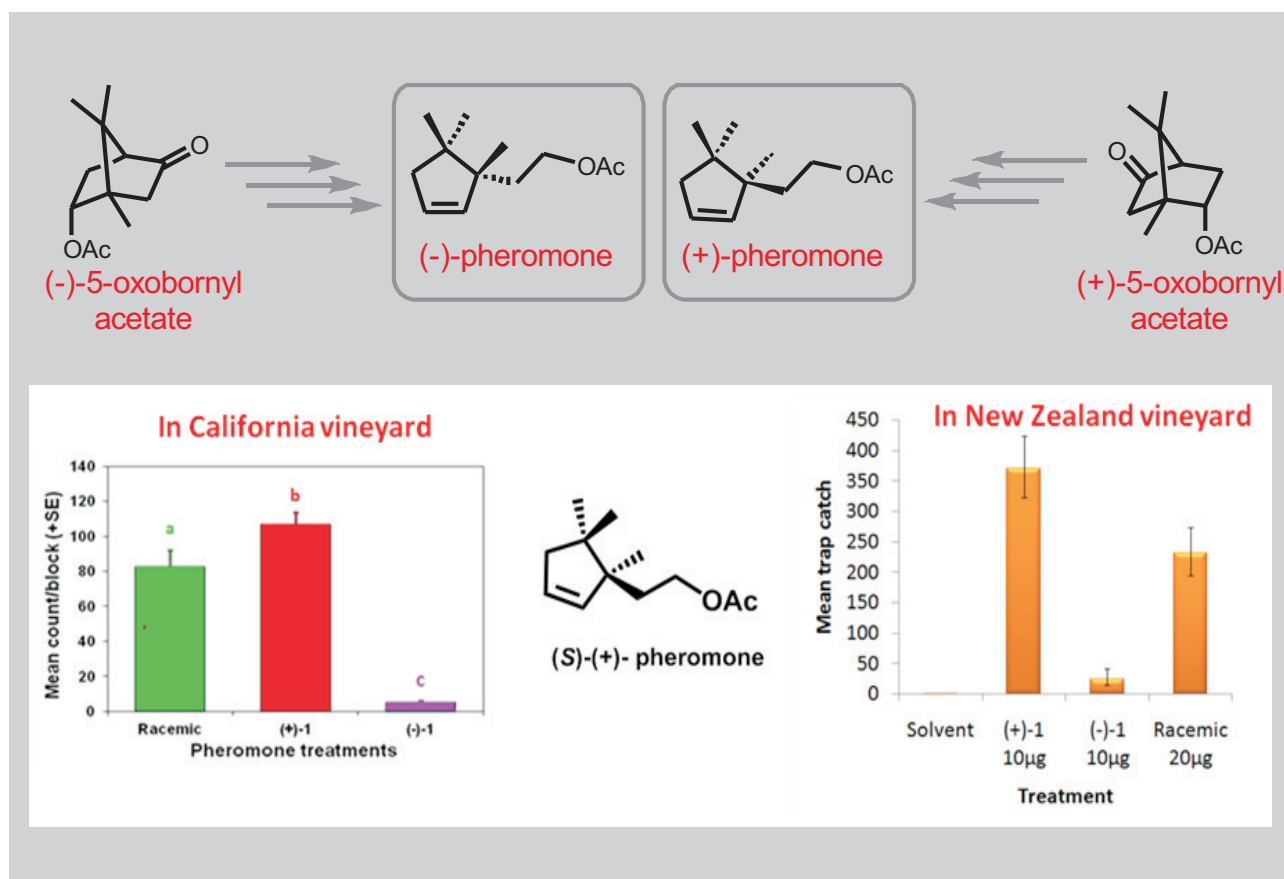
## Agriculture, Food and Nutrition

### Crop protection

Srinivasa Reddy | ds.reddy@ncl.res.in

**Enantiospecific synthesis of the longtailed mealybug pheromone enantiomers:** The longtailed mealybug is a pest that infests various crops such as avocado, coffee, citrus, guava, mango, orchids, pineapple, potato, sugarcane etc. The sex pheromone secreted by the female longtailed mealybug was isolated and characterized by Millar's group. Recently, in collaboration with the Millar group, the group showed that the (S)-(+)-enantiomer was

highly attractive and the (R)-(-)-enantiomer was inactive, suggesting that female longtailed mealybugs produce the (S)-enantiomer. Following this, an enantiospecific route was developed for the synthesis of pheromones starting from corresponding bornyl acetates. The highlights of this synthesis are use of cheap chiral pool starting material and translocation of [3.2.1] bicyclic lactone (*J. Org. Chem.* **2015**, *80*, 7785).



## Agriculture, Food and Nutrition

### Crop protection

Narendra Kadoo | ny.kadoo@ncl.res.in

**OMICS analyses reveal the mechanism of resistance to chickpea pathogen:** *Fusarium* wilt caused by *Fusarium oxysporum* sp. *ciceri* (Foc) is a major threat to global chickpea production. High-throughput metabolomics, proteomics and transcriptomics analyses revealed that resistant plants produced more flavonoids, isoflavonoids, phytoalexins, reactive oxygen species and had higher carbon and nitrogen metabolism and lignification compared to susceptible plants. Several antifungal metabolites like aurantion-obstine  $\beta$ -glucosides,

quercetin and pathogenesis-related proteins were induced in resistant plants. It was also characterized in planta pathogen progression and colonization using GFP-transformed pathogen with confocal microscopy and quantitative PCR (Fig), which revealed that the pathogen could successfully colonize and reproduce in the susceptible cultivar, but resistant plants severely restricted this (*Phytochemistry* **2015**, *116*, 120; *Plant Biotechnol. J.* **2016**, *14*, 1589; *PLoS ONE* **2016**, *11*, e0156490).

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

**Identification and characterization of insect growth inhibitors:** Plant-insect interactions were studied aiming for developing crop protection strategies from insect attack using plant defensive molecules such as protease inhibitor genes, proteins, peptides and secondary

metabolites. RNA-interference strategies were explored for *Helicoverpa armigera* control. These investigations supposed to help for developing eco-friendly methods for crop protection (*Colloid. Surface. B*, **2015**, *130*, 84; *Insect Sci.* **2016**, *23*, 68; *Insect Biochem. Molec.* **2016**, *74*, 1).

### Plant secondary metabolites and pathway analysis

Sushama Gaikwad | sm.gaikwad@ncl.res.in

**Functional and conformational transitions of *Bacopa monniera* mevalonate diphosphate decarboxylase:** Functional and conformational transitions of mevalonate diphosphate decarboxylase (MDD), a key enzyme of mevalonate pathway in isoprenoid biosynthesis, from *Bacopa monniera* (BmMDD), cloned and overexpressed in *E. coli* were analyzed. Thermal denaturation of BmMDD caused rapid structural transitions at and above 40°C leading to aggregation of the protein. Information on the

structural elements responsible for the protein aggregation will be useful in deducing the mechanism of aggregation prone diseases. Ribbon diagram of BmMDD homology model representing the residues surrounding the tryptophan residues exposed on the surface. Tryptophan residues are shown in green, basic and acidic residues are highlighted in blue and red color, respectively (*Int. J. Biol. Macromol.* **2016**, *83*, 160).

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

**Biosynthesis of steroidal alkaloids and their precursor in tomato:** Elucidation of the cholesterol and steroidal glycoalkaloid biosynthesis pathway and their regulators in Solanaceous vegetable crop plants namely potato and tomato was undergone to improve the nutritional value of

tuber and fruits. The findings provided the insight into the regulation of SGA biosynthesis and means for manipulating these metabolites in crops (*Nat. Commun.* **2016**, *7*, 10654).



# Resource Centers

**Central NMR Facility:** This Resource Center provides NMR support to all the scientific activities of the laboratory. The scientists associated with this Resource Center 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 Center maintains and operates five NMR spectrometers operating at 200, 300, 400, 500 and 700 MHz and a JEOL ECX 400 spectrometer. Bruker AV300 is a wide bore spectrometer dedicated to solid state NMR while the standard bore Bruker AV500 and JEOL ECX 400 spectrometers are equipped with solid state accessories. The recently acquired 700 MHz spectrometer is equipped

with accessories for solution state and solid state NMR. Although, the primary users of this facility are from the research community within the laboratory, the facility is open to researchers in other educational institutions and industries. Apart from technical support, the Center also plays an integral part in the basic and applied research activities of the Laboratory.

During the current year, the NMR Facility analyzed about 46000 samples in solution state and 900 samples in solid state of which about 300 samples were from industries, other R&D and academic institutes generating an ECF of about Rs. 30 lakhs.

**Catalyst Pilot Plant:** Catalyst Pilot Plant (CPP) houses all the scale-up facilities required for the translation of the processes for the preparation of the solid catalysts/adsorbents/ supports and the environmentally benign catalytic conversion of batch processes from the 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. The process for the preparation of the proprietary catalyst for the direct conversion of carbon dioxide and methanol to dimethyl carbonate was scaled up and the reproducibility of the product quality was checked at the desired scale of operation. Several formulation trials were conducted and shaped catalysts were tested for their catalytic

performance while translating the batch process to a continuous one. The process of the synthesis of proprietary catalyst developed by BPCL R&D Centre, Noida was also scaled up to yield higher product yield/batch level. The behavior of the hydrothermal crystallization process was examined in order to check the feasibility of molecular sieve scale up at desired different scale of operations. CPP attempted to prepared and supplied the catalysts for the R&D purpose at client's end. The activities were focused in the research areas like zeolite-based micro/ mesoporous composites for specialty chemicals, direct conversion of cellulose/ glucose to levulinic acid, one step pretreatment of biomass with selective extraction of lignin by liquid ammonia and epoxidation of renewable feedstocks.

**Network Administration Unit:** The fully reliable, scalable, robust and redundant 'DATA CENTER' constructed by the unit is now fully operational. The unit deployed some of the high throughput Network devices such as a network router, a pair of 'Core switch chase' and a pair of 'Firewall' that are capable of delivering up to 10 Tbps of system bandwidth capacity. The unit provided LAN connectivity in the newly constructed 'HoR-IV' hostel Building, by providing 300 network ports all across the hostel. The unit also completed an activity of establishing LAN / WAN connectivity in the newly created 'Indus Magic' building by providing about 125 wired / wireless network

points at various locations in the premises, installing 12 IP based surveillance cameras at various locations as well as a Video Conferencing system. The unit also revamped the entire guest house Wi-Fi by deploying 10 strong wireless devices of higher capacity. The unit also looks after the web based 'Access Control and Time Management' system, while maintaining more than 60 biometric readers as well as boom barriers and turn styles, installed at various locations in the lab. This year, the center has also laid about 5 km worth redundant Fiber cable from DIRC to more than 70% hub centers in the lab.

**Knowledge Resource Centre:** Knowledge Resource Centre (KRC)/Library manage both print and digital resources. During the year KRC subscribed to more than 276 journals out of which around 250 are electronic journals and 26 are print journals. KRC provides access to various journals and databases through NKRC consortia which covers 39 CSIR labs and 26 DST institutes. During the year library users were provided access to various databases such as iThenticate plagiarism software, Web

of Science, Sci-Finder, Questal/Orbit, Thompson/Innovations. More than 300 documents were added in the library collection of which 150 were print books, 105 Hindi Books and around 66 theses. During the year 40 casual visitors, 33 students, 6 corporate members, 13 retired scientists and 1 institutional member availed services of the library. KRC could generate Rs 1.34 Lakhs of revenue from various services provided by the library.

**Centre for Materials Characterization:** Centre for Materials Characterization (CMC) is a central facility for routine and advanced characterization of materials. The centre caters to the requirements of entire research community at CSIR-NCL as well as the industrial and academic clients including our sister concerns on payment basis. The centre is equipped with various instruments, such as Single Crystal and powder X-ray diffractometers (SCXRD/XRD), Scanning electron microscopes (SEM/e-SEM), Transmission electron

microscopes (TEM), High Resolution TEM (HRTEM), X-ray photoelectron spectroscope (XPS), Mass spectrometers (MS), High Resolution Mass Spectrometer (HRMS), Maldi-TOF MS, LC-MS, Triple TOF LC-MS, SQUID magnetometer, Raman Spectrometer, Vibrating Sample Magnetometer, etc that are used for R & D projects of the institute. During the year, more than seventeen thousand samples were analysed out of which about one percent comprised industrial samples. This generated some amount of ECF for the laboratory.

**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 units 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 ~ 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.

# S & T Support Services

## Publication and Science Communication:

Publication and Science Communication (PSC) Unit works as a channel for the communication 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.

## Engineering Services:

The support includes basic building structure for the work and there after necessary setup inside the building like Lab furniture, fume hoods, exhaust systems, air-conditioning etc. The basic services to run the research activity include water, electricity and services like vacuum, compressed air etc. The unit makes arrangement of liquid nitrogen, glass blowing services etc. Engineering services has a major setup of workshop unit, pump house unit, electrical substations etc. It manages the services with sectional staff related to basic

engineering services like Civil, Electrical, Mechanical and Glass blowing.

CSIR-NCL has a major set up of Colony having about 545 staff quarters. In addition to this, there are common centers like community hall, guest house, students' hostels, dispensary etc. ESU takes care of all these major installations. CSIR-NCL organizes many national and international seminars. ESU takes care of required back up for these Seminars related to Electrical, air-conditioning, and civil engineering services.

No.	Work Category	Percentage
1	Major new constructions	14
2	Renovation works	15
3	Major work of Electrical Substation & D.G. set installations.	26
4	New Fume hood & Furniture setup	14
5	New road works	9
6	Utility services setup (Vacuum, Air, Gas)	13
7	Air-conditioning installations.	9

## Instrumentation and Communication:

Innovative development was done for soft PID development using LabVIEW developer suite and PID tools. For considerable big pilot plant, it is mandatory to have PIDs for process parameter settings and control should be at the desktop of the Technical Manager/engineer. The developed work takes care of setting, resetting, control feedback and real time measurements from the desktop – soft PIDs and LabVIEW Vis on PC. It is not only cost effective but also needs very low time to correct any problem in the plant. The unit takes care of

servicing of instruments, fault finding and rejuvenation of the instrument (TGA/DTA).

Communication system Alcatel Omni PCX Enterprise (OXE) was updated with latest Release 11.2 Operating system, Call billing software and Voice messaging software. In addition to this underground copper telephone cable and 12 core OFC cables were laid from main building Communication room for newly constructed MSM building and NRM buildings near KG lab area. Separate underground and OFC cables were laid up to Security gate near CMC building and also upto DIRC building.

## S & T Support Services

**Human Resource Management: Project Training:** More than 430 intern students pursuing the courses such as M.Sc., M.Pharm., B.E., M.E., B.Tech., M.Tech. at various colleges, universities and institutes including IITs, IISERs, and NITs as well as foreign institutes completed their Summer/Winter Projects at CSIR-NCL.

**Guest workers:** Seventy guest-workers worked at CSIR-NCL including fellows of various Indian Sciences and Engineering Academies. Three students from abroad were also trained.

**Institutional visits:** The Unit coordinated twenty institutional visits 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 21, 2015 and Dec 20, 2015 for 18605 and 15452 registered candidates, respectively.

### वित्त एवं लेखा

1.	निधि की उपयोगिता सीएसआईआर अनुदान राशि परियोजनाएँ नेटवर्क (सी/एफ सहित) गैर-नेटवर्क NMITLI परियोजनाएँ ईएमआर एवं वैज्ञानिक पूल प्रयोगशाला आरक्षित निधि बाहरी वित्तपोषित परियोजनाएँ विविध जमा राशि बाहरी निकायों की ओर से भुगतान प्रायोजित सम्मेलनों/संगोष्ठियों हेतु अमानत	(रु. लाख में) 3779.359 15109.040 108.606 1082.400 88.188 2065.631 52.853 549.294 65.292
	कुल	22900.663
2.	प्रयोगशाला आरक्षित निधि का अर्जन वर्ष के दौरान अतिरिक्त निधि (सीएसआईआर के अलावा) के निवेश पर अर्जित ब्याज के माध्यम से प्रयोगशाला आरक्षित निधि का अर्जन अन्य लेखा शीर्षों से	(रु. लाख में) 231.556 706.025
	कुल	937.581
3.	31.3.2016 को अतिरिक्त निधि का निवेश (रु. लाख में)	2699.900
4.	आपत्ति-पुस्तिका मदों का निपटारा वर्ष के दौरान किए गए समायोजन निजी यात्रा भत्ता /छुट्टी यात्रा रियायत स्थानीय	836.628 52.742 48.794
	कुल	938.164
	कुल मदें	385
5.	निम्न लिखित प्रकार के वाउचर तैयार किए गए भुगतान प्राप्त राशि टी.ई.	18139 4522 248
	कुल	22909

# S & T Support Services

## Finance and Accounts

1.	<b>Funds Utilization</b>	
	CSIR Grant	
	Projects	(₹ in lakh)
	Network (including C/F)	3779.359
	Non – network	15109.040
	NMITLI Projects	108.606
	EMR & Scientist Pool	1082.400
	Laboratory Reserve	88.188
	Externally Funded Projects	2065.631
	Misc. Deposits	52.853
	Payment on behalf of outside bodies	549.294
	Deposits for Sponsored conf. / seminars	65.292
	<b>Total</b>	<b>22900.663</b>
2.	<b>Generation of Lab Reserve</b>	(₹ in lakh)
	Through earning of interest on investment of surplus funds (other than CSIR) during the year	231.556
	From other heads	706.025
	<b>Total</b>	<b>937.581</b>
3.	<b>Investment of surplus funds as on 31.3.2016 (₹ in lakh)</b>	2699.900
4.	<b>Clearance of OB items</b>	
	Adj. made during the year	(₹ in lakh)
	Private	836.628
	TA/LTC	52.742
	Local	48.794
	<b>Total</b>	<b>938.164</b>
	No. of items	385
5.	<b>Following types of vouchers were generated</b>	
	Payment	18139
	Receipt	4522
	TE	248
	<b>Total</b>	<b>22909</b>



## S & T Support Services

### भंडार एवं क्रय

भंडार एवं क्रय में निम्नलिखित गतिविधियों हेतु पहल की गई:

- ❖ ऑनलाइन मांगपत्र के द्वारा एक दिन के भीतर आर्डर पूरा करके, दो दिन के भीतर आपूर्ति की जाना जारी है ।
- ❖ साल्वेंट गोडाउन का नवीनीकरण किया गया तथा संबंधित मुद्दों को हल किया गया ।
- ❖ स्टेशनरी स्टॉक की जांच की गई तथा स्थानीय खरीद को कम करने के लिए इसमें नई वस्तुएं जोड़ी गई ।
- ❖ FVC बिल प्रमाणन को सुव्यवस्थित किया गया ।
- ❖ नॉन मूविंग एवं स्लो मूविंग आइटम्स की समीक्षा की गई ।
- ❖ ईआरपी कार्यान्वयन जारी है ।
- ❖ उच्च मूल्य वाली विभिन्न प्रकार की वस्तुओं की उपलब्धता हेतु वर्ष 2015.16 के दौरान 3 प्रेस निविदाएं जारी की गई ।

भंडार एवं क्रय: उपलब्धियां

मद	संख्या		मूल्य (रु. करोड़ में )	
	2014 -15	2015 -16	2014 - 15	2015 -16
कुल प्राप्त एवं निष्पादित मांगपत्र	1523	2547	29.81	49.53
कुल दिए गए ऑर्डर (आयातित )	193	385	15.16	27.80
कुल दिए गए ऑर्डर (स्वदेशी : ऑनलाइन आरसी ऑर्डर सहित)	1216	2173	22.54	22.01
कुल प्राप्त सामग्री (आयातित )	1007	202	11.31	17.58
कुल प्राप्त सामग्री (स्वदेशी )	2376	1190	18.57	13.42
स्थानीय खरीद (ऑनलाइन आरसी ऑर्डर सहित)	8852	7300	5.29	11.11
भंडार से जारी की गई कुल सामग्री	24160	27800	-	
वित्तीय वर्ष 2015-16 के दौरान समायोजित बकाया शेष			17.07	20.83
वित्तीय वर्ष 2015-16 के दौरान सीमा शुल्क से छूट प्राप्त राशि का उपयोग			07.07	13.54
वित्तीय वर्ष 2015-16 के दौरान उत्पाद शुल्क से छूट प्राप्त राशि का उपयोग	-		8.54	2.25



## Patents Granted: Indian(1-1-2015 to 31-12-2015)

Title	Inventor(s)	Grant No.
A Process For The Preparation Of Substituted Cycloalkanones	Satya Varahala Nadimpalli Raju, Smita Atmaram Mule, Kumar Venkatraman Srinivasan, Chelanattu Khizhakke Madath Raman Rajan, Surendra Ponrathnam	267532
Process for the simultaneous conversion of methane and organic oxygenate to C <sub>2</sub> -C <sub>10</sub> hydrocarbons using bifunctional pentasil zeolite catalyst	Chaudhary V R, Mondal K C, Mulla S A	271061
Process for preparation of S-(-)- betaxolol hydrochloride	Ramesh Anna Joshi, Murugan Muthu Krishnan, Dinesh Ramesh Garud, Sanjay Pandurang Borikar, Mukund Keshav Gurjar	264715
A enzyme composition for controlling investation of wooly aphid and sooty mould on sugarcane plant and a method of treatment thereof	Mukund Vinayak Deshpande, Santosh Bhikulal Chavan, Medha Prashantkulkarni	269370
An improved process for the preparation of alkyl and aryl carbamates	Darbha Srinivas, Rajendra Srivastava, Paul Ratnasamy	267959
Novel reusable transition metal complex catalyst useful for the preparation of high pure quality 3, 3-diaminobenzidine and its analogues and a process thereof	Ravi Kant Shukla, Lourduswamy Emmanuvel, Chidambaram Ramesh Kumar, Suryavanshi Gurunath, Arumugam Sudalai, Swati Kulkarni, Swaminathan Sivaram	267647
A process for the preparation of copolymer - 1 (cop-i), composed of l-alanine, l-lysine, l-glutamic acid and l-tyrosine-drug for the treatment of multiple sclerosis	Garnaik Baijayantimala	270977
Sulfonic acid functionalized SWCNTS a key to increase the conductivity of NAFION membranes for PEMFCS applications	Vijayamohan K Pillai, R Kannan, Bhalchandra A Kakade	268022
A single step hydrolytic process for the conversion of hemicellulose into value added chemicals	Dhepe Pares, Sahu Ramakanta	270095
Room temperature electrochemical process for synthesizing titanium dioxide nanoneedles	Rajeshkumar Shankar Hyam, Reshma Kanta Bhosale, Satishchandra Balkrishna Ogale	269059
A process for deacidification using membranes	Ulhas Kanhaiyalal Kharul, Ramchandra Vitthal Gadre, Vithal Venkatrao Jogdand, Yogesh Jayasing Chendake	271304

## Patents Granted: Foreign (cont'd)...

Sr. No.	Title	Inventor (s)	Country/ Region :Patent No.
31	Cu-mediated annulation strategy for the production of 1-amino-2-naphthalenecarboxylic acid derivatives	Rekula Santhosh Reddy, Pragati Kishore Prasad, Brij Bhushan Ahuja, Arumugam Sudalai	US: 9233911
32	Cu-mediated one pot production of o-cyanocinnamionitrile derivatives	Brijbhushan Ahuja, Reddy Santosh Rekula, Arumugam Sudalai	US: 9096498
33	Depolymerization of lignin using solid acid catalysts	Paresh Laxmikant Dhepe, Deepa Ak	US: 9051244
34	Electrochemical process for synthesis of graphene	Dhanraj Bhagwanrao Shinde, Vijayamohanan Kunjikrishnan Pillai	DE: 2616392 a1 EP: 2616392 a1 ES: 2616392 a1 GB: 2616392 a1
35	Electronically conducting carbon and carbon based nano-composites by pyrolysis of dead leaves and other similar natural waste in reducing ambient	Mandakini Biswal, Abhik Banerjee, Satischandra Ogale	US: 9212285
36	Enantiomers of fluconazole analogues containing thieno-[2,3-d]pyrimidin-4(3h)-one moiety	Hanumnat Bapurao Borate, Suleman Riyasaheb Maujan, Sangmeshwar Prabhakar Sawargave, Subhash P Chavan, Mohan A Chandavarkar, Ramakrishnan Iyer, Vikas Nawathye, Gajanan Chavan, Amit Tawte	NZ: 614359 US: 9181269
37	Enzymes from <i>Beauveria</i> sp and process for preparation thereof	Seeta Laxman Ryali, Shiv Shankar, Snehal Vijay More, Harish Bansilal Khandelwal, Chandra Babu Kannan Narasimhan, Saravanan Palanivel, Padmanabhan Balaram	DK: 2531596 NL: 2531596 CN: Zl201180017172.4 EP: 2531596 US: 9217140
38	Enzymes from <i>Conidiobolus brefeldianus</i> and process for preparation thereof	Seeta Laxman Ryali, Harish Bansilal Khandelwal, Snehal Vijay More, Kamalakar Motiram Kalal, Chandra Babu Kannan Narasimhan, Saravanan Palanivel, Padmanabhan Balaram	EP: 2539431
39	Fluorescent grafting and chemical modification of silk ( <i>Bombyx mori</i> ) for optoelectronic application	Asha Syamakumari, Kaushlendra Kumar, Anuya Nisal	US: 9290601 EP: 2872591
40	Fractal impeller for stirring	Amol Kulkarni, Bhaskar Dattatraya Kulkarni	US: 9138699
41	Graft copolymer composition with pH dependent behaviour	Ramesh Muthusamy, Mohan Gopalkrishna Kulkarni	US: 9012574
42	Highly efficient, three-dimensional, ordered, mesoporous titanosilicates, process to prepare and uses thereof	Darbha Srinivas, Anuj Kumar	US: 8932980
43	Hybrid molecules containing pharmacophores of fluconazole as antifungal agents and their preparation	Hanumant Bapurao Borate, Sawargave Prabhakar Sangmeshwer, Chavan P Shubhash, Chandavarkar A Mohan, Iyer Ramakrishnan, Tawte Amit, Rao Deepali	NZ: 610143

## Patents Granted: Foreign (cont'd)...

Sr. No.	Title	Inventor (s)	Country/ Region :Patent No.
44	Improved process for production of tert-butyl amine	Vijay Vasant Bokade, Praphulla Narahar Joshi, Prashant Suresh Niphadkar	EP: 2582656 JP: 5791711
45	Inhibitory activity of <i>Bytteneria</i> species	Dhiman Sarkar, Swati Pramod Joshi, Upasana Singh, Ketki Dilip Shurpali, Roshan Rajan Kulkarni	US: 9028893
46	Method for the preparation of biofuels from glycerol	Dharbha Srinivas, Lakshmi Saikia, Paul Ratnasamy	TW: 498315
47	Methodology for the continuous flow manufacturing of beta-amino crotonate	Amol Arvind Kulkarni, Ramesh Anna Joshi, Rohini Ramesh Joshi	US: 9199913
48	Methodology for the continuous flow synthesis of meta aminoacetphenone	Amol Arvind Kulkarni, Ramesh Anna Joshi, Rohini Ramesh Joshi	US: 9150497
49	New method for the preparation of highly enantiopure (s)-2-ethyl-n-(1-methoxypropan-2-yl)-6-methyl aniline, a precursor of (s)-metolachlor	Murugan Muthukrishnan, Prashant Pramod Mujumdar	US: 9199930
50	New process for the synthesis of methyl 3-epi-shikimate and oseltamivir	Argumugam Sudalai, Varun Rawat, Soumen Dey	US: 9150498
51	New process for the production of 4-substituted chromanes via gold catalysis	Pandurang V Chouthaiwale, Dattatray A Devalankar, Arumugam Sudalai	US: 9102646
52	New process route to cyclic carbonates directly from aldehydes and CO <sub>2</sub>	Arumugam Sudalai, Boopathi Senthil Kumar, Ravindra Dattatray Aher	US: 9266854
53	Novel processes for the preparation of pure methyl lactate from alkali metal lactate using carbon dioxide and methanol	Prashant Purushottam Barve, Bhaskar Dattatraya Kulkarni, Milind Yashwant Gupte, Sanjay Narayan Nene, Ravindra William Shinde	JP: 5680085
54	Perylenebisimidepolyester blend films for photovoltaic applications	Asha Syama Kumari, Nisha Simon Kumari	US: 9048432
55	pH sensitive graft copolymer	Muthusamy Ramesh, Mohan Gopalkrishna Kulkarni	JP: 5674686
56	Phenolytic kinetic resolution of azido and alkoxy epoxides : process for the production of enantiomerically pure $\alpha$ -aryloxy $\alpha'$ -azido/alkoxy alcohols	Pratibha Uttam Karabal, Dayanand Kamble Ambadast, Arumugam Sudalai	US: 8975430
57	Pimarane diterpenes from <i>anisochilus verticillatus</i>	Swati Pramod Joshi, Roshan Rajan Kulkarni	US: 9024043
58	PIP 3 antagonist	Ramana Venkata Chepuri, Alexei Degterev	US: 9040585
59	Polymeric form of ionic liquids	Ulhas Kanhaiyalal Kharul, Santosh Chandrakant Kumbharkar,, Rupesh Sudhakar Bhavsar	DE: 2616499 EP: 2616499 FR: 2616499 GB: 2616499 RU: 2575849 US: 9200118

## Patents Granted: Foreign (cont'd)...

Sr. No.	Title	Inventor (s)	Country/ Region :Patent No.
60	Process for delta-valerolactone via catalytic hydrogenation of levulinic acid	C V Rode, A M Hengne	US: 8975421
61	Process for making dimethyl carbonate	Darbha Srinivas, Pulikkeel Unnikrishnan	US: 9073849
62	Process for preparing amides	Darbha Srinivas, Anuj Kumar, Nepak Devadutta	US: 9221749
63	Process for preparing biodegradable lubricant base oils	Darbha Srinivas, Mehejabeen Kotwal	US: 9174919
64	Process for producing fatty acids	Darbha Srinivas, Satyarthi Jitendra Kumar, Thirumalaiswamy Raja, Deshpande Shilpa Shirish	JP: 5830019
65	Process for producing hydrocarbon fuel	Darbha Srinivas, Rajendra Srivastava, Paul Ratnasamy	EP: 1934312
66	Process for the preparation hyperbranched polyesters	Darbha Srinivas, Joby Sebastian	CN: Zl201280018710.6 EP: 2678370
67	Process for the preparation of hydroxyacetone via glycerol dehydration	Chandrashekhar Vasant Rode, Amol Mahalingappa Hengne, Ajay Ashok Ghalwadkar, Rasika Bharat Mane, Pravinkumar Hansraj Mohite, Hari Shankar Potdar	CN: 102781897 b
68	Process for the preparation of pseudo indoxyl derivatives and studied their optical properties	Chepuri V Ramana, Yogesh Mansukhabhai Goriya	US: 9145364
69	Pulsatile release composition of therapeutic agent	Muthusamy Ramesh, Kulkarni Mohan Gopalkrishna	JP: 5698683
70	Selective detection and analysis of small molecules	Venkateswarlu Panchagnula, Dipankar Ghosh, Deepika G Dhaware	EP: 2676287
71	Shape preserving transformations from ZnO and Cu <sub>2</sub> O to TiO <sub>2</sub> by TiCl <sub>4</sub> treatment	Subas Kumar Muduli, Vivek Vishnu Dhas, Onkar Sharad Game, Ashish Prabhakar Yengantiwar, Abhik Banerjee, Satishchandra Balakrishna Ogale	US: 9290392
72	Short and efficient synthesis of antibiotic CJ-15, 801 and its isomers	D Srinivasa Reddy, Komirishetty Kashinath, Pandrangi Siva Swaroop,	US: 9193674
73	Sila analogs of oxazolidine derivatives	D Srinivasa Reddy, Seetharam Singh Balamkundu, Remya Ramesh	US: 9233989
74	Substituted 1,4-dioxo-8-azaspiro [4,5] decanes useful as fungicides and a process for the preparation thereof	Mukund Vinayak Deshpande, Sunita Ranjan Deshpande, Fazal Shirazi, Chaudhary Preeti Madhukar, Rao Nelavelli Malleswara, Mohanty Baidyanath, Sharma Nageshwar, Nath, Bachhawat Anand Kumar, Kaliannan Ganesan, Paul Sanjoy, Kumar Raj, Rao Bommenna Vittal, Gawali Bhimrao Bo	JP: 5738268
75	Synthesis of disuphonic acids starting from cashew nut shell liquid: crosslinking catalysts for silane functionalized polyolefins	Prakash P Wadgaonkar, Bhimrao D Sarwade, Bhausheh Vilas Tawade	US: 9133089
76	Titanium gel composition for the removal of organic dyes and other organic contaminants from aqueous solution	Mohan Keraba Dongare, Shubhangi Bhalchandra Umbarkar	JP: 5716928 US: 9149673

## Network Projects

<b>Title</b>	<b>Project Leader</b>
Catalysts for Specialty Chemicals (CSC)	Dr. Dhepe Paresh
Hydrogen Energy: Overcoming materials challenges in PEMFC towards generation, separation, storage and conversion of hydrogen (HYDEN)	Dr. Kharul U. K.
Innovate, develop and up-scale modular, agile, intensified and continuous (Indus MAGIC) processes and plants	Dr. Ranade Vivek Vinayak
Encapsulated Microorganisms for Environmental Protection (EMEP)	Dr. Gadre R.V.
Creating Intellectual Property and capabilities for the development of improved security features and substrates for the Indian currency note (FUTURE)	Dr. Premnath V.
A multi-scale Simulation and Modeling Approach to Designing Smart Functional Materials for use in Energy, Electrochemistry and Bio-mimetics (MSM)	Dr. Kumar Vanka
Centre for Surface and Interface Science Research (CSISR)	Dr. Gopinath C. S. Dr. Vinod C. P.
Nuclear Magnetic Resonance Centre for Advanced Research (NMRCAR)	Dr. Rajamohan P. R.
National Repository of Molecules (NORMS)	Dr. Sarkar Dhiman
Up gradation of facilities/National Repository of molecules and National Collection of Industrial Micro Organisms Resource Centre (NCIMRC)	Dr. Dharne Mahesh S.
New Approaches towards Understanding of Disease Dynamics and to Accelerate Drug Discovery (UNDO)	Dr. Sarkar Dhiman
Emerging and re-emerging challenges in infectious disease: System based drug design for infectious diseases (SPLenDID)	Dr. Argade N. P.
Bioprospection of plant resources and other natural products (BioprosPR)	Dr. Kadoo N. Y.
Genomics of medicinal plants and agronomically important traits (PlaGen)	Dr. Giri A. P.
Plant Diversity: Studying adaptation biology and understanding/exploiting medicinally important plants for useful bioactives (SIMPLE)	Dr. Kadoo N. Y.
Integrated NextGen approaches in health, disease and environmental toxicity (INDEPTH)	Dr. Kulkarni Mahesh J.
Nanomaterials: Applications and impact on Safety, Health and Environment (NanoSHE)	Dr. Ahmad Absar
Host Interactome analysis: Understanding the Role of Host molecules in Parasitic Infection (HOPE)	Dr. Ram Rup Sarkar
Neurodegenerative Diseases: Causes and Corrections (miND)	Dr. Kulkarni Mahesh J.

## Network Projects...cont'd

Title	Project Leader
Plant-Microbe and Soil Interactions (PMSI)	Dr. Kadoo N. Y.
Man as a Superorganism: Understanding the Human Microbiome (HUM)	Dr. Suresh C. G.
Centre for BIOtherapeutic Molecule Discovery (BioDiscovery)	Dr. Sanjayan G. J. Dr. Giri A. P.
Genome Dynamics in cellular organization, differentiation and enantiostasis (GenCODE)	Dr. Fernandes Moneesha
CSIR-NCL-IGIB Joint Research Initiative: Interfacing Chemistry and Biology	Dr. Thulasiram H. V.
Towards Understanding Skin Cell Homeostasis (TOUCH)	Dr. Fernandes Moneesha
Clean Coal Technology (TapCoal)	Dr. Srinivas D.
Membrane and Adsorbent Technology Platform for Effective Separation of Gases and Liquid (MATES)	Dr. Desale Girish R.
Inherently Safer Practices for Industrial Risk Reduction (INSPIRE)	Dr. Karthikeyan M.
Organic reactions in generating innovative and natural scaffolds (ORIGIN)	Dr. Ramana C. V.
Non-Infringing Chemistry and Engineering for Pharmaceuticals - (NICE-P)	Dr. D. Srinivasa Reddy
Metabolic profiling of human body fluids by MS and NMR (CMET)	Dr. Venkateswarlu Panchagnula
Screening molecules in lead exploration (SMiLE)	Dr. Kulkarni Mahesh J.
Development of sustainable processes for edible oils with health benefits from traditional and new resources (PEOPLE-HOPE)	Dr. Kadoo N. Y.
Development of Sustainable Waste Management Technologies for Chemical and Allied industries (SETCA)	Dr. Bhandari V. M. Dr. Kamble Sanjay P.
Energy Efficient Technologies (E2++)	Dr. Kharul U. K.
Catalysts for Sustainable Energy (Ecat)	Dr. Srinivas D.
Research Initiative for Low Emissions (RILE)	Dr.(Mrs.) Umbarkar S. B.
Natural products as Affordable Healthcare Agents (NaPAHA)	Dr. Thulasiram H. V.
Development of Functional food and their formulations for potential health benefits of common man (FUNHEALTH)	Dr. Giri A. P.
Molecules to Materials to Devices (M2D)	Dr. Prasad B. L. V
Affordable Cancer Therapeutics (ACT)	Dr. Chavan S. P.
Advanced Drug Delivery System (ADD)	Dr. Sen Gupta Sayam
CSIR-NCL OSDD Outreach Center	Dr. Karthikeyan M. Dr. Ramana C. V.
Biocatalysts for Industrial Applications & Greener Organic Synthesis (BIAGOS)	Dr. Thulasiram H. V.



## Network Projects...cont'd

Title	Project Leader
Technologies and Products for Solar Energy Utilization through Networks (TAPSUN)	Dr. Krishnamoorthy K.
Innovative solutions for Solar Energy storage	Dr. Gopinath C. S. Dr. Shelke Manjusha Dr. Avadhani Chilukuri Ver
Zero Emission Research Initiative for Solid Wastes from Leather (ZERIS)	Shri Deenadayalan
Recovery of water from domestic waste water using membrane based systems	Dr. Kamble Sanjay P.
CSIR Knowledge Gateway & Open Source Private Cloud Infrastructure (KNOWGATE)	Dr. Sunita Barve

## NCL Customers

<b>Indian Customers</b>	
<ul style="list-style-type: none"> <li>• Dr. Reddy's Laboratories Ltd.</li> <li>• Benefuel Incorporation</li> <li>• Hari Om Chemicals</li> <li>• Reliance Industries Ltd.</li> <li>• Vijay Chemical Industries</li> <li>• Green Vision Life Sciences Pvt. Ltd.</li> <li>• Expanded Polymer Systems Pvt. Ltd.</li> <li>• Sumitomo Chemical India Pvt. Ltd.</li> <li>• Lupin Ltd. (Lupin Research Park)</li> <li>• Tata Chemicals Ltd.</li> <li>• Godrej Consumer Products Ltd.</li> <li>• Gulbrandsen Chemicals Pvt. Ltd.</li> <li>• Deccan Nutraceuticals Pvt. Ltd.</li> </ul>	<ul style="list-style-type: none"> <li>• Galaxy Surfactants Ltd.</li> <li>• Emcure Pharmaceuticals Ltd.</li> <li>• Godrej Industries Ltd. (GIL)</li> <li>• Syngenta India Ltd.</li> <li>• Hicare Services Pvt. Ltd.</li> <li>• Serum Institute of India Ltd.</li> <li>• Jay Chemicals</li> <li>• KanBiosys Pvt. Ltd.</li> <li>• Deepak Nitrite Ltd.</li> <li>• D. J. Malpani</li> <li>• Uniphos Envirotronic Pvt. Ltd.</li> <li>• Gujarat Fluorochemicals Ltd.</li> <li>• UPL Limited</li> <li>• ATGC Biotech Pvt. Ltd.</li> <li>• Vijay Chemical Industries</li> </ul>

<b>Foreign Customers</b>	
<ul style="list-style-type: none"> <li>• General Cable Corporation</li> <li>• GlaxoSmithKline LLC</li> </ul>	<ul style="list-style-type: none"> <li>• Solvay Speciality Polymers, Italy</li> <li>• Benefuel Inc., USA</li> </ul>

<b>Publicly Funded Clients</b>	
<ul style="list-style-type: none"> <li>• Bharat Petroleum Corporation</li> </ul>	<ul style="list-style-type: none"> <li>• GAIL (India) Limited</li> </ul>

## Dateline CSIR-NCL

12/06/2015	Workshop on Industrial Automation and Process Control
03/08/2015	Acharya P. C. Ray Memorial Lecture by Dr. R. R. Sonde, Executive Vice President, Research Technology & Innovation Center, Thermax Ltd. Pune
26/09/2015	CSIR Foundation Day Lecture by Prof. Devang Khakhar, Director, IIT Bombay on "A New Era for R&D in India: The Role of CSIR"
18/11/2015	Prof. Mc Bain Memorial Lecture on Adv. Particle design for Therapeutic delivery by interfacing materials science and Biology by Prof. Frank Caruso fr. university of Melbourne
04/01/2016	Workshop on Synthesis, Characterization and Application of Nanoparticle Assemblies
07/01/2016	CSIR - NCL foundation day Lecture by Prof. Ramgopal Rao, Dept of Electrical Engg. IIT – Mumbai
19/01/2016	Dr.L.K. Doraiswamy Memorial Lecture by Prof. Maria Flytzani of Tufts University, Medford
02/02/2016	Visit of Dr. Harsh Vardhan, Vice President, CSIR and Union Minister for Science & Technology and Earth Sciences
03/02/2016	Address of Dr. Girish Sahni, DG, CSIR to the CSIR-NCL staff
29/02/2016	National Science Day lecture on "Chemical Engineering Forays in Rural India" by Prof. A.B. Pandit Institute of Chemical Technology Mumbai



## Awards/Recognitions

Name	Award
Amol Kulkarni	SwarnaJayanti Fellowship
	OPPI Young Scientist Award 2015
Anil Kumar	Chairman of CODATA National Committee of International Council of Scientific Union, Paris
C. S. Gopinath	A member of the Editorial Board of Indian Journal of Chemical Technology
H. V. Thulasiram	Member of Editorial Board of Scientific Reports
M. Karthikeyan	2015 Legal Tech Open Innovation Challenge—Docket Analytics
M. V. Deshpande	Vice President of Mycological Society of India
Mahesh Kulkarni	Raman Research Fellowship
Manohar Badiger	Member of the Research Council for the Biomedical Technology wing of the Sree Chitra Tirunal Institute for Medical Sciences and Technology
Narshinha Argade	Member of American Chemical Society
Pradeep Kumar	National Representative of the IUPAC Chemistry and Environment Division for the term 2016-2017
Sourav Pal	Member of Executive Council of Federation of Asian Chemical Society (FACS)
	A special issue as a Sourav Pal Festschrift to recognize and honour
Sreekumar Kurungot	Associate Editor for the RSC Advances
Srinivasa Reddy	Shanti Swarup Bhatnagar Prize 2015
	NASI- Reliance Industries Platinum Jubilee Award
	CRSI Bronze Medal
Vidya Gupta	Late Smt. Pushpalata Ranade National Woman Award 2015
Vivek Ranade	Associate Editor of Industrial & Engineering Chemistry Research, An international Journal
	Fellow of the Indian National Science Academy

## सीएसआईआर-एनसीएल की राजभाषा कार्यान्वयन संबंधी रिपोर्ट

भारत सरकार की राजभाषा नीति तथा राजभाषा संबंधी नियमों का अनुसरण करने की दृष्टि से सीएसआईआर-राष्ट्रीय रासायनिक प्रयोगशाला(एन.सी.एल.) में प्रत्येक स्तर पर गहन प्रयास किए जाते हैं। सीएसआईआर-एन.सी.एल. एक वैज्ञानिक प्रयोगशाला है, जहां अधिकांश कार्य वैज्ञानिक तथा तकनीकी स्वरूप का होता है तथा शेष प्रशासनिक कार्य अधिकांशतः हिन्दी भाषा में किया जाता है। इस प्रयोगशाला में किए जा रहे राजभाषा कार्यान्वयन संबंधी उल्लेखनीय प्रयास निम्नानुसार हैं।

- प्रत्येक तिमाही में एनसीएल की राजभाषा कार्यान्वयन समिति की तिमाही बैठक नियमित रूप से निदेशक महोदय की अध्यक्षता में आयोजित की जाती है एवं इन बैठकों में प्रयोगशाला में राजभाषा हिन्दी के प्रगामी प्रयोग तथा राजभाषा कार्यान्वयन संबंधी प्रयासों की समीक्षा की जाती है। इन बैठकों में प्रयोगशाला के प्रत्येक प्रभाग/ अनुभाग प्रमुख सदस्य के रूप में उपस्थित रहते हैं।
- एनसीएल के स्टाफ को हिन्दी कार्य करने में आ रही समस्याओं का निदान करने तथा हिन्दी में कार्य करने हेतु प्रोत्साहित करने की दृष्टि से प्रत्येक तिमाही में नियमित रूप से हिन्दी कार्यशाला का आयोजन किया जाता है। इन कार्यशालाओं में स्टाफ को भारत सरकार की राजभाषा नीति की जानकारी देने के साथ-साथ अपना दैनंदिन सरकारी कार्य हिन्दी में करने तथा कंप्यूटर पर यूनिकोड प्रणाली के माध्यम से हिन्दी में काम करने का प्रशिक्षण दिया जाता है।
- प्रतिवर्ष हिन्दी गृहपत्रिका "एनसीएल-आलोक" का प्रकाशन नियमित रूप से किया जाता है। गृहपत्रिका प्रकाशन का मूल उद्देश्य हिन्दी भाषा में लिखे गए वैज्ञानिक लेखों का प्रचार-प्रसार तथा कर्मचारियों की हिन्दी में लेखन और अभिव्यक्ति क्षमता को प्रोत्साहित करना है।
- एनसीएल में प्रतिवर्ष हिन्दी पखवाड़ा समारोह का भव्य आयोजन किया जाता है। इस वर्ष 15-29 सितंबर, 2015 के दौरान हिन्दी पखवाड़ा आयोजित किया गया। इस अवसर पर स्टाफ के लिए विभिन्न हिन्दी प्रतियोगिताओं तथा कार्यक्रमों का आयोजन किया जाता है। हिन्दी पखवाड़ा के आरंभ में हिन्दी दिवस के अवसर पर प्रतिवर्ष प्रयोगशाला की वार्षिक गृहपत्रिका "एनसीएल-आलोक" का विमोचन किया जाता है।
- हिन्दी कक्ष द्वारा प्रतिदिन हिन्दी सुविचार तथा अंग्रेजी शब्द के अर्थ का प्रेषण मेल द्वारा सभी कर्मचारियों को किया जाता है, ताकि कर्मचारियों में हिन्दी भाषा के प्रति रुचि उत्पन्न हो सकें।
- राजभाषा अधिनियम की धारा 3(3) के अंतर्गत जारी होने वाले सभी दस्तावेज द्विभाषी जारी किए जाते हैं।

- इस प्रयोगशाला में राजभाषा विभाग द्वारा जारी वार्षिक कार्यक्रम में निर्धारित किए गए लक्ष्यों की प्राप्ति की ओर विशेष ध्यान दिया जाता है ।
- केंद्र सरकार, राजभाषा नियम 1976 (संघ के सरकारी प्रयोजनों के लिए प्रयोग) के नियम 10 (4)के अंतर्गत इस प्रयोगशाला को ऐसे कार्यालयों के रूप में , जिसके 80% से अधिक कर्मचारी वृंद ने हिन्दी का कार्यसाधक ज्ञान प्राप्त कर लिया है, राजपत्र में अधिसूचित किया गया है ।
- प्रयोगशाला के 98%कर्मचारियों को हिन्दी, हिन्दी टंकण एवं आशुलिपि का प्रशिक्षण दिया जा चुका है ।
- प्रशासन अनुभाग के कुछ अधिकारियों/कर्मचारियों तथा वैज्ञानिक स्टाफ को कंप्यूटर पर हिन्दी में कार्य करने हेतु प्रशिक्षित किया गया है तथा शेष स्टाफ को प्रशिक्षित करने की प्रक्रिया जारी है ।
- प्रयोगशाला में सभी मानक प्रपत्र, फार्म तथा आवेदन पत्रइत्यादि द्विभाषी रूप में तैयार किए गए हैं ।
- प्रयोगशाला की वेबसाइट को द्विभाषी रूप में प्रदर्शित किया गया है ।
- प्रयोगशाला के सभी कम्प्यूटरों में द्विभाषी रूप से कार्य करने की सुविधा उपलब्ध है ।
- प्रयोगशाला के सभी साइनबोर्ड, नाम-पट्टों तथा रबर की मोहरों को द्विभाषी बनाया गया है ।
- प्रशिक्षण कार्यक्रमों में मिली-जुली भाषा का उपयोग किया जाता है ।
- प्रयोगशाला के निदेशक एवं हिन्दी अधिकारी नगर राजभाषा कार्यान्वयन समिति की बैठकों में नियमित रूप से भाग लेते हैं ।
- प्रयोगशाला की शीर्ष स्तर की प्रबंध परिषद की बैठकों की कार्यसूची द्विभाषी रूप में तैयार की जाती है और इन बैठकों में हिन्दी में भी चर्चा की जाती है ।
- प्रयोगशाला के पुस्तकालय हेतु प्रतिवर्ष हिन्दी पुस्तकें खरीदी जाती हैं ।
- प्रयोगशाला में आयोजित होने वाले समारोहों, व्याख्यानों एवं संगोष्ठियों की रिपोर्ट हिन्दी एवं अंग्रेजी दोनों भाषाओं में सीएसआईआर-समाचार में प्रकाशनार्थ राष्ट्रीय विज्ञान संचार एवं सूचना स्त्रेत संस्थान (निसकेयर), नई दिल्ली को नियमित रूप से भेजी जाती है ।



- सीएसआईआर मुख्यालय की मौलिक (विज्ञान) पुस्तक लेखन योजना, वैज्ञानिक कार्यों में हिन्दी पुरस्कार योजना तथा विज्ञान चिंतन लेखमाला आदि योजनाएँ इस प्रयोगशाला में लागू हैं। इन सभी योजनाओं में प्रयोगशाला के वैज्ञानिक और कर्मचारी उत्साहपूर्वक भाग लेते हैं।
- इसके अतिरिक्त प्रयोगशाला में आयोजित होने वाले विभिन्न वैज्ञानिक कार्यक्रमों तथा अन्य समारोहों का संचालन भी हिन्दी माध्यम से किया जाता है। दिनांक 2 फरवरी, 2016 को माननीय मंत्री हर्षवर्धन जी के एनसीएल आगमन के समय आयोजित कार्यक्रम का संचालन भी हिन्दी भाषा में किया गया।
- इस प्रयोगशाला के वैज्ञानिक देश के विभिन्न संस्थानों में राजभाषा के माध्यम से आयोजित होने वाली संगोष्ठियों तथा विज्ञान सम्मेलनों में भाग लेकर हिन्दी भाषा में अपना शोध पत्र प्रस्तुत करते हैं।
- प्रयोगशाला से जारी होने वाली सभी निविदा सूचनाएँ तथा विज्ञापन इत्यादि द्विभाषी रूप में प्रकाशित किए जाते हैं।
- विज्ञान शिक्षा के प्रति रुचि उत्पन्न करने तथा राजभाषा के माध्यम से विज्ञान के प्रचार-प्रसार के उद्देश्य से प्रयोगशाला के निदेशक महोदय विभिन्न विद्यालयों तथा महाविद्यालयों के विद्यार्थियों के लिए विज्ञान संबंधी व्याख्यान हिन्दी में देते हैं।
- प्रयोगशाला के स्टाफ को हिन्दी में कार्य करने हेतु प्रोत्साहित करने की दृष्टि से यहाँ विभिन्न राजभाषा प्रोत्साहन योजनाएँ लागू हैं।
- प्रयोगशाला में हिन्दी काम-काज को बढ़ावा देने तथा राजभाषा नीति के अनुपालन हेतु 9 अनुभागों को हिन्दी में कार्य करने के लिए निर्दिष्ट किया गया है।
- प्रयोगशाला में प्राप्त हिन्दी पत्रों के उत्तर अनिवार्य रूप से हिन्दी में ही दिये जाते हैं तथा क तथा ख क्षेत्रों को जाने वाले अधिकांश पत्रों के लिफाफों पर पते हिन्दी भाषा में लिखे जाते हैं।
- राजभाषा विभाग के वार्षिक कार्यक्रम तथा राजभाषा संबंधी निर्देशों से सभी विभाग/प्रभाग प्रमुखों को अवगत कराया जाता है।

## हिन्दी पखवाड़ा रिपोर्ट

सीएसआईआर-एनसीएल में दिनांक 14 से 30 सितंबर, 2015 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 प्रयोगशाला के स्टाफ एवं शोध छात्रों ने बड़ी संख्या में उत्साहपूर्वक प्रतिभाग लिया।

हिन्दी पखवाड़ा समारोह के दौरान निम्नांकित गतिविधियां आयोजित की गईं-

- दिनांक 14 सितंबर, 2015 - हिन्दी पखवाड़ा शुभारंभ एवं गृहपत्रिका 'एनसीएल आलोक' का लोकार्पण
- दिनांक 15 सितंबर, 2015 - हिन्दी कार्यशाला एवं सामान्य ज्ञान प्रतियोगिता
- दिनांक 16 सितंबर, 2015 - तात्कालिक भाषण प्रतियोगिता
- दिनांक 18 सितंबर, 2015 - हिन्दी शुद्धलेखन प्रतियोगिता
- दिनांक 21 सितंबर, 2015 - हिन्दी काव्यपाठ प्रतियोगिता
- दिनांक 22 सितंबर, 2015 - हिन्दी निबंध प्रतियोगिता
- दिनांक 29 सितंबर, 2015 - हिन्दी में वैज्ञानिक प्रस्तुतिकरण
- दिनांक 30 सितंबर, 2015 - पखवाड़ा समापन एवं पुरस्कार वितरण समारोह

दिनांक 14 सितंबर, 2015 को प्रयोगशाला में हिन्दी पखवाड़ा शुभारंभ तथा वार्षिक राजभाषा पत्रिका 'एन.सी.एल.आलोक' का लोकार्पण कार्यक्रम आयोजित किया गया। इस अवसर पर मुख्यप अतिथि के रूप में नगर के प्रख्यात हिन्दी लेखक तथा 'हम लोग' पत्रिका के संपादक श्री संजय भारद्वाज तथा अध्यक्ष के रूप में प्रयोगशाला के उपनिदेशक डॉ. विवेक रानाडे उपस्थित थे। सर्वप्रथम मंचासीन अधिकारियों का स्वागत तुलसी पौधे से किया गया। तत्पश्चात सरस्वती वंदना प्रस्तुत की गई। इसके उपरांत एनसीएल की पत्रिका 'एनसीएल आलोक - के 19 वें अंक का विमोचन किया गया।



मुख्य अतिथि श्री संजय भारद्वाज 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 हिन्दी मीडिया, वाणिज्य, उद्योग-व्यापार इत्यादि क्षेत्रों में केवल भारत ही नहीं बल्कि समूचे विश्व में अपने पंख पसार रही 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 उपनिदेशक डॉ. विवेक रानाडे 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।' उन्होंने उपस्थित स्टाफ सदस्यों से अपील की कि 'सभी वैज्ञानिक/अधिकारी/कर्मचारी बिना किसी हिचक के राजभाषा हिन्दी 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 स्वयं भी हिन्दी में कार्य करें तथा अपने अधीनस्थ कर्मचारियों को हिन्दी में कार्य करने के लिए प्रोत्साहित करें।'

तत्पश्चात इस कार्यक्रम में हिन्दी अधिकारी श्रीमती स्वाति चड्ढा द्वारा 'हिन्दी के विकास में विभिन्न विद्वानों का योगदान' विषय पर एक पावरपॉइंट प्रस्तुतिकरण भी किया गया। कार्यक्रम के अंत में प्रशासन अधिकारी श्री अजित बैनर्जी ने सभी के प्रति आभार व्यक्त किया।

दिनांक 30 सितंबर, 2015 को आयोजित हिन्दी पखवाड़ा समापन एवं पुरस्कार वितरण समारोह आयोजित किया गया। समारोह के आरंभ में हिन्दी अधिकारी, श्रीमती स्वाति चड्ढा ने हिन्दी पखवाड़े की प्रासंगिकता एवं इस दौरान आयोजित गतिविधियों की जानकारी दी। कार्यक्रम के दौरान मुख्य अतिथि के रूप में उपस्थित डॉ. राजबहादुर (वरिष्ठ हिन्दी अधिकारी, उच्च उर्जा पदार्थ अनुसंधान केंद्र, पुणे) ने कहा कि - 'हिन्दी भाषा सभी भाषा-भाषियों के बीच एक महत्वपूर्ण सेतु का और संपर्क बनाने का कार्य करती है। देश के आर्थिक/ सामाजिक विकास और राष्ट्रीय अखंडता में हिन्दी भाषा की महत्वपूर्ण भूमिका है। हम सभी को अपनी भाषा के विकास और संरक्षण में अपना योगदान देना चाहिए।'

इस अवसर पर अध्यक्ष के रूप में उपस्थित उपनिदेशक डॉ. विवेक रानाडे ने कहा कि 'जिस प्रकार हम अपने राष्ट्र ध्वज और राष्ट्र गीत का सम्मान करते हैं, उसी तरह हम सबको अपनी राजभाषा - राष्ट्र भाषा 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।

अंत में श्रीमती पूजा कुलकर्णी, प्रशासन अधिकारी ने सभी के प्रति धन्यवाद ज्ञापित किया। समारोह की कार्यवाही का संचालन हिन्दी अधिकारी श्रीमती स्वाति चट्ढा ने किया।



## Outreach Programme

The Outreach Programme is the science activity of CSIR- National Chemical Laboratory and Faculty from Indian Institute of Science, Education and research, Pune. The objective is to boost the excitement of science and technology with school children. Following talks were organized during the year.

Date	Topic	Speaker
19 Apr, 2015	Hydrogen Energy and Fuel Cells: Exciting Opportunities in India	Dr. Ashish Lele, CSIR-NCL, Pune
31 May, 2015	Color, Art and Chemistry	Dr. Sakya Sen, CSIR-NCL, Pune
28 June, 2015	The Smart One Behind Smart Phones	Prof. Bhas Bapat , IISER, Pune
19 July, 2015	Chemistry of the Cell Membrane: And How Does it Affect Us ?	Dr. Durba Sengupta, CSIR-NCL, Pune
30 August, 2015	Pushing and Pulling by Protein Filaments	Dr. Gayathri Pananghat, IISER, Pune
20 September, 2015	From Molecules to Life	Dr. Shekhar Mande, NCCS, Pune
18 October, 2015	Stem Cells: Superheroes of the past, present and future	Dr. Deepa Subramanyam, NCCS, Pune
29 November, 2015	Understanding how activity in the brain produces movements	Dr. Raghav Rajan, IISER-Pune
13 December, 2015	"Present Physics - Future Devices"	Dr. T. S. Mahesh, IISER-Pune
19 December, 2015	How Drones Work? The Science of Automation!	Nitin Gupta, NavStik Labs
3 January, 2016	"Do liquids have a "skin"?"	Chirag Kalelkar, IIT-Kharagpur
23 January, 2016	"Role of Experiments in developing Physical Theories"	Prof. H. C. Verma, IIT-Kanpur
20 February, 2016	Gravitational Waves Astronomy - Indian Perspective	Manish Jain, IUCAA, Pune
20 March, 2016	"Where are my genes?" - A journey through the nucleus of a human cell	Dr. Kundan Sengupta, IISER Pune