

CSIR National Chemical Laboratory



75 Years of
CSIR Touching Lives

Annual Report 2016-17



सीएसआईआर - राष्ट्रीय रासायनिक प्रयोगशाला
वैज्ञानिक तथा औद्योगिक अनुसंधान परिषद
वार्षिक प्रतिवेदन 2016 - 17



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सीएसआईआर-राष्ट्रीय रासायनिक प्रयोगशाला

वैज्ञानिक तथा औद्योगिक अनुसंधान परिषद



वार्षिक प्रतिवेदन 2016 - 17

With Best Compliments from...

Prof. Ashwini Kumar Nangia
Director

CSIR-National Chemical Laboratory

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निदेशक

की कलम से...



सीएसआईआर-राष्ट्रीय रासायनिक प्रयोगशाला की वर्ष 2016-17 हेतु वार्षिक प्रतिवेदन 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। बाहरी नकदी आय हमारे बजट का लगभग 20 प्रतिशत है और हम इस प्रतिशत को और अधिक बढ़ाने का प्रयास कर रहे हैं ताकि आत्मनिर्भरता की दिशा में आगे बढ़ा जा सके।

वर्ष के दौरान बहुत से महत्वपूर्ण कार्यक्रमों का आयोजन हमारे द्वारा किया गया। रिलायंस इंडस्ट्रीज़ लि., मुंबई के अनुसंधान एवं विकास अध्यक्ष डॉ. अजीत सप्रे ने सीएसआईआर-स्थापना दिवस समारोह में “Frontiers of Hydrocarbon Business- Molecules to Materials to Markets: One Perspective” नामक विषय पर व्याख्यान दिया। प्रो. आशुतोष शर्मा, सचिव, विज्ञान एवं प्रौद्योगिकी विभाग, नई दिल्ली द्वारा एनसीएल – स्थापना दिवस समारोह में “Science, Technology and Innovation: Closing the Circle of Knowledge” नामक व्याख्यान प्रस्तुत किया गया। राष्ट्रीय विज्ञान दिवस के उपलक्ष्य में प्रो. पुष्पितो के. घोष, के. वी. मारीवाला- जे. बी. जोशी विशिष्ट प्राध्यापक, रासायनिक अभियांत्रिकी विभाग, रासायनिक प्रौद्योगिकी संस्थान, मुंबई द्वारा “Simple Illustrations of the Interplay between Science and Innovation” विषय पर व्याख्यान प्रस्तुत किया गया।

वर्ष के दौरान प्रयोगशाला के द्वारा विभिन्न कार्यशालाओं, संगोष्ठियों एवं सम्मेलनों का आयोजन किया गया, जिसमें ‘Sustainable Development for Energy and Environment’ विषय पर अंतर्राष्ट्रीय संगोष्ठी तथा Microbial Ecology and Systematics विषय पर संगोष्ठी; Current Trends in Catalysis for Energy विषय पर राष्ट्रीय संगोष्ठी; “Scanning Probe Microscopy Techniques and Conference on Advanced Organic Synthesis – 2016” विषय पर कार्यशाला; “Advances in Organic Synthesis –2017” विषय पर संगोष्ठी के अलावा ‘सीएसआईआर-एनसीएल : समग्र अनुसंधान’ विषय पर हिन्दी वैज्ञानिक संगोष्ठी के आयोजन सम्मिलित हैं।

रिसर्च स्कालर्स सम्मेलन में प्रो. जयंत नार्लीकर, एमरेटस प्रोफेसर, IUCAA, पुणे द्वारा “The interaction between Physics, Mathematics & Astronomy” विषय पर संबोधित किया गया। प्रयोगशाला द्वारा राष्ट्रीय तथा अंतर्राष्ट्रीय स्तर के विशेषज्ञ समीक्षित जर्नल्स में 600 से भी अधिक शोधपत्र प्रकाशित किए गए, जो कि वैज्ञानिक प्रकाशन के क्षेत्र में एक बड़ी उपलब्धि है। प्रयोगशाला ने प्रौद्योगिकियों को विकसित करने एवं उन्हें उद्योगों को स्थानांतरित करने के अपने प्रयास को जारी रखा है। सीएसआईआर-एनसीएल का एच इंडेक्स 134 है और प्रति शोधपत्र औसत साइटेशन 20.81 है।

प्रयोगशाला ने प्रौद्योगिकियों को विकसित करने और उद्योगों को स्थानांतरित करने के अपने प्रयासों को जारी रखा है। वर्ष के दौरान व्यावसायिक रूप से विकसित प्रौद्योगिकियों और प्रक्रियाओं में batch to continuous nitration process for the production of pendimethalin; Modeling framework for underground coal gasification; Basic Engineering Package for p-aminophenol plant - Phase II; Molecular sieve scale up: Pilot scale synthesis एवं characterization and Process for folic acid synthesis का समावेश है

इन अनुसंधान गतिविधियों के दायरे में कार्बनिक एवं अकार्बनिक रसायन, बहुलक एवं यौगिक, प्रक्रिया अभियांत्रिकी एवं प्रतिक्रिया अनुकूलन, उत्प्रेरण डिजाइन एवं संश्लेषण, सिंथेटिक रूपांतरण एवं ड्रग अणु, स्पैक्ट्रोस्कोपिक तकनीक एवं विश्लेषणात्मक लक्षण वर्णन, जैवरासायनिक प्रक्रियाएं, एंजाइम्स इत्यादि क्षेत्र शामिल हैं।

मैं सीएसआईआर-एनसीएल के अनुसंधान परिषद और प्रबंधन परिषद के साथ ही महानिदेशक, सीएसआईआर एवं सीएसआईआर, 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।

अश्विनी कु. नांगिया

(अश्विनी कुमार नांगिया)





From the
Director's
Desk...

The Annual Report of CSIR-NCL for the year 2016-17 summarizes the achievements in the areas of basic sciences as well as processes and technologies developed. The laboratory has progressed in the number and quality of publications and strengthened its association with industry partners. The external cash flow generated was about 20% of our budget, and we are striving to increase this percentage towards greater self-sufficiency.

Several important events took place during the year. The CSIR Foundation Day lecture was delivered by Dr. Ajit Sapre, President R&D, Reliance Industries Ltd., Mumbai, on the topic "Frontiers of Hydrocarbon Business- Molecules to Materials to Markets: One Perspective". NCL Foundation Day Lecture was presented by Prof. Ashutosh Sharma, Secretary, Department of Science & Technology, New Delhi on the theme "Science, Technology and Innovation: Closing the Circle of Knowledge". The National Science Day lecture was given by Prof. Pushpito K. Ghosh, K. V. Mariwala - J. B. Joshi Distinguished Professor, Department of Chemical Engineering, Institute of Chemical Technology, Mumbai on the theme of "Simple Illustrations of the Interplay between Science and Innovation".

The Laboratory hosted different workshops, conferences and symposia that included International conference on Sustainable Development for Energy and Environment and symposium on Microbial Ecology and Systematics; National Conference on Current Trends in Catalysis for Energy; Workshop on Scanning Probe Microscopy Techniques and Conference on Advanced Organic Synthesis – 2016; a Symposium on "Advances in Organic Synthesis – 2017 besides a Hindi Seminar on "CSIR-NCL-Overall Research".

The Research Scholars meet was addressed by Prof. Jayant Narlikar, Emeritus Professor, IUCAA, Pune on the topic "The interaction between Physics, Mathematics & Astronomy". 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. The H index of CSIR-NCL stands at 134 and average citation per paper is 20.81.

The laboratory has continued the efforts to develop the technologies and transfer it to the industries. The technologies and processes commercialized during the year included batch to continuous nitration process for the production of pendimethalin; Modeling framework for underground coal gasification; Basic Engineering Package for p-aminophenol plant - Phase II; Molecular sieve scale up: Pilot scale synthesis and characterization and Process for folic acid synthesis.

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 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 the Annual Report.

Ashwini Nangia

(Ashwini Kumar Nangia)



Vision, Mission, Guiding principles & Values



V I S I O N

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

M I S S I O N

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 Principle Values

To be deeply committed to the success of our stakeholders

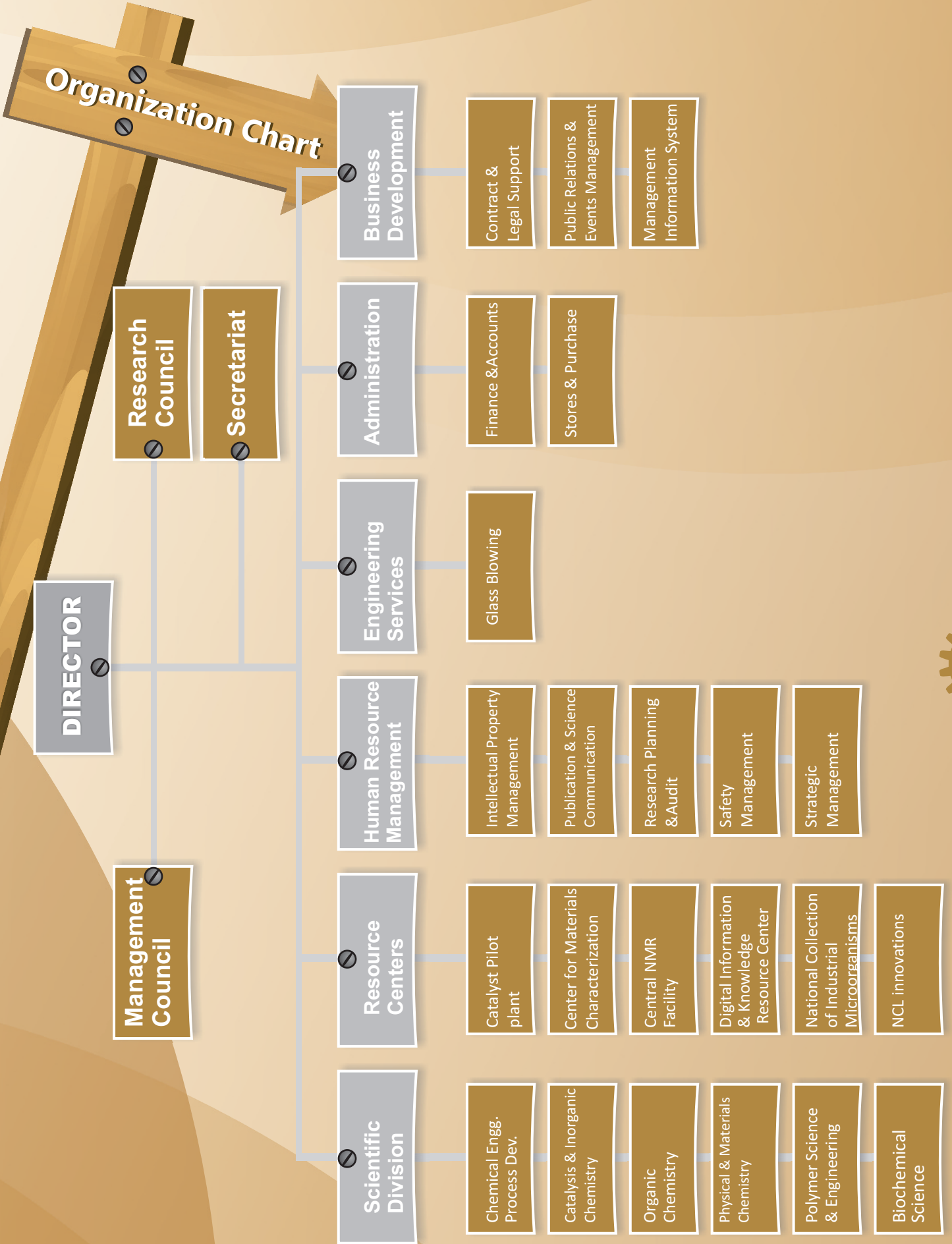
To create and sustain a self - driven and self - managed learning organization with a high degree of internal and external transparency

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



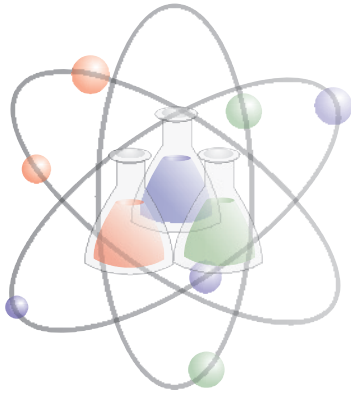




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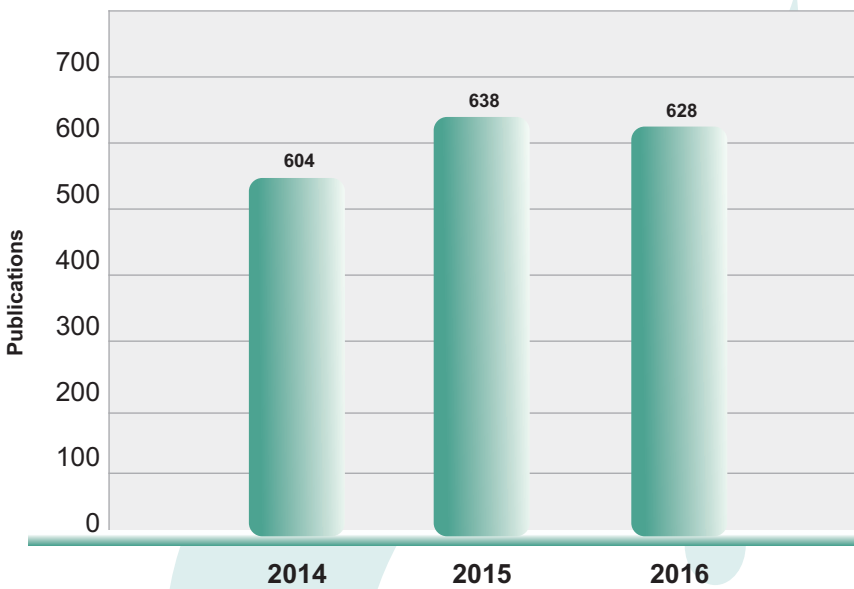


Performance Indicators

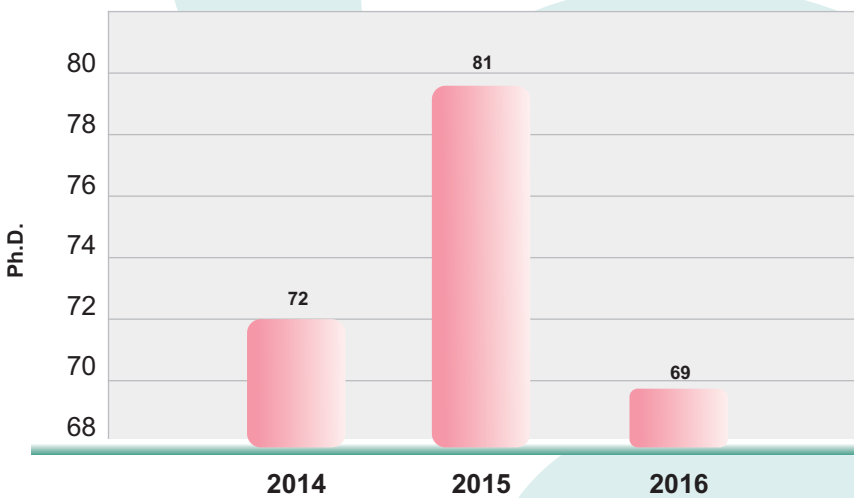


Science Performance Indicators

Research Output



Publications

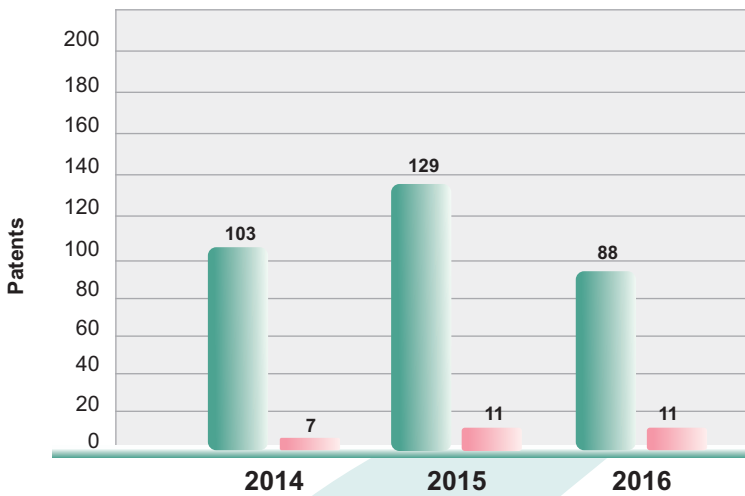


Ph.D. Theses



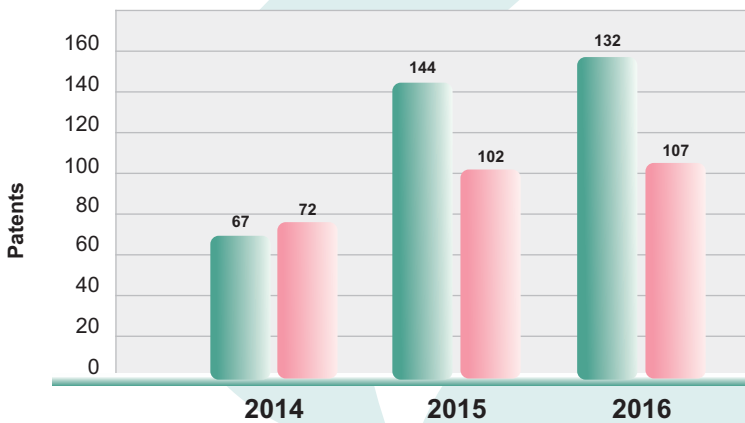


Technology Performance Indicators



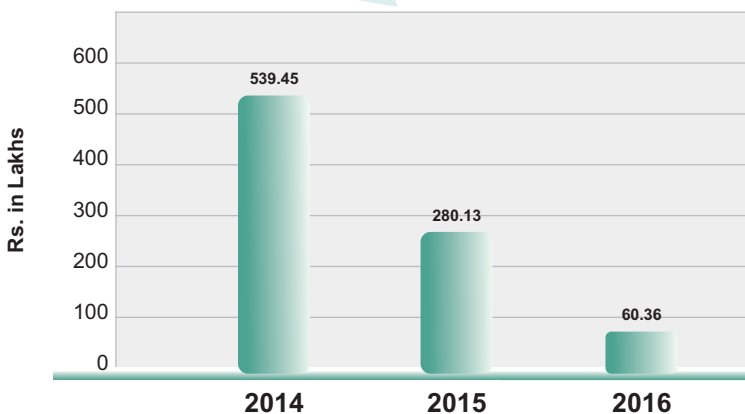
■ Filed
■ Granted

Indian Patents



■ Filed
■ Granted

Foreign Patents



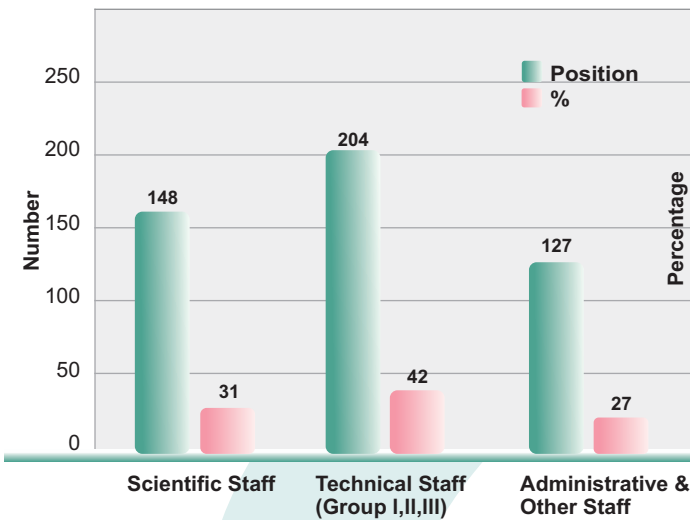
Premia / Royalty Earnings



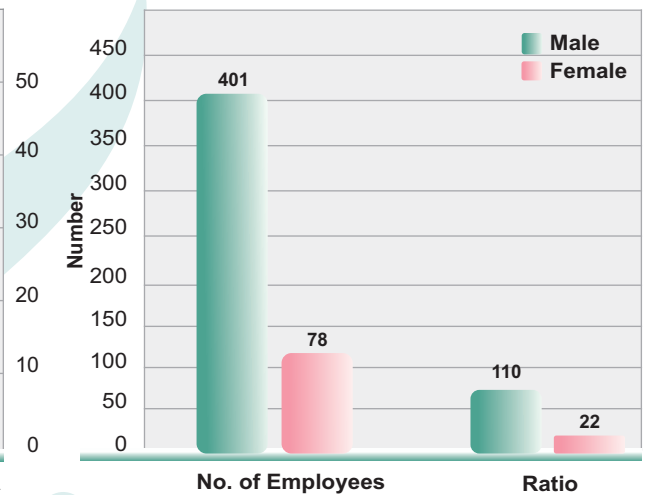


Human Resource Indicators

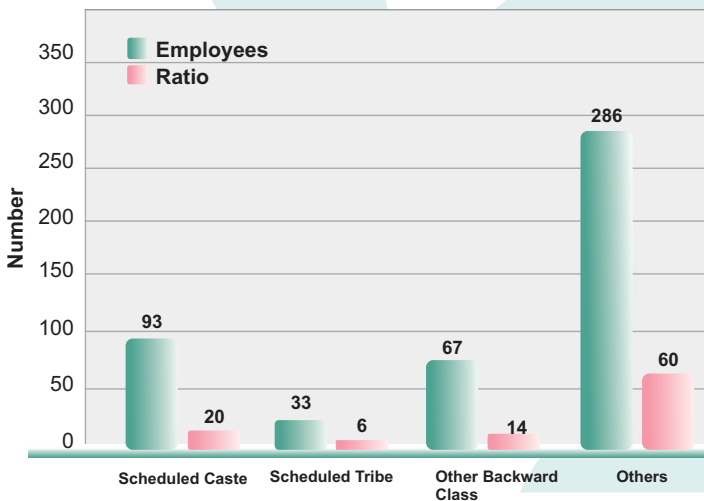
Total Staff: 511



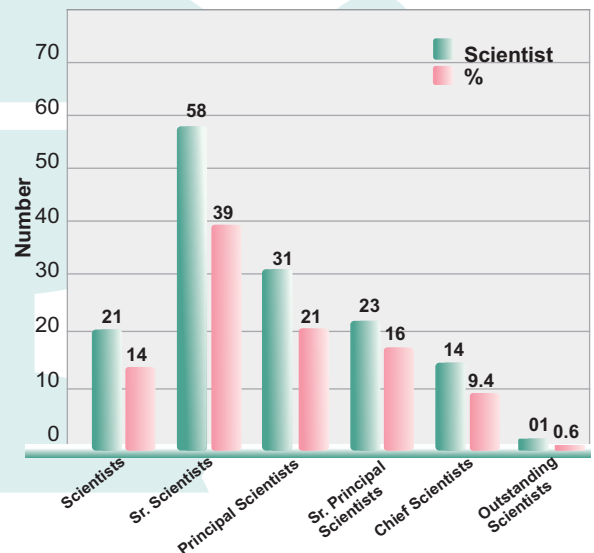
Male / Female Ratio



SC,ST, OBC & Others



Scientific Staff Distribution



WE WELCOME



Mr. Rajendra Kumar (23.08.2016)

Process Development and Process Safety

- M. Tech in Chemical Engineering, Indian Institute of Technology Bombay (2011)
- B. Tech in Chemical Engineering, Indian Institute of Technology Kanpur (2008)



Dr. KoteswaraRao Vamkudoth (07.09.2016)

Fungal Biotechnology and Microbiology

- Post-Doctoral Research Scholar, Kakatiya University,
- UGC-India (2013- 2016) Ph.D. Kakatiya University, (2009-2012)



Dr. Mrs. M. Banu (08.12.2016)

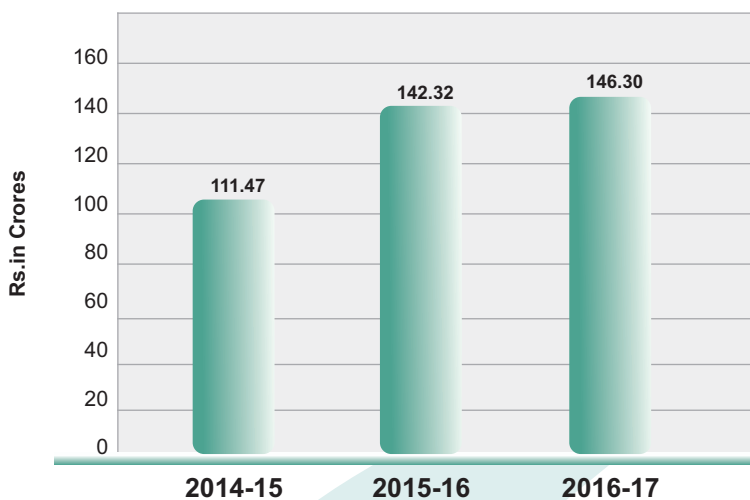
Catalysis and Carbohydrate Chemistry

- Post-Doctoral Research Scholar, UNIST, Ulsan, South Korea (2013-2015)
- Post-Doctoral Research Scholar, POSTECH, Pohang, South Korea (2012-2013)
- Ph.D. Bharathidasan University & NCCR, IIT Madras (2011)

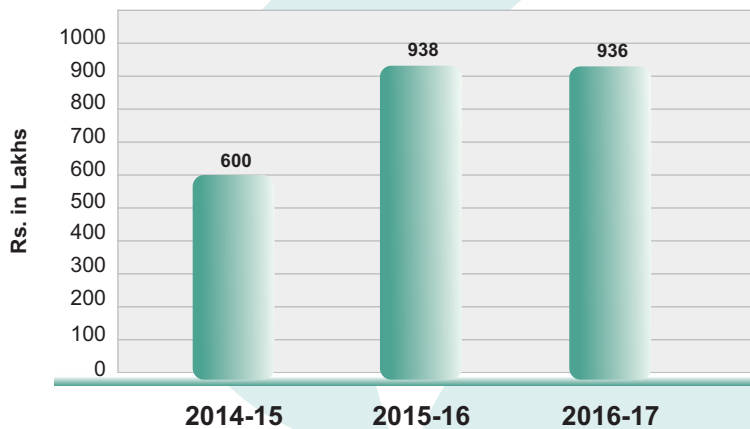




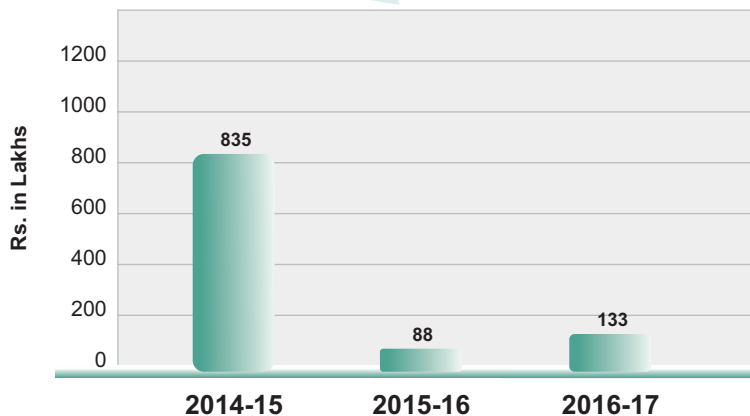
Financial Performance Indicators



CSIR Budget



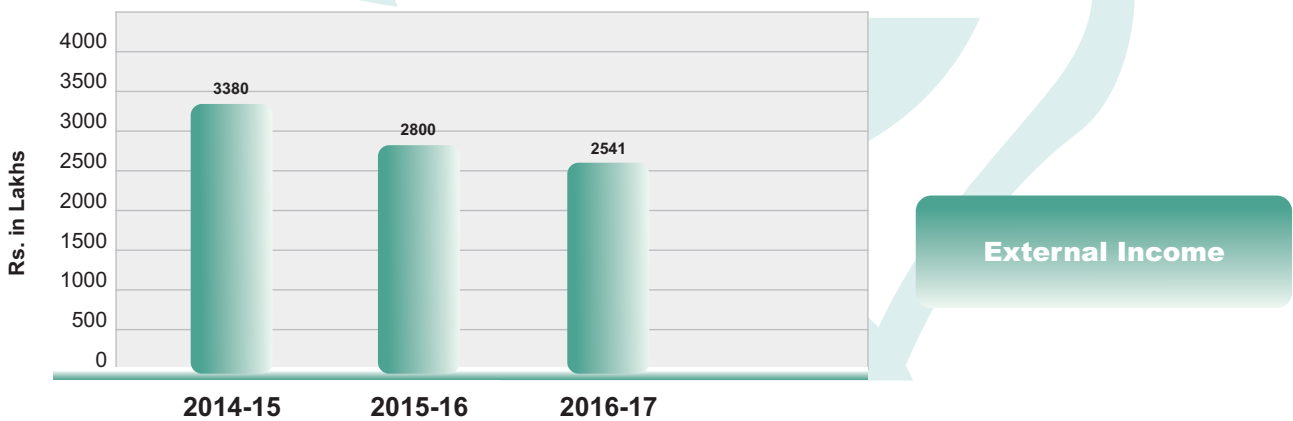
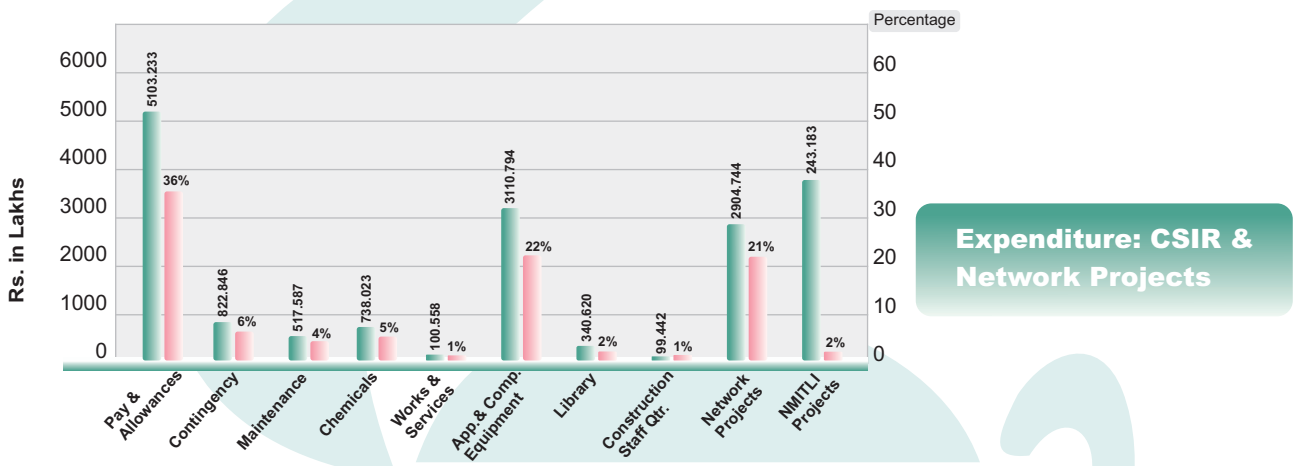
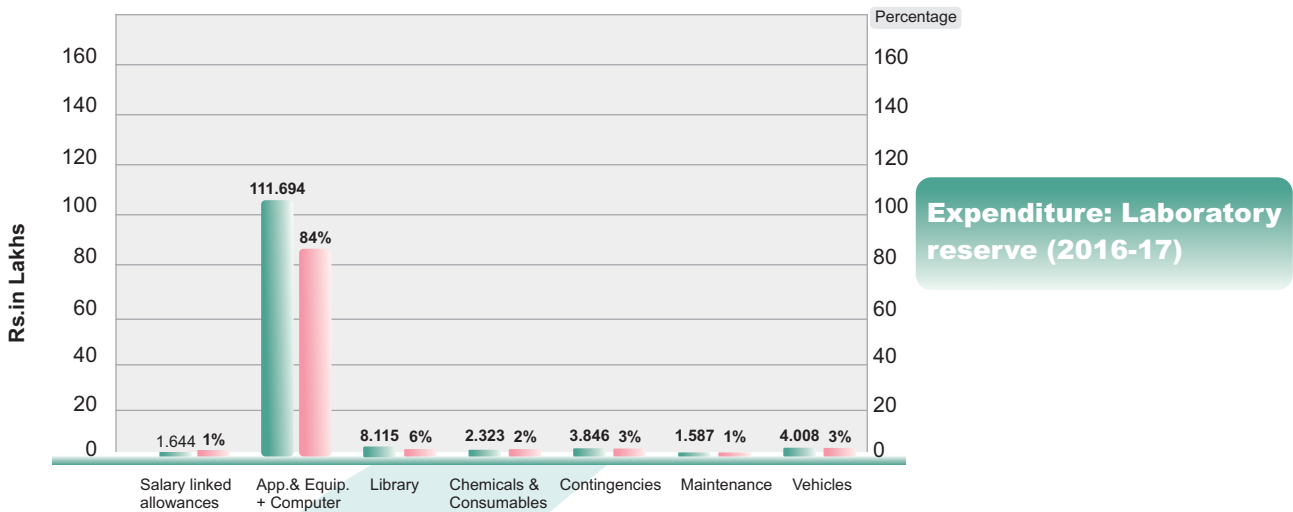
Laboratory reserve: Receipts



Laboratory reserve: Expenditure



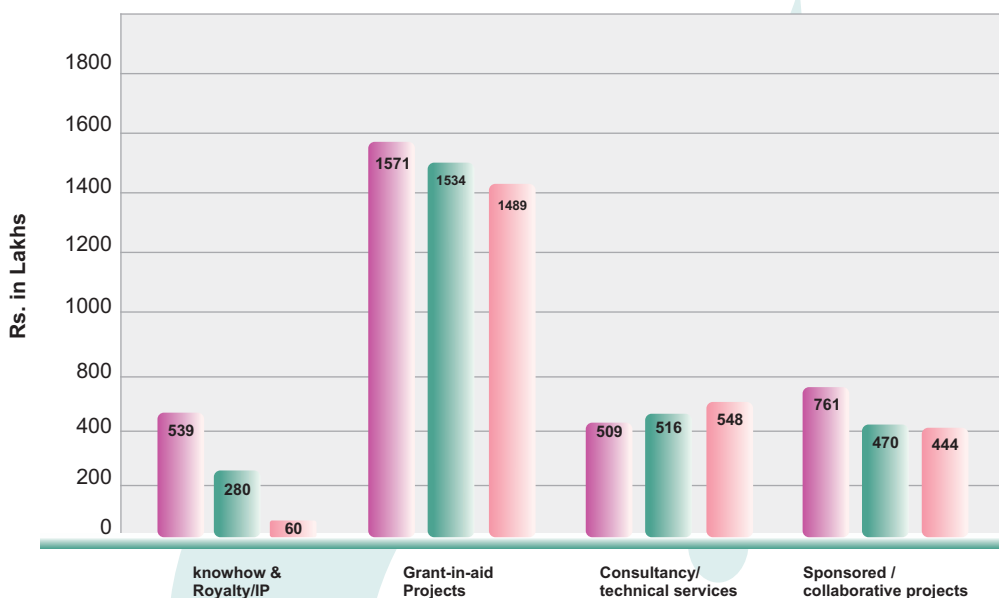
Financial Performance Indicators



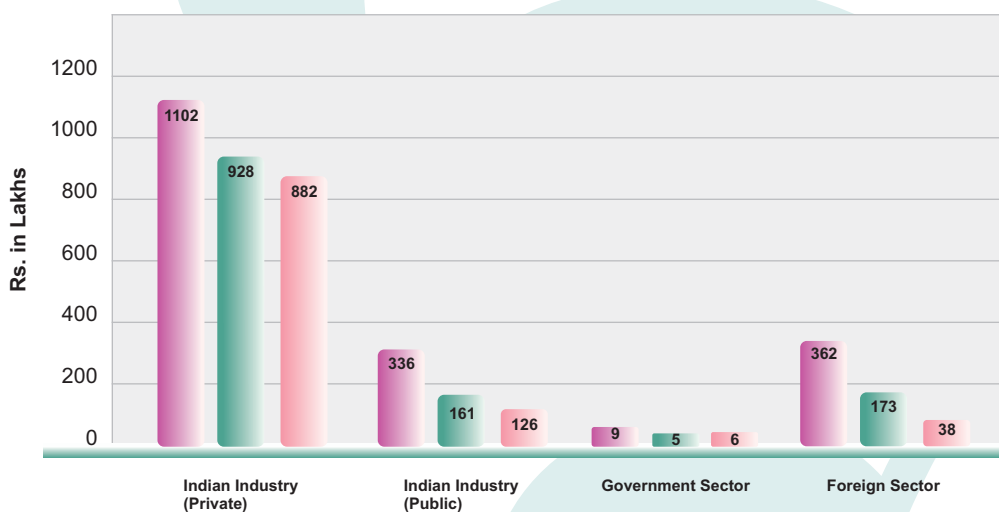
Financial Performance Indicators

- 2014-15
- 2015-16
- 2016-17

Research Output

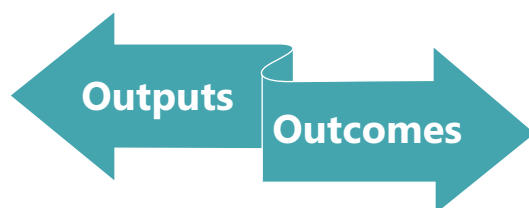


ECF by Source



ECF from Industry





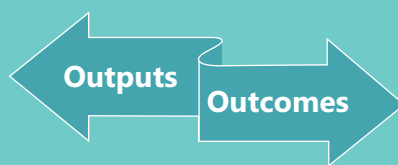
Outputs & Outcomes

Category of Benefits	Benefit	Indicators	2014-15	2015-16	2016-17
Public and social goods	Generation of and dissemination of generic knowledge	Number of papers published (Calendar year)	540	637	628
		Number of invention disclosure (Calendar year)	150	105	-
		Number of patents filed in India (Calendar year)	112	97	88
		No of foreign patents filed ** (Calendar year)	78	120	132
		Number of PCT applications filed (Calendar year)	77	44	49
		No of US applications filed	50	58	-
	Highly trained man-power	Number of PhDs produced (Calendar year)	72	81	69
		Number of NET/GATE qualified students joined (including DBT JRF)	88	57	71
	Science awareness, popularization etc.	Number of popular S&T articles published (in all languages)	3	2	4
		Number of national and regional workshops, seminars organized	7	2	7
	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)	49	88	107
	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	8	8

1 Crore = 10 Million

Performance Indicators





Category of Benefits	Benefit	Indicators	2014-15	2015-16	2016-17
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)	18.09	12.67	10.52
	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)	5.39	2.80	0.80
	Other tactical and strategic developments	Total earnings from patent related transaction(` in crore)	-	-	-
		No. of patents in new Licensing /assignment/ option arrangements	1	-	-
		No. of unique Licensing /assignment/ option cases	-	-	-
		No. of Indian patents granted (Calendar year)	7	8	11
	Contributions to projects involving valuable opportunities in the form of technology options	No of foreign patents granted** (Calendar year)	49	88	107
		Money inflow from NMITLI projects and other similar strategic projects (` in Crore)	1.65	0.13	10.05
		Money inflow from Technology Mission & GIA projects (other than NMITLI) projects (` in Crore)	15.71	15.34	14.89
Intellectual assets and reputation	Quality, reputation and standing of scientific manpower	No. of Indian patents granted (Calendar year)	7	14	11
		No. of foreign patents granted** (Calendar year)	49	88	107
		Number of PhDs granted where lab scientists were research guides	72	81	69
		Number of staff who are members of National academies (Cumulative)	32	32	32
		Number of Bhatnagar awardees (Cumulative)	15	16	16
	Number of Padma awardees (Cumulative)	5	5	5	
Lab's standing with industry	Total worth of projects with industry (only industry: both Indian & foreign) (excluding Grant-in-Aid)(` in Crore)	18.09	12.67	10.52	

* - 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

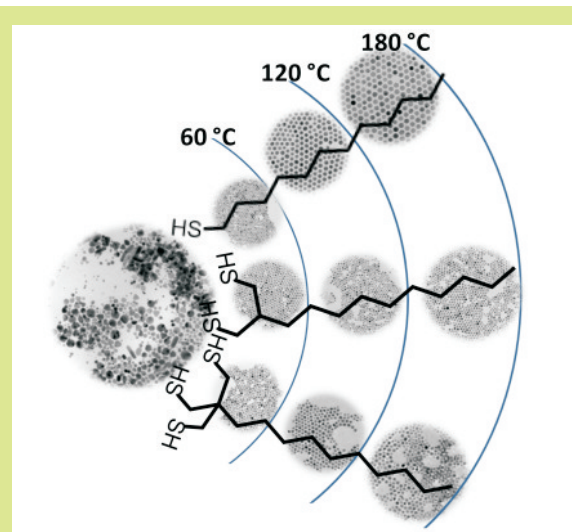
Advanced Materials

Nanostructured materials

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Demonstration of the governing parameters for controlling the monodispersity of metal nanocrystals

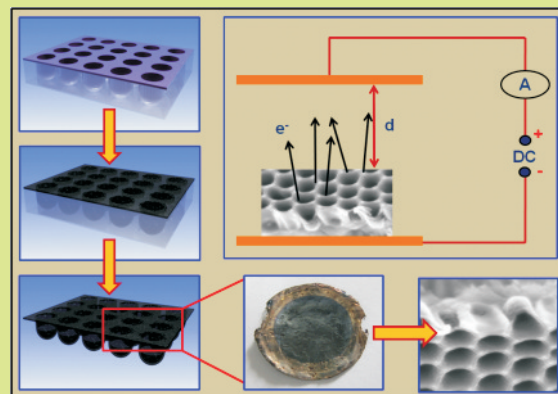
The governing parameters and their correlation on the controlling the size distribution of metal nanocrystals was investigated. More specifically, it was shown how nature of surface passivating ligands (i.e. structure, binding efficiency) can influence the size distribution of the metal nanoparticles (Langmuir 2017, 33, 1943, 9491).



Schematic resolution of the control of particle size distribution through digestive ripening

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Field emission properties of highly ordered low aspect ratio carbon nanocup arrays: A high performance field emission of cup-stacked carbon nanotubes (CSCNTs) were designed and developed. These 3D high-aspect ratio carbon nanocup structures were synthesized by a combination of anodization and chemical vapor deposition techniques. The morphological analysis revealed that CSCNTs have low-aspect ratio structures with a cup diameter of ~ 50 nm and length of ~ 100 nm. The enhanced field emission behavior observed for the CSCNTs was attributed to a high field enhancement factor of 1645, high field emission current density of $1 \mu\text{A}/\text{cm}^2$ and low turn-on field $2.30 \text{ V}/\mu\text{m}$ with better emission current stability. The enhancements observed in CSCNTs arrays were attributed synergic effect of high aspect ratio, atomically sharp diameter of the cups, and uniform distribution of the emitters over the whole area of specimen and lower screening effect of the CSCNTs. These obtained results provide new information about the effect of the stacking carbon layers on their electronic properties and open up possibilities to integrate new morphologies of graphitic carbon in nanotechnology applications.



Schematic illustrating the fabrication process

First, the CVD process synthesized the highly porous carbon nanocup structure on AAO template, then AAO template was dissolved using hydrofluoric acid solution and resulting the three-dimensional porous architectures of a connected arrays of cup-stacked carbon nanotube film was formed. (RSC Adv. 2016, 6, 9932).

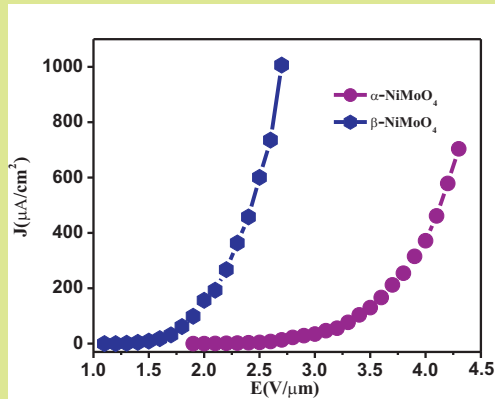
Advanced Materials

Nanostructured materials

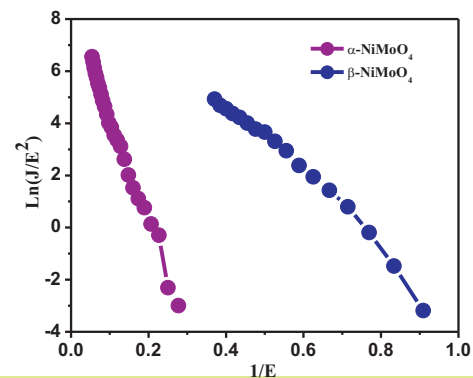
Enhanced field emission performance of NiMoO₄ nano sheets by tuning the phase

Large scale synthesis of α - and β -NiMoO₄ by a facile hydrothermal method was reported and it was observed that urea played important role on the growth of β -NiMoO₄ nanosheets. Field emission (FE) investigations of α - and β -NiMoO₄ at a base pressure of $\sim 1 \times 10^{-8}$ mbar was also carried out. The obtained turn-on field at emission current density of $1 \mu\text{A}/\text{cm}^2$ for β -NiMoO₄ nanosheets and α -NiMoO₄ was $1.3 \text{ V}/\mu\text{m}$ and $2.2 \text{ V}/\mu\text{m}$, respectively were observed. The maximum(-)

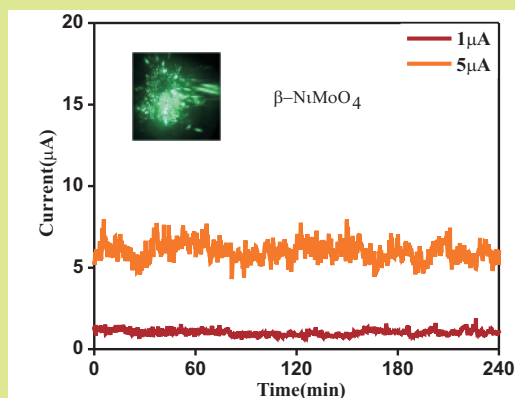
field emission current density of $1.006 \text{ mA}/\text{cm}^2$ was achieved for β -NiMoO₄ nanosheets at an applied electric field of $2.7 \text{ V}/\mu\text{m}$. Furthermore, it was found that the β -NiMoO₄ nanosheets possessed good field emission performance compared to α -NiMoO₄. The results indicated that NiMoO₄ can be used as a promising material in FE applications with possibility of tuning field emission performance by controlling the phase.



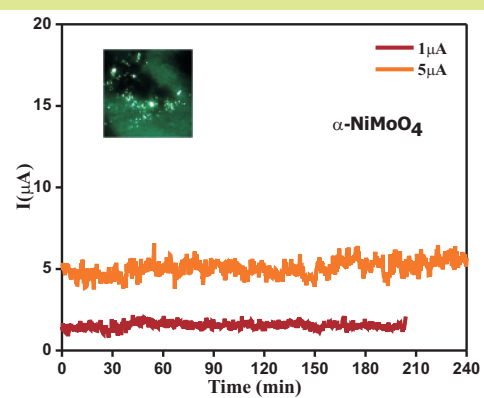
J-E characteristics



F-N plots



Field emission current stability for β -NiMoO₄ sample showed corresponding field emission pattern



Field emission current stability for α -NiMoO₄ sample and inset showed corresponding field emission pattern.

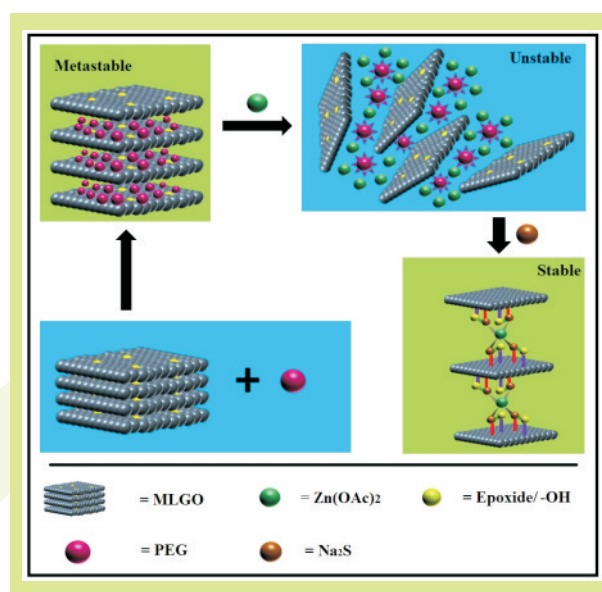
Advanced Materials

Nanostructured materials

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

Nanogates: A new chemical bond entity: The group has worked on the novel sandwich material of GO and ZnS which led to the discovery of nanogate structure between the GO layers. The formation of the defects in the GO sheets with the incorporation of nanogates was explained by a step-wise reaction mechanism, charge transfer process, frontier MO theory, theoretical structure elucidation and various experimental analyses. This work explained experimentally for the first time how hydrogen is consumed in the defect formation. Coordinate bond between Zn and S was also observed in the sandwich materials which is rarely found in previously reported materials, which was clearly explained by the MO theory in this present work. The sandwich material GO-ZnS has a superior photocatalytic activity over the GO and ZnS materials which are due to the transfer of electron from the excited ZnS to GO sheets through the nanogates structure.

The formation of the hetero nanogates structure in the GO-ZnS sandwich materials will have a huge potential in the field of drug delivery, biocompatible devices, solar cell, energy storage, water splitting etc. (Patent: IN 201711033660).



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Selective synthesis of WO₃ and W₁₈O₄₉ nanostructures: Simple inorganic routes for the synthesis of WO₃ and W₁₈O₄₉ nanostructures with variable size and self-assembly were reported. The morphologies and formation of stoichiometric WO₃ as well as substoichiometric W₁₈O₄₉ single-crystal phase were controlled by changing the pH of the reactions medium. This synthesis strategy has the advantages that it is one step, aqueous medium-based, and requires no surfactant or stabilizing agent.

Furthermore, it enabled the self-assembly of 1D nanorods of WO₃ and W₁₈O₄₉ into hierarchical nanostructures as nanorods bundles, cocoons, urchins, fishbones, etc. This synthesis method may open up a new way to control and tune the stoichiometric and substoichiometric composition of metal oxide nanostructures. Efficient sunlight-driven photocatalytic performance to degrade Rhodamine B (100 mL; 40 mg L⁻¹) with these tungsten oxide nanostructures was also demonstrated (*CrystEngComm*. 2017, 19, 2096).

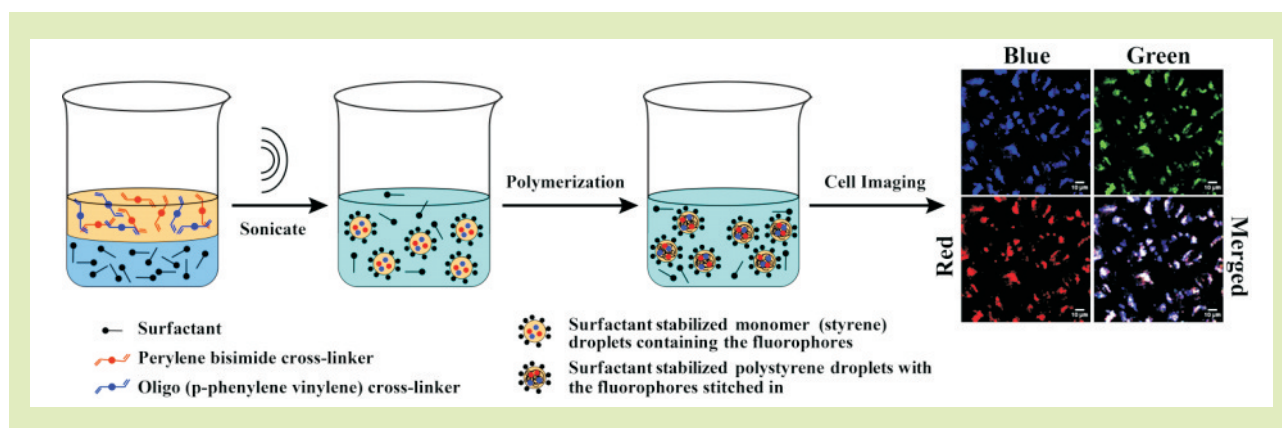
Advanced Materials

Functional materials

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

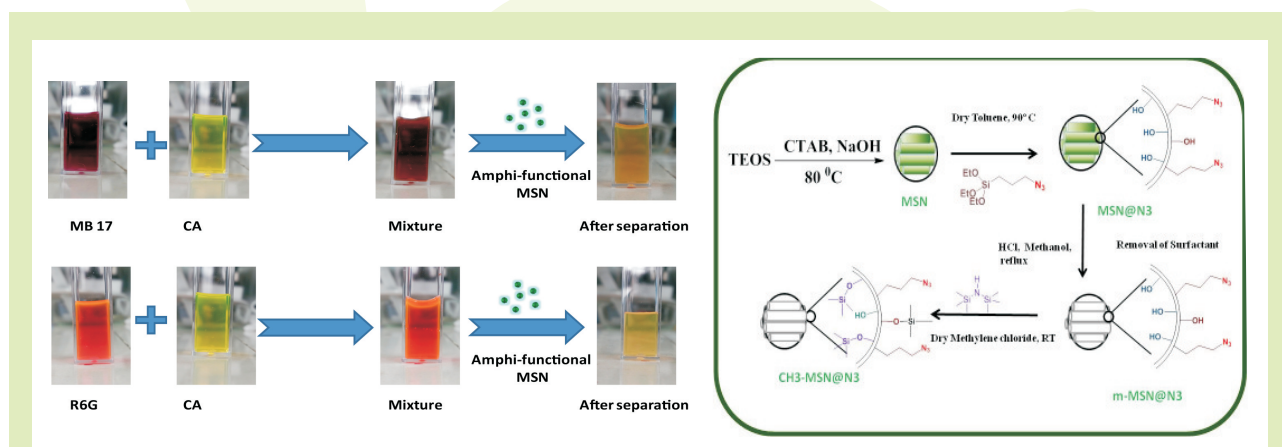
Fluorescent polystyrene beads for bioimaging applications: Fluorescent Polystyrene (PS) nanobeads in the size range $\sim 70 - 120$ nm incorporating perylene bisimide (PBI-PS) and oligo (p-phenylene vinylene) (OPV-PS) were developed by mini emulsion polymerization technique. The covalent incorporation

of the fluorophores ensured the absence of dye leakage and the PS in addition to being biocompatible also reduced aggregation induced self-quenching of fluorescence of the dyes. These fluorescent PS nanobeads could access multiple excitation wavelengths for imaging applications. The ability for multicolor imaging showed the potential to overcome the cellular autofluorescence and to enhance the resolution contrast of the image (*ACS Biomater. Sci. Eng.* **2017**, *3*, 1788).



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Amphi-functional mesoporous silica nanoparticles for dye separation: Amphi-functional mesoporous silica nanoparticles were synthesized by a stepwise chemical modification approach. These surface functionalized porous adsorbents/ carriers could selectively uptake particular single dye out of mixture of dyes (*J. Mater. Chem. A* **2017**, *5*, 14914).



Schematic of amphi-functional mesoporous silica synthesis strategy and its use for selective separation of the dyes from mixture of dyes

Advanced Materials

Functional materials

Janardan Kundu j.kundu@ncl.res.in

Functional nanomaterials for applications in energy and environment: The synthetic strategies for preparing metallic dendrites (monometallic, bimetallic) that found useful applications in catalysis and self-cleaning surfaces were reported. These nanostructures have potential for acting as material

for making "Dry Urinals". The synthesis of metal-semiconductor heterostructures (Ag-Cu₂O) for applications in chemical sensing and cleaning waste water utilizing photocatalysis was reported. The group had also recently reported on Mn²⁺ doping of 2D layered perovskite material for lighting applications (RSC Adv. **2016**, 6, 8416; ChemistrySelect **2017**, 2, 5552; CrystEngComm. **2017**, 19, 1669; Chem. Mater. **2017**, 29, 7816).

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

Sintered ceramic magnetostrictive materials: Ceramic magnetostrictive smart materials were extensively studied for their wide range of technologically driven applications. Cobalt ferrite is one of the important ceramic magnetostrictive materials with potential applications. It was shown that the magnetostriction parameters of sintered cobalt ferrite can be tuned by selective replacement of Fe by other divalent or trivalent ions in the tetrahedral and octahedral coordination environments in the spinel ferrite lattice. Co-substitution of divalent ions in cobalt ferrite was found to give higher strain sensitivity and high magnetostriction strain at low magnetic fields, at low degrees of substitution (*J. Appl. Phys.* **2017**, 121, 93904; *Mater. Lett.* **2017**, 192, 169).

Structure-property correlation studies on magneto-electric materials: Magnetolectric materials showing coupled magnetic and electric orders are interesting materials with potential applications. Bismuth ferrite, BiFeO₃ is one of the very few room temperature magnetolectrics. Due to the poor magnetic parameters, magnetolectric coupling is very low in bismuth ferrite and therefore, the material is not much useful for practical applications. Simultaneous substitution for Bi and Fe in BiFeO₃ is a suitable method for tuning of the magnetic and electrical properties. It was found that enhanced magnetic and dielectric properties can be obtained in the morphotropic phase boundary region containing both rhombohedral and orthorhombic phases (*Mater. Res. Exp.* **2017**, 4, 16104).

Sapna Ravindranathan s.ravindranathan@ncl.res.in

Host-guest systems: One of the methods to control conformational flexibility is the formation of host-guest inclusion complexes of triphenyl amine TPA derivatives with different macrocyclic hosts like cyclodextrin (CD), cucurbit[7]uril (CB[7]) etc. The CB[7] and β-CD based inclusion complexes of a unique TPA derivative, with two decoupled excited states were examined. It showed dual emission behavior in solution at room temperature. A detailed NMR study of the association and dynamics of the host-guest systems formed by host molecules β-Cyclodextrin (β-CD) and cucurbit[7]uril (CB[7]) with a newly synthesized triphenylamine derivative (1) showed that

the two host molecules form inclusion complexes that are significantly different in character. CB[7] formed a 1:3 host-guest complex while a 1:1 complex was formed by β-CD. The latter complex exists in a dynamic equilibrium in which only one of the three arms of 1 was bound to a β-CD molecule at a given time. The structural and dynamics information obtained by NMR readily correlated with the emission behavior of the two inclusion complexes (*J. Org. Chem.* **2016**, 81, 512).

Silk Fibroin Sophorolipid gelation mechanism: An aqueous solution of silk fibroin (SF) undergoes gelation over a period of few days to weeks. Addition of sophorolipid which is a biosurfactant reduces the gelation time to 2-3 hours. Since sophorolipid (SL) from *candida bombicola* is largely comprised of acidic

Advanced Materials

Functional materials

(ASL) and lactonic (LSL) forms, the interaction of SF with each of these forms independently and as a mixture (MSL) was investigated. NMR studies helped to understand the differences in the nature of molecular self assembly in the different types of sophorolipids. The difference in the self assembling

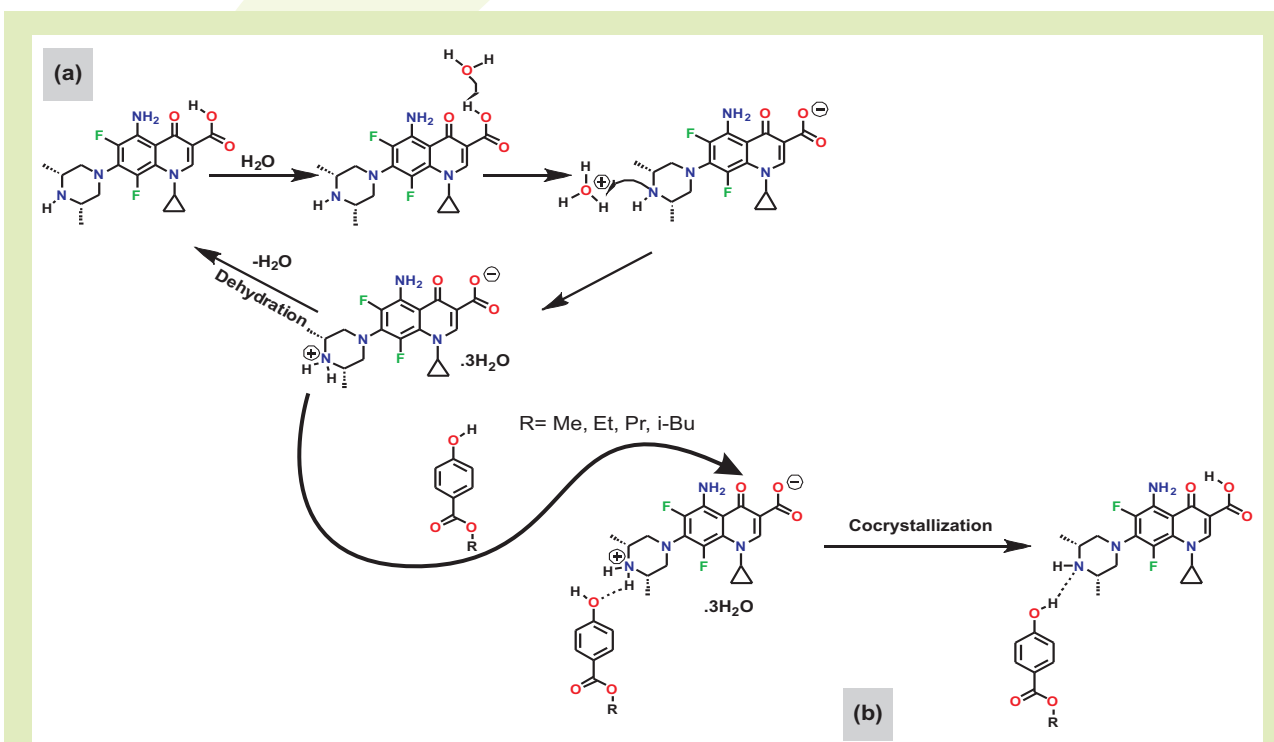
behavior also led to differences in their interactions with SF. The rate of gelation followed the order LSL+SF > MSL+SF > ASL+SF >> SF. It was showed that preferential binding of LSL to SF results in rapid unfolding of the SF chain thereby accelerating the gelation process (*Biomacromolecules* **2016**, *17*, 3318).

Biomaterials

Ashwini Kumar Nangia ak.nangia@ncl.res.in

Crystal engineering of a zwitterionic drug to neutral cocrystals: Crystal engineering of the neutral form of an important floxacin drug via a phenol-amine heterosynthon was demonstrated. The O–H...N hydrogen bond drives the migration of the proton from the zwitterionic structure to the neutral drug molecule in the cocrystal with paraben. All cocrystals showed enhanced dissolution profiles compared to the

zwitterionic and neutral forms of SPX. This method can be specifically used for oral drug delivery of amphoteric drugs in the neutral form and high solubility (good bioavailability and absorption rate). There are several antibacterials, anti-allergies and diuretics as amphoteric drugs, which occur as zwitterions in the solid state with poor membrane permeability. Therefore cocrystallization of these drugs could stabilize the neutral form with improved solubility (*Chem. Commun.* **2016**, *52*, 12610).



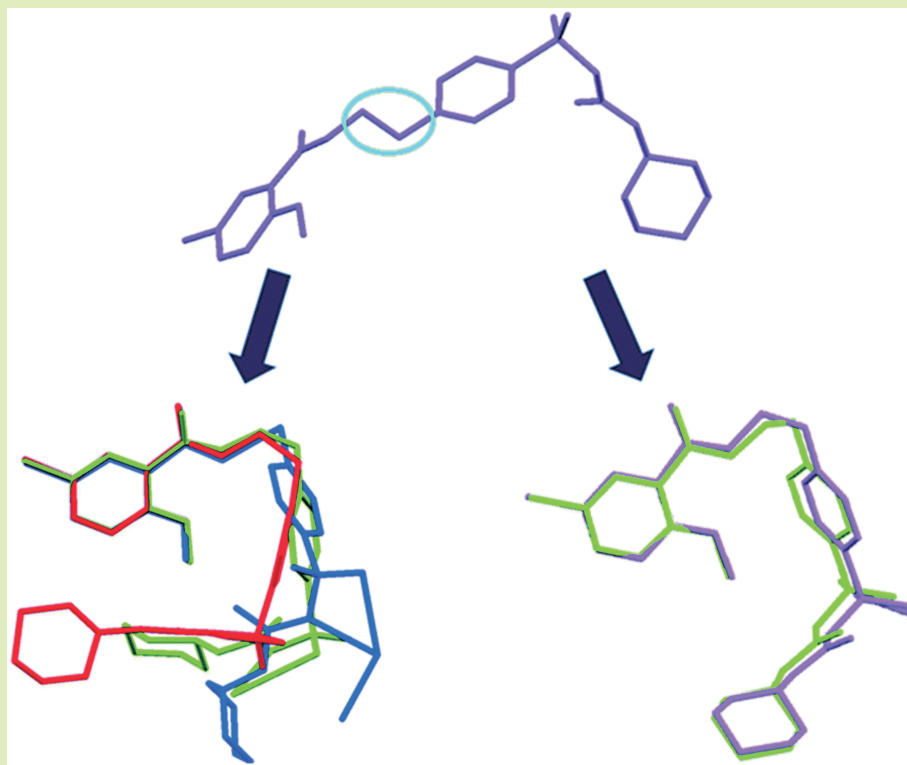
Proposed mechanism of (a) neutral to zwitterion transformation of SPX in the presence of water. (b) Zwitterion to neutral form of SPX conversion in the presence of paraben cocrystal.

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Biomaterials

Polymorphism, isostructurality and physicochemical properties of glibenclamide salts: Driven by aim to enhance the solubility of glibenclamide salts such as Na, K and NH₄ were synthesized. The products were characterized by different spectroscopic, thermal and diffraction techniques as well as X-ray crystal structures. The crystal structure of GBA-Na form I showed a square pyramidal geometry while forms II and III adopt a distorted octahedral geometry of the central sodium ion. Dimorphism of GBA-Na was the first example of polymorphism for sulfonyl urea salts in the CSD. XPac analysis, powder diffraction and packing similarities showed that GBA-Na form I and GBA-NH₄ and GBA-K form I and GBA-NH₄ were isostructural with similar packing and powder

XRD pattern by exchange of the monovalent cations. Thermal analysis and controlled heating showed conversion of GBA-Na form III and GBA-K form II (hydrates) into their anhydrate form I. GBA salts exhibited excellent solubility in water and phosphate buffer media. These salts adsorbed water (0.4 to 6.2% range) at high humidity but showed weight loss in the desorption cycle. Thus these crystalline forms were reversible without any hysteresis. The solubility and stability of glibenclamide salts increased in the salts with GBA-K form I exhibiting good stability and high solubility for pharmaceutical development (*CrystEngComm* 2017, 19, 918).



Overlay of GBA molecule extracted from the crystal structure of the guest free form (purple), GBA-Na form I (green), GBA-Na form II (red), GBA-Na-H₂O form III (blue), GBA-K form I (magenta), and GBA-NH₄ (light green).

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CMC grafted mesoporous silica nanogels for enhanced cellular uptake and release of curcumin: Amine functionalized mesoporous silica nanoparticles (MSNs) were synthesized which were further reacted with carboxylic groups on carboxymethyl cellulose

(CMC) using EDC coupling chemistry. Synthesis of MSNs with a particle size of 120-130 nm and pore size of 2-3 nm was confirmed from TEM, SEM and N₂ adsorption-desorption studies. The external surface of MSNs was grafted with amine moieties which were then reacted with the carboxylic groups on CMC using EDC coupling chemistry. The pores of the MSN were incubated with hydrophobic drug curcumin,

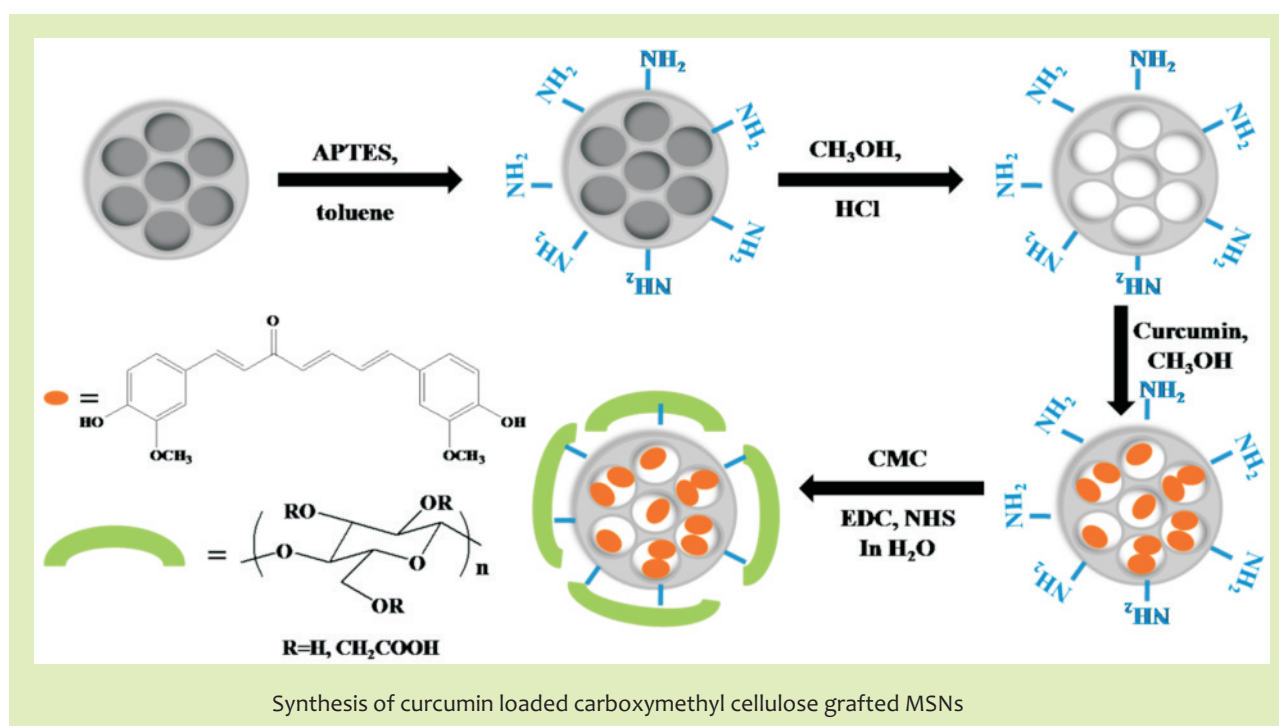
Research & Development

Advanced Materials

Biomaterials

which has both anticancer and antibacterial activity. The drug release profile in 0.5% SLS solution showed only 15% release of curcumin molecules from MSN-cur-CMC as compared to that of 45% from MSN-cur-NH₂ over a period of 72 h. This showed that CMC helped in preventing curcumin molecules from premature leaching over a longer period of time. MTT assay showed negligible toxic effect of MSN-NH₂ and MSN

-CMC on breast cancer cell line MDA-MB-231 up to a concentration of 200 µg/ml, thus indicating the biocompatibility of the functionalized MSNs. Curcumin loaded CMC functionalized particles showed enhanced cellular uptake and per cent cytotoxicity of MSN-cur-CMC compared to that of MSN-cur-NH₂ as observed in the MTT assay (from GI₅₀ values) and fluorescence studies on the breast cancer cell line MDA-MB-231



All the mentioned observations indicated that CMC grafting on the surface of MSN enhanced the cellular uptake and cytotoxicity of the cells at remarkably less concentration of curcumin molecules. This showed that MSN-CMC nanogels could be used as a model system successfully for the enhanced cellular uptake and drug delivery of hydrophobic moieties.

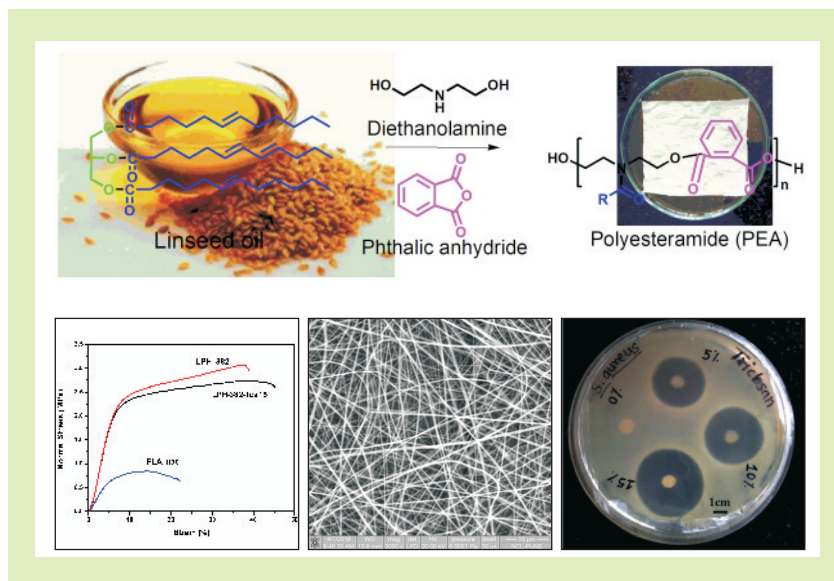
G. V. N. Rathna rv.gundlori@ncl.res.in

Mechanically strong nano-matrices of linseed oil based polyesteramide blends: New nanomaterials of bio-origin with improved mechanical properties are in demand for biomedical application. Therefore, it was proposed to develop bioactive nano-matrices using polyesteramides. Polyesteramide was synthesized from linseed oil and blended with poly (L-lactide) and human serum albumin and fabricated nano-matrices

with antibacterial drugs, triclosan and metranidazole. The morphology of the bioactive nano-matrices represented smooth and fine nanofibers, which were non toxic and antibacterial. The uniqueness of the developed nano-matrices of polyesteramide blends is that their mechanical strength is 3-fold higher than the nano-matrices of poly (L-lactide), which is one of the essential features of these to be used as a biomaterial for biomedical application (*MedChemComm* **2016**, 7, 2299).

Advanced Materials

Biomaterials



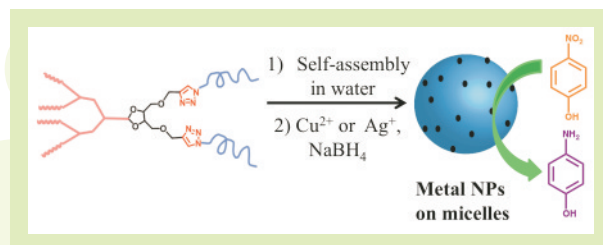
Polymers

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Metal nanoparticles stabilized by polymeric micelles in water: Conversion of toxic pollutants in water effluents into relatively benign and useful chemicals is important for water management. Copper and silver nanoparticles were fabricated in aqueous solution using micellar assemblies of dendritic amphiphiles containing triazole rings that were synthesized using click chemistry.

The micelle-stabilized nanoparticles, at ppm concentrations, efficiently catalyzed the reduction of up to 1 ppm of 4-nitrophenol to 4-amino-phenol in aqueous solution (*New J. Chem.* **2017**, *41*, 4546)



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

Organometallic chemistry of small and macromolecules

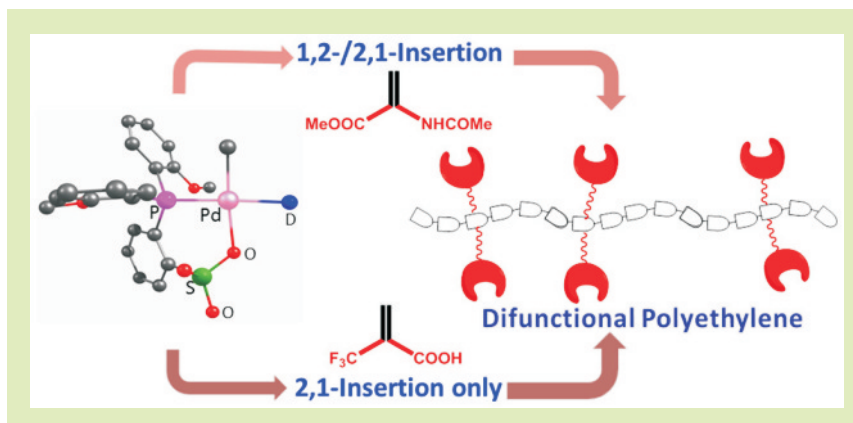
Water loving polyethylene: More than half of the total polymers produce is polyethylene or the humble carry-bag. The usual water hating polyethylene cannot be used for applications such as paints, primers and adhesives. A catalyst and a process to make water loving polyethylene was developed (*Macromolecules* **2017**, *50*, 5748; *Inorg. Chem.* **2017**, *56*, 12448).

Chemicals and polymers from renewable resources:

The organometallic catalysts were tailored to refine plant oils to feed stock chemicals and sugars to polymers. A case of converting non-edible cashew nut shell liquid based oil to useful monomers and polymers was reported. The second case in consideration is utilization of sugars to make degradable polymers (*ChemCatChem* **2017**, *9*, 3997; *Green Mat.* **2017**, *5*, 63).

Advanced Materials

Polymers



Composite materials

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Development of shear thickening fluids for personal protective system: Conventional body armor materials are typically comprised of many layers of polyaramidpoly (phenylenediamine terephthalamide) fabric sold by DuPont under the registered name of Kevlar®, with optional ceramic tile inserts. These materials are too huge and rigid for application in extremities protection. Therefore, there is a need to

Reinforced cellulose papers with enhanced tear strength: Strategies to enhance tear strength of papers include adding various wet and dry strengthening resins, coating the paper with varnish, laminated paper containing synthetic polymer layer in between cellulosic layers. Reinforced cellulosic papers with 50% higher tear strength and 40% higher tensile modulus were developed by incorporating only 20 wt% nanocellulose fibrils derived from waste cotton rags. The increase in specific surface area arising from reduced fibre diameter enhanced colloidal interaction, mechanical interlocking and hydrogen bonding between the fibres when water was drained out. Nanocellulose reinforced paper was processed in existing paper machinery that did not contain any synthetic polymer and also provided additional advantages in smoothness and folding endurance apart from tear strength.

develop a material which can offer the equivalent ballistic performance of existing body armor materials with significantly more compactness and flexibility. Monodispersed silica nanoparticles were synthesized at pilot scale using 20 L stirred glass reactor having particle sizes of 500 nm, 250 nm, 125 nm etc. 5 kg monodispersed silica nanoparticles material was supplied to TBRL, Chandigarh. A novel methodology has been established for the preparation of shear thickening fluids (STF) using monodispersed silica nanoparticle and polyethylene glycol.

Kadhiravan Shanmuganathan k.shanmuganathan@ncl.res.in

Cellulose or melanin fibres with enhanced dye uptake: Melanins constitute a class of bio-macromolecules that are abundant in nature. Their unique molecular structure has precluded their dissolution in common solvents and facile processing into functional materials. It was found that commercially available 40 wt% tetrabutyl ammonium hydroxide solution (TBAH) yielded stable solutions of synthetic and natural melanins at ambient conditions and the dissolution rate was accelerated by microwave radiation. Since the same solvent dissolved the most ubiquitous biopolymer cellulose, composite fibres of cellulose/ melanin were successfully prepared and these fibers exhibited significant dye absorption capacity (62% reduction) with methylene blue (*Green Mater.* **2017**, *5*, 85).

Advanced Materials

Materials for environmental and healthcare applications

Bhushan Pradosh Chaudhari bp.chaudhari@ncl.res.in

Biosynthesis of nanoparticles for healthcare and diagnostics applications: A one pot green protocol was demonstrated for the synthesis of highly monodispersed silver nanoparticles using leaves of *Salvadora persica* plant. When the leaf extract of *Salvadora persica* plant reacted with silver nitrate (AgNO_3) solution, it resulted in the synthesis of highly monodispersed silver nanoparticles with an average size of 3 nm. These nanoparticles were then characterized by UV-Visible spectroscopy, Transmission Electron Microscopy, Energy Dispersive Analysis of X-Rays, X-ray diffraction analysis and Fourier Transform Infrared analysis. These nanoparticles can be used for various healthcare applications like anti-infectious, drug delivery, sensor etc.

Guruswamy Kumaraswamy g.kumaraswamy@ncl.res.in

Lipid nanoparticles for improved pesticide delivery: Agricultural run-off due to pesticide overuse contaminates soil and ground water, posing a significant environmental challenge. Since leaves are coated with a microcrystalline layer, they repel aqueous pesticide sprays, leading to excessive spraying of pesticides. An aqueous nanoparticle dispersion of food grade was demonstrated, non-toxic lipids exhibits significantly enhanced retention when impinging on a hydrophobic surface. Lipid nanoparticles enhance drop adhesion by changing the surface wettability. They diffuse to the leaf surface and reorganize to form a thin wetting film within the millisecond time scales of drop impact. Lipid nanoparticle drops do not roll off inclined lotus leaf surfaces and form continuous films on spraying.

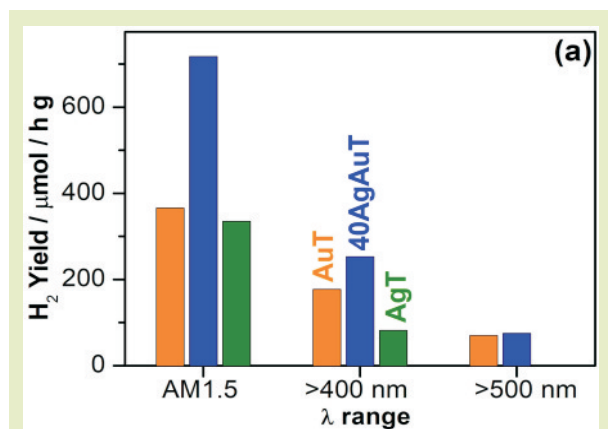
Advanced Materials

Materials for energy

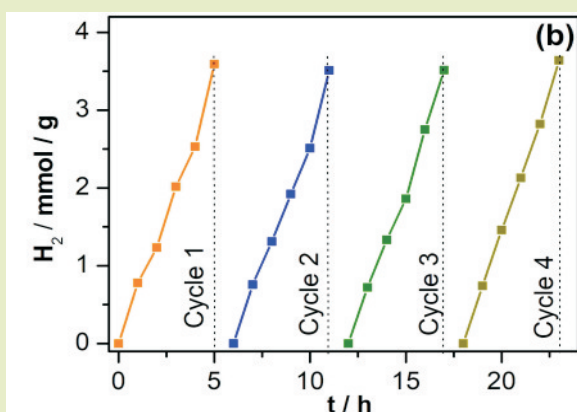
C. S. Gopinath cs.gopinath@ncl.res.in

Solar energy conversion and solar water splitting

Solar water splitting: Photocatalytic production of hydrogen was demonstrated using a semiconductor bimetal (Ag-Au) nanocompo-site, namely, Ag-Au/TiO₂. Metal-metal and metal-semiconductor junction property is essential for solar hydrogen generation activity. Hydrogen production was shown with >500 nm filtered light and it demonstrated the role of gold (*ChemCatChem* **2016**, 8, 3294).

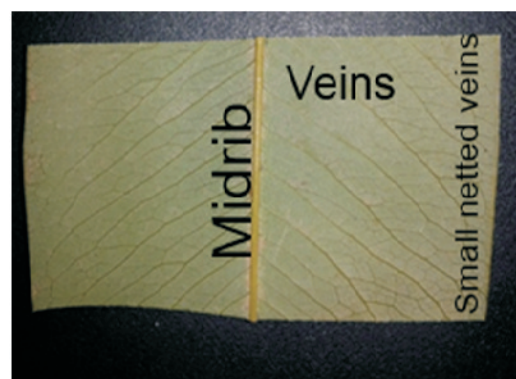


Photocatalytic H₂ evolution activity of bimetallic Ag-Au/TiO₂



Sustainable activity demonstrated for 24 h and after every 5 h the gaseous products are evacuated.

Green leaf to inorganic leaf: Is it possible to use green leaves, available freely in our gardens, as a template for making inorganic leaf, while retaining the nanospace available within the leaf architecture? The answer is 'yes'. It was demonstrated with inorganic leaf made up of ZnO, by intercalating Zn²⁺ ions into the porous channels of the champa (*Plumeria, Magnolia champaca*) tree leaves. TEM studies revealed a variety of macro-micro-nanospace available in the inorganic leaf ZnO (IL-ZnO), and suggested the possibility of exploiting the same to produce natural nano-architecture for various applications. A speciality of the present work is the maximum suppression of defects in photoluminescence of IL-ZnO leaf, compared to the commercial ZnO, which was exploited for light harvesting through chemical conversion. Benzene to phenol conversion was studied in UV light and IL-ZnO showed significant conversion and yield demonstrating C-H activation at ambient temperature (*J. Nanosci. Nanotechnol.* **2016**, 16, 9203).



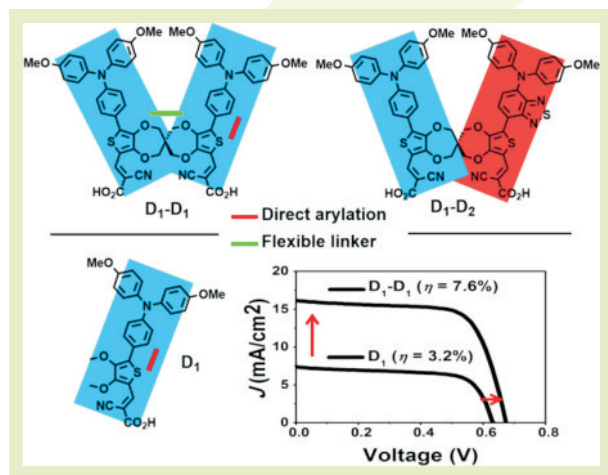
A typical cut-piece of fresh leaf from champa tree. Entire (above); a typical inorganic ZnO leaf (below)

Materials for energy

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Orthogonally functionalized donor/acceptor homo- and heterodimeric dyes for dye-sensitized solar cells:

A series of homodimeric (D_1 - D_1 and D_2 - D_2) and heterodimeric (D_1 - D_2 and D_2 - D_1) donor/acceptor (D/A) dyes was designed and synthesized containing spiroBiProDOT π -spacer by utilizing Pd-catalyzed direct arylation reaction. It correlated the device performance with monomeric dyes (D_1 and D_2). Both the thiophenes (π -spacer) of spiroBiProDOT were functionalized with same or different donor groups which led to homodimeric and heterodimeric chromophores in a single sensitizer. The homodimeric spiro-dye D_1 - D_1 showed higher power conversion efficiency (PCE) of 7.6% with a open-circuit potential (V_{oc}) and photo current density (J_{sc}) of 0.672 V and 16.16 mA/cm². The monomeric D_1 exhibited a PCE of 3.2% (V_{oc} of 0.64 V and J_{sc} of 7.2 mA/cm²), which is lower by 2.4 fold compared to dimeric analogue (ACS Appl. Mater. Inter. **2017**, 9, 34875).

**Interplay between π -bridge and position of branched-alkyl groups of unsymmetrical D-A-D- π -A squaraine in DSSC:**

Far-red absorbing squaraines possessing high molar absorptivity ($>10^5$ M⁻¹ cm⁻¹) are being attracted as high efficiency chromophores in dye-sensitized solar cell (DSSC). A series of donor-acceptor-donor- π spacer-acceptor (D-A-D- π -A) unsymmetrical squaraines, PSQ1-5, with indoline donor, and squaric/cyanoacetic acid acceptor units were designed for sensitized solar cells. Benzene (PSQ1-2) and thiophene (PSQ3-5) π -spacers and out-of-plane branched alkyl groups

at the indoline which is away (PSQ1, PSQ3 and PSQ5) or near (PSQ2 and PSQ4) anchoring group were introduced to extend the absorption towards near-infrared region and controlling orientation on TiO₂ surface. Dynamic aggregation tendency of PSQ1 and PSQ3 than their isomers systematically modulated the orientation on the TiO₂ surface that enhanced photovoltaic performance. DSSCs sensitised with PSQ5 achieved a PCE of 8.15% under simulated AM 1.5G illumination (100 mW cm⁻²), with a current density (J_{sc}) and open-circuit voltage (V_{oc}) of 19.73 mA cm⁻² and 630 mV. A clear comparison of incident photon-to-current conversion efficiency (IPCE) versus light harvesting efficiency correlated the structure-property relationship with J_{sc} obtained for PSQ dyes (ACS Appl. Mater. Inter. **2017**, 9, 32698).

Molecular control of overpotential and recombination process in donor-acceptor hemicyanine sensitized solar cells:

A series of donor-acceptor (D-A) hemicyanine dyes was synthesized utilizing a planar heterotriangulene (HT) or triphenylamine (TPA) donor and alkyl functionalized indolium carboxylic acid acceptor unit. The photophysical, and electrochemical properties of D-A dyes are significantly modulated by introducing strong HT donor instead of TPA. The strong donor nature of HT and effective passivation of surface by hydrophobic alkyl chains close to the anchoring group for NC3 dye exhibited an average PCE of 4.34% with a V_{oc} of 0.416 V, J_{sc} of 20.04 mA cm⁻², and fill factor (ff) of 52.03% under simulated AM 1.5G illumination (100 mW cm⁻²) without 3 α ,7 α -dihydroxy-5 β -cholic acid co-adsorbent (J. Phys. Chem. C. **2017**, 121, 21836).

Heterotriangulene-based unsymmetrical squaraine dyes:

Unsymmetrical squaraine sensitizers with two different donor moieties, triphenylamine and heterotriangulene (NSQ1-3), for dye-sensitized solar cell were designed and synthesized. These dyes utilized the indolium moiety to control charge recombination dynamics at TiO₂-dye-electrolyte interface by connecting linear and branched alkyl functionalities. An efficient heterotriangulene donor and branched alkyl group at sp³-C atom were strategically incorporated to increase the power conversion efficiency of zwitterionic dyes by improving photocurrent density (J_{sc}) and open-circuit potential (V_{oc}) of the cell. Among these four dyes, NSQ3 exhibited

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the highest efficiency of 6.73% with a J_{sc} of 18.74 mA/cm², V_{oc} of 0.53 V, and fill factor (ff) of 68.3%, without any co-adsorbent under irradiance of 100 mW/cm² (AM 1.5G sunlight). In presence of chenodeoxycholic acid, NSQ1, NSQ2 and NSQ3 showed efficiency of 7.07%, 7.38% and 7.14%, respectively. Despite the low V_{oc} , far red light harvesting efficiency, reduced dye aggregation, long life time (t) of

injected electron and high quantum efficiency (QE) played constructive role to achieve high PCE efficiency. Deceleration of charge recombination for NSQ dye cells were further studied by electro-chemical impedance spectroscopy and open-circuit photovoltage decay measurements of DSSC devices (*J. Mater. Chem. A* **2016**, *4*, 18910).

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Renewable Energy

Blocking layer to improve DSSC efficiency: Dye regeneration and recombination of electrons residing in photoanode with that of electrolyte are two key events impacting the DSSC efficiency. A polymer-graphene composite with specific band edges was used to improve the rate of dye regeneration and decrease the recombination. The efficiency of the DSSC was found to be 10.4% (*Chem. Commun.* **2017**, *53*, 6629).

Compressible supercapacitor: Devices with flexibility and compressibility are required for the wearable electronics. A cross-linked polymer gel was found to be compressible. However, they are not conducting. Green tea extract was used as reductive coating to coat gold. PEDOT was used as capacitive material. The capacitors efficiency didn't vary as a function of compression and expansion (*J. Phys. Chem. C* **2017**, *121*, 3270).

Band edge modulated polymer to enhance DSSC efficiency: A polymer with specific HOMO and LUMO

energy levels was identified in order to decrease the recombination in the DSSC. This polymer blocked the electron transfer from photo anode to the electrolyte due to unfavorable energy levels. The DSSC efficiency with the polymer was found to be ~ 25% higher than that of the cells without polymer (*Adv. Energy Mater.* **2016**, *6*, DOI:10.1002/aenm.201502334).

Hydrophobic blocking layer to enhance OPV efficiency: In organic solar cells, PEDOT-PSS has been widely used as hole transport layer (HTL). This layer is hydrophilic. On the other hand, photoactive layers are hydrophobic. Thus, there is a mismatch between photoactive layer and HTL. SDS micelles were disassembled on top of PEDOT to prepare HTL. The hydrophobic HTL imparted gradation to donor and acceptor increased the efficiency of the cells by 22% (*Chem. Commun.* **2016**, *52*, 3486).

BODIPY polymer with high charge transport

BODIPY is a fluorescent molecule with poor charge transport properties. BODIPY polymer showed an impressive hole mobility of 0.01 cm²/Vs due to combination of dipole and quadrupole. It is a likely candidate for energy conversion (*J. Phys. Chem. C* **2016**, *120*, 26199).

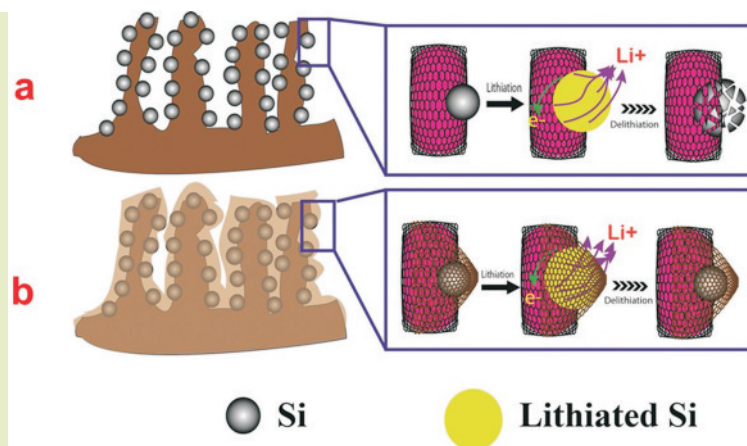
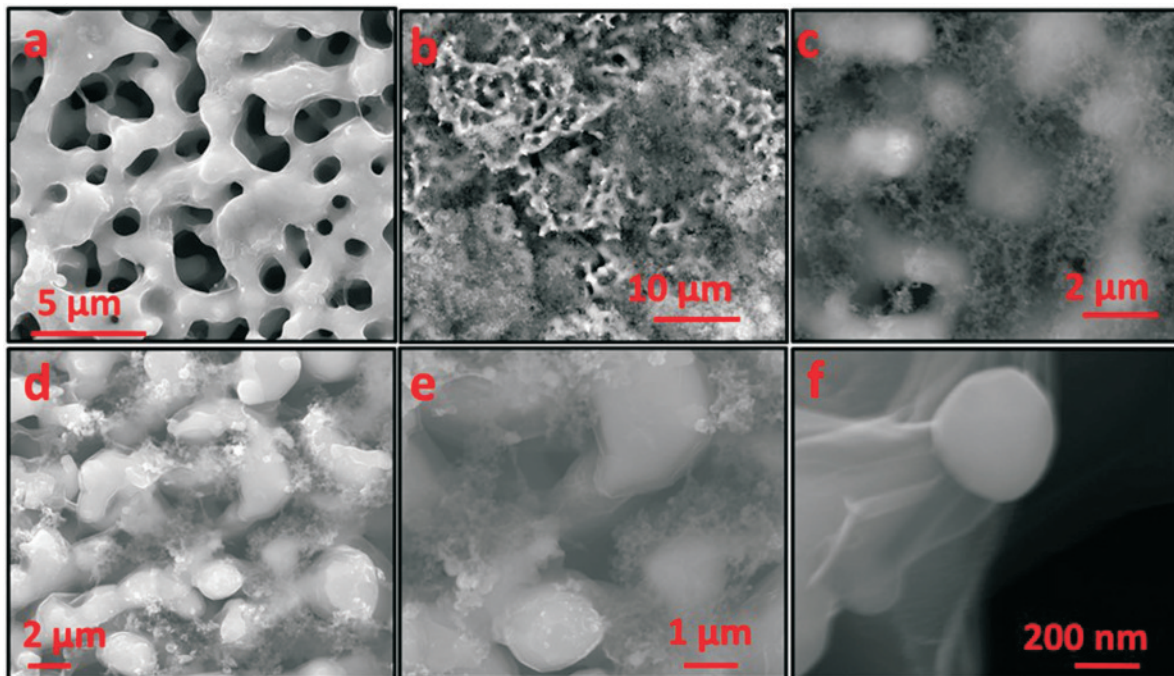
Advanced Materials

Materials for energy

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Facile synthesis of 3D anode assembly with Si nanoparticles : An innovative 3D electrode assembly was fabricated in an effort to tame volume expansion and structural disintegration during cycling that involved continuous layer of graphene coated on porous current collector and Si nanoparticles sealed in as an active material. Graphene deposition and pore formation in metal current collector was achieved in a unique single step synthesis. All the active components

like current collector, reacting material, and conducting material were manipulated in a way to produce synergistic architecture in a chemical vapor deposition process. Highly pure graphene deposited in this process enabled efficient electron transfer from all over of the surface of silicon nanoparticles and prevented continuous solid electrolyte interphase layer formation. This binder free anode assembly showed extremely stable lithium storage performance for over 1000 cycles with 88% of initial capacity retention and 100% Coulombic efficiency (*Adv. Mater. Interfaces* **2017**, *4*, 1601043).



Characterization and Schematics representation (lithiation/delithiation) of si-nanoparticles in 3D anode assembly

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Facile synthesis and electrochemical evaluation of PANI/CNT/MoS₂ ternary composite: Synthesis of a novel ternary composite consisting of polyaniline (PANI), functionalized multi-walled carbon nanotubes (CNTs) and molybdenum disulfide (MoS₂), via an in-situ polymerization method was reported. Detailed structural and electrochemical characterization showed that incorporation of a small amount of MoS₂ in PANI/CNT composite tended to eliminate agglomeration problem of CNT. The PANI/CNT/MoS₂ ternary composite reached a specific capacitance of 350 F/g at the current density 1 A/g corresponding to a 5% MoS₂ content. This ternary composite showed good cycling stability even at a higher energy density of 10 A/g. Further, PANI/CNT/MoS₂ composite electrode showed higher energy density (7.77 Wh/kg) and power density (2140 W/kg) as compared to PANI/CNT composite without MoS₂ (*Mater. Sci. Eng. B* **2017**, 223, 24).

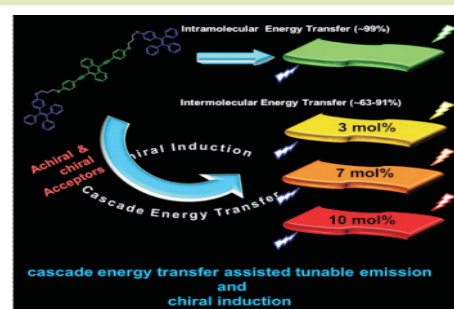
One-step synthesis of MoS₂-CuS composite with high electrochemical activity: A one-step in-situ solvothermal method was developed to synthesize MoS₂-CuS composite. MoS₂ sheets increased the electron transfer ability assisting the improvement in catalytic activity of the MoS₂-CuS counter electrode. The charge transfer resistance derived from impedance spectroscopy for MoS₂-CuS composite counter electrode at the electrode/electrolyte interface was very low, when compared to MoS₂, mostly due to more number of active catalytic sites for the reduction of polysulfide electrolyte. Tafel polarization plot showed excellent electrocatalytic activity of MoS₂-CuS composite towards the polysulfide electrolyte. Finally the CdS/CdSe sensitized solar cell achieved a power conversion efficiency of about 5 % upon optimization of MoS₂-CuS composition (*ChemElectroChem*. **2017**, 4, 1984).

Co-catalytic metal oxide nanoparticles decorated silicon/ hematite core shell nanowire arrays: A co-catalytic nanoparticles decorated Silicon nanowire (SiNWs)/ Hematite (Fe₂O₃) core shell structures were fabricated as photo anodes and studied the PEC water oxidation properties. As Fe₂O₃ possessed weak oxidation kinetics, decoration of NiO

and Co₃O₄ nanoparticles on SiNW/Fe₂O₃ by hydrothermal method acted as co-catalysts improving the water oxidation reactions. It was found that decoration of Co₃O₄ nanoparticles enhanced the photocurrent up to 2.6 times, whereas for NiO nanoparticles improvement is of 1.5 times when compared to the undecorated electrodes. Along with enhancement of photocurrents, it also showed shift of onset potentials. The effect of the co-catalytic nanoparticles on the enhancement of photocurrent and charge transfer resistance at the interface of electrode-electrolyte was studied by electrochemical impedance spectroscopy. The flat band potentials of the photo electrodes were measured by using Mottschottky analysis (*ChemistrySelect* **2017**, 2, 2544).

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Cascade energy transfer from self- assembled nanosheet hybrids: In an attempt to improve the light harvesting efficiency of an acceptor doped assembly, a donor-acceptor-donor triad was designed and synthesized that exhibited an exceptional intramolecular energy transfer with ~99% efficiency. Moreover, a facile cascade energy transfer (energy funnelling) was observed in the presence of a series of second acceptors (63-91% efficiency) with tunable emission colors. Self-assembled nanosheets formed by the triad in the presence of acceptors, exhibit cascade energy transfer assisted tunable emission. In addition, use of chiral acceptors induced the chirality to the triad and resulted in the formation of chiral nanosheets along with cascade energy transfer. Here chiral induction, nanosheet formation and cascade energy transfer in the presence of chiral acceptor were used as a tool to probe the intercalation of acceptor molecules in the donor scaffold (*Chem. Commun.* **2017**, 53, 7072).



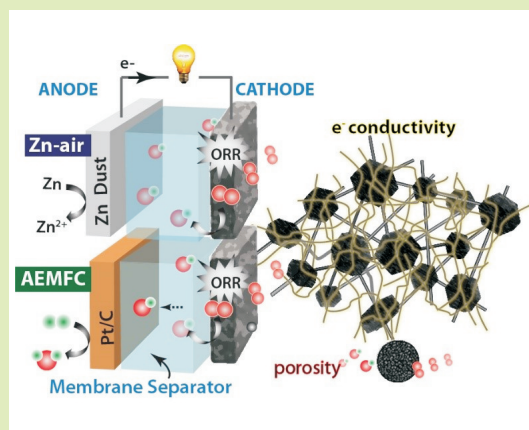
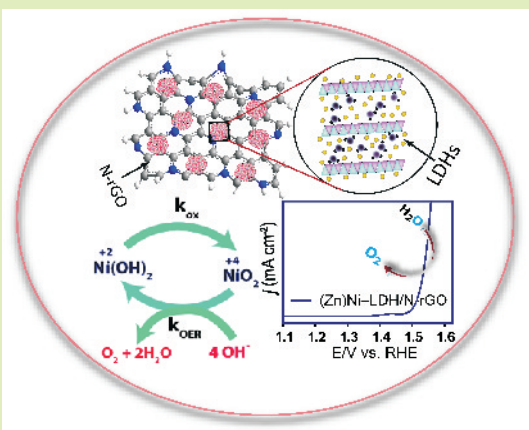
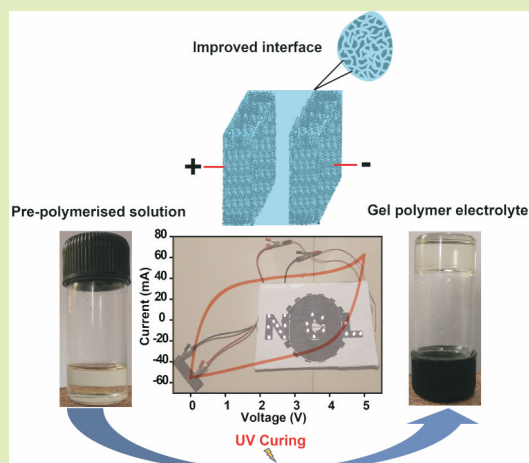
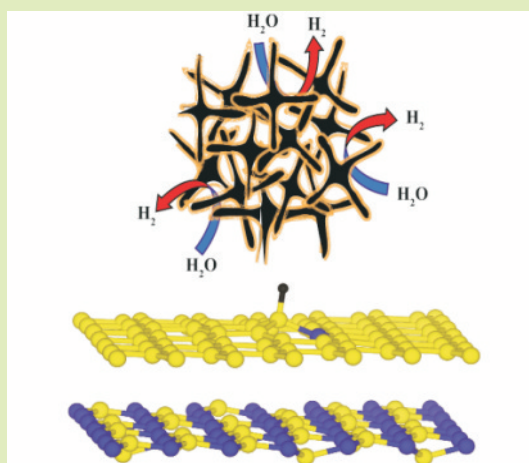
Advanced Materials

Materials for energy

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Electrode and electrolyte designing towards all-solid-state flexible supercapacitors: It was proved that polyaniline (PANI) is more apt to be adopted as the negative electrode in asymmetric SCs (ASCs). Such a device in which PANI and carbon are used as the negative and positive electrodes respectively exhibited stable electrochemical performance for more than 27000 continuous cycles with a high specific capacitance of 510 F/g corresponding to the PANI negative electrode. A Grafoil-Scotch tape-derived highly conducting flexible substrate was demonstrated as a potential SC electrode.

The practical utility of the substrate was demonstrated by fabricating a high-performance solid supercapacitor through electrodeposition of MnO_2 'nanograss' over the anodized substrate. Apart from the research in electrode materials, a major breakthrough in the device fabrication strategy was achieved. The *in-situ* synthesis of a non-aqueous solid-state gel polymer electrolyte (GPE) which can extend to the nano-regime of high surface area carbon was exhibited to mimic the electrode-electrolyte interface close to that of a liquid electrolyte. ASC device prepared by means of the *in-situ* strategy exhibited a specific capacitance of 111 F g^{-1} at a current density of 0.25 A g^{-1} , when operated at a voltage window of 2.5 V (*ChemElectroChem* **2016**, *3*, 1; *Nanoscale*, **2017**, *9*, 3593; *Mater. Chem. A*, **2017**, *5*, 8461).



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Electro catalysts for oxygen reduction reaction for fuel cell and zinc-air battery applications: Self-sacrificial Co-based ZIF was used to derive Co-embedded highly porous carbon/MWCNTs composite which was found to consistently perform in par with that of the standard Pt/C electrocatalyst when implemented in both Zn-air battery and AEMFC systems. CoMn alloy oxide nanoparticles supported on N-doped porous graphene was designed for ORR catalyst in alkaline medium displaying remarkably high ORR activity. This catalyst was used for fabricating and testing single-cells of an anion-exchange membrane fuel cell (AEMFC) and a primary Zn-air battery. A noble metal alloyed catalyst was developed having trigonal bipyramidal and truncated cube-type mixed morphologies, anchored on the nitrogen-doped graphene (CuPt-TBTC/NGr-90) exhibiting 2.1 times higher mass activity and 2.2 times higher specific activity, compared to Pt/C at 0.90 V (vs. RHE). A peak power density of 300 mW cm^{-2} was achieved by fabricating a zinc-air battery with this catalyst, showing much higher peak power density than that of the state-of-the-art Pt/C catalyst. The effect of Zn substitution in the cobalt ferrite matrix towards ORR was also explored and the obtained catalyst ($\text{CoFe}_{1.7}\text{Zn}_{0.3}\text{O}_4$ composite anchored over NGr) showed significantly low ORR onset potential (80 mV shift from the 20% Pt/C catalyst) (*ChemElectroChem*, **2017**, *4*, 1; *ACS Catal.* **2017**, *7*, 6700; *Nanoscale* **2017**, *9*, 9009; *ChemistrySelect* **2017**, *2*, 7845).

Electrocatalysts for oxygen evolution reaction and hydrogen evolution reaction: Several electrocatalysts were developed for improving the sluggish kinetics of the half-cell reactions of electrochemical water splitting, i.e. OER and HER, the anode and cathode reactions in a water electrolyzer, respectively. The synthesis of NiZn double hydroxide was reported over nitrogen doped graphene which is enriched with the OER active $\gamma\text{-NiOOH}$ phase. The thin, porous and open layered structure of the as synthesized (Zn)Ni-LDH/N-rGO augments the efficiency of the catalytic activity towards OER in alkaline medium. The very low over potential of 290 mV obtained at a current density of 10 mAcm^{-2} compared to the benchmark catalyst all the while possessing a low Tafel slope of 44 mV per decade made this catalyst an excellent candidate in real electrochemical water splitting devices. A highly efficient metal-free electrocatalyst for HER was reported. This catalyst was synthesized by the high-temperature annealing of graphene oxide-coated melamine foam. The low over-potential of 193 mV exhibited by the catalyst is far lower than that of the several other metal-free catalysts and some metal based catalysts reported elsewhere. Moreover, DFT studies were also performed which confirmed Volmer-Heyrovsky mechanism operated during HER (*Nanoscale* **2017**, *9*, 12590; *ChemElectroChem.* **2017**, *4*, 1).

Energy and Environment

Renewable and alternative energy technologies

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Effect of out-of-plane alkyl group's position in dye-sensitized solar cell efficiency: A series of indoline based unsymmetrical squaraine (SQ) dyes that contain alkyl chains at sp^3 C- and N- atoms of indoline moieties with a carboxylic acid anchoring group was 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, however, remarkable changes with respect to the power conversion efficiencies (PCE) were observed depending upon the position of alkyl groups in the dye. Careful analysis of incident photon-to-current conversion efficiency (IPCE) profiles indicated the presence of aggregated structure on the TiO_2 surface that contributed to the charge injection in the presence of a co-adsorbent. A dye-sensitized solar cell (DSSC) device made out of SQ5 was achieved an efficiency of 9.0%, with an open-circuit potential (V_{oc}) of 660 mV and short-circuit current density (J_{sc}) of 19.82 mA/cm^2 , under simulated AM 1.5G illumination (100 mW/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 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 (*ACS Appl. Mater. Inter.* **2016**, *8*, 35353).

Panchromatic sensitizer for dye-sensitized solar cells: Metal-free near-infrared (NIR) active unsymmetrical squaraine dyes, RSQ1 and RSQ2, with benzo-dithiophene (BDT) π -spacer and cyanoacrylic acid acceptor were synthesized by utilizing palladium catalyzed direct (hetero)arylation reaction. Methyl and 2-ethylhexyl groups were strategically placed at the BDT unit for RSQ1 and RSQ2 respectively, to investigate the effect of alkylated π -spacer on dye aggregation on the TiO_2 surface and recombination reactions at TiO_2 /dye/electrolyte interface. RSQ2 performed better than RSQ1 owing to its higher open-circuit voltage (V_{oc}) and fill factor (ff) in spite of having comparable short-circuit current density (J_{sc}). The panchromatic incident photon-to-current conversion efficiency (IPCE) response was also observed for both the dyes. RSQ2 showed power conversion efficiency (PCE) of 6.72% with short-circuit current density (J_{sc}) of 18.53 mA/cm^2 , open circuit voltage (V_{oc}) of 0.538 V, and fill factor (ff) of 67.4%, without any co-adsorbent. Attenuation of the charge recombination for RSQ2 was revealed by electrochemical impedance analysis (EIS) and open-circuit potential decay transients (OCVD), which attributed to its higher V_{oc} and ff in comparison to RSQ1 (*J. Org. Chem.* **2017**, *82*, 1920).

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Solid base catalyzed depolymerization of lignin: The depolymerization of high molecular weight lignin (60,000 Da) over various recyclable solid base catalysts at 250°C in an hour was reported. Most of the zeolitic catalysts (NaX, NaY, NaP) showed very high yields of low molecular weight products than other catalysts (MgO, CaO, HT, HAP) under these conditions. Particularly, over NaX maximum yield (51%) of low molecular weight products was achieved. Identification and quantification of products was done by GC, GC-MS, HPLC, LC-MS, CHNS, NMR and FT-IR techniques. The revelation of retention of most of the

functional groups on products present in lignin was done by FT-IR studies. It was observed that efficiencies of catalysts were dependent on pH, cation, type and concentration of basic sites etc. A unique study on products adsorption capacities on solids recognized that as strength of basic sites increases adsorption enhances (*Green Chem.* **2017**, *19*, 778).

Acidic ionic liquid catalyzed valorization of hemicellulose into furfural: Valorization of hemicellulose to valuable chemicals such as C5 sugars and furfural in the one-pot fashion was performed. The acidic ionic liquids in presence of water showed high yields of C5 sugars ($>80\%$) with $>99\%$ conversion of hemicelluloses at 160°C . Within 4 hours 85% furfural yield was obtained

Research & Development

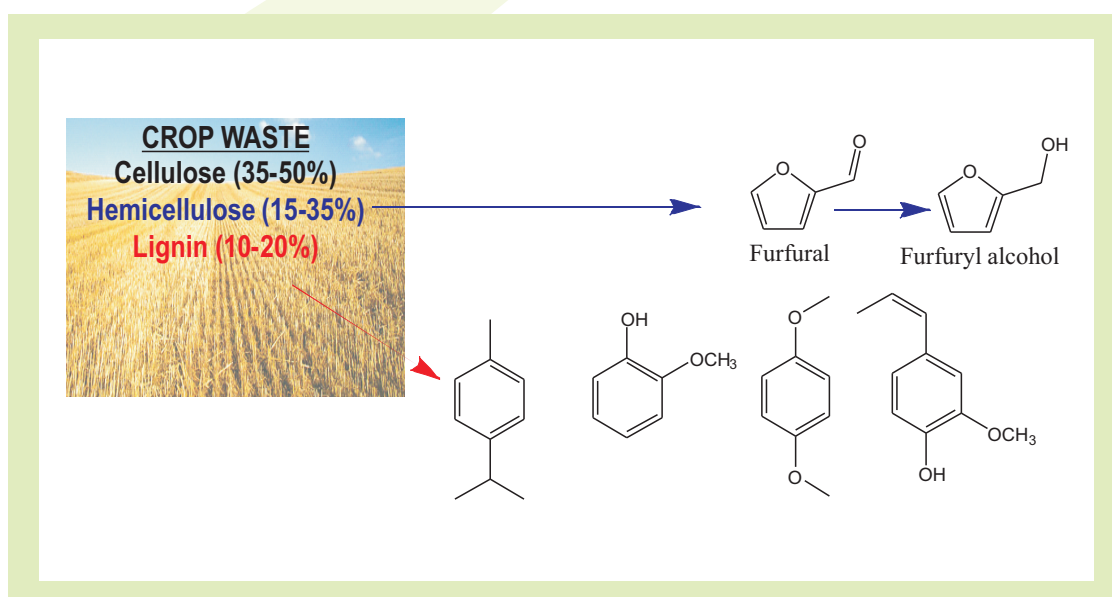
Energy and Environment

Renewable and alternative energy technologies

with water +toluene biphasic solvent system directly from hemicellulose in a one-pot fashion using the catalytic amount of 1-methyl-3-(3-sulfopropyl)-imidazolium hydrogen sulfate. It was seen that BAILs perform better than solid acid [Faujasite and Mordenite zeolites; ion exchange resin, Amberlyst-15] and mineralcatalysts [HCl and H₂SO₄]. The higher activity of BAILs compared to solid acids and mineral acid was correlated to Hammett acidity function (H₀) and ion-dipole type of interaction. The catalysts were characterized using NMR (¹H and ¹³C), elemental analysis and TGA to confirm that those are stable under reaction conditions and thus were recyclable (*New J. Chemistry*, 2017, 41, 6137).

Ambient condition high concentration furfural hydrogenation: Furfural (FAL), a major biomass-derived chemical, can be hydrogenated to yield the industrially important platform chemical, furfuryl

alcohol (FOL). Although heterogeneous catalyst-based methods are known to yield FOL from dilute solutions of FAL, they mainly operate at high temperatures and/or high pressures of hydrogen and in the presence of organic solvents. Bimetallic PtCo/C catalysts were employed with varying metal concentrations to achieve the maximum possible FOL yield (100%) at 35 °C under 0.1 MPa H₂ in water. Yield of 86% FOL was observed with concentrated FAL (40 wt%) at 50 °C and under 1 MPa H₂ pressure. Moreover, efficient catalyst recycling was observed over at least four runs with marginal loss in activity due to handling error and isolation of FOL in pure form confirmed by NMR and HPLC. Characterization of catalysts with several physico-chemical techniques revealed the presence of electron-rich Pt and ionic Co species in proximity with each other and it worked synergistically to facilitate maximum possible yield of FOL under ambient conditions and in water medium (*Green Chem.* 2017, 19, 1144).



Energy and Environment

Emission and effluent control including water and soil management

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Newer developments in Environmental Pollution Control

Desulfurization of transportation fuels and organics :

Governments worldwide now mandate ultra-low sulfur levels in transportation fuels below 10 ppm. Sulfur in the fuels has been a major concern not just from environment point of view due to SO_x emissions, but also from the viewpoint of application of gasoline in Fuel Cells that require much more stringent conditions of < 1 ppm, to avoid poisoning of the catalyst due to sulfur. The group is engaged in developing newer technology in the form of hydrodynamic cavitation and newer materials for adsorption to offer

an economically viable option to the existing desulfurization processes (*Sci. Rep.* **2016**, DOI:10.1038/srep33021).

Industrial wastewater treatment: A hydrodynamic cavitation technology was developed using vortex diode for the removal of refractory pollutants. The technology is effective in the treatment of dye wastewaters for removal of variety of dyes, fertilizer industrial wastewaters and has immense potential for other wastewater treatment applications. It can also be combined with other conventional processes such as anaerobic biological treatment for increased energy recovery, especially useful for Distillery Industry. Extensive studies in this regard are in progress (*Environ. Prog. Sustain.* DOI 10.1002/ep.12674).

Water: treatment, disinfection, purification

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Treatment of domestic sewage water

Recovery of water from domestic/industrial wastewater using membrane based systems: The natural microbial flora / consortium, enriched with the rapidly growing algae, standard algal isolates along with MBR were effectively utilized for the treatment of sewage as economical alternatives. The performance of microalgae and mixed culture consortia were studied

for the removal of nutrients as well as organic matter using open raceway pond and treated water was separated from the microalgae by using MBR. Thus it was found that the microalgae coupled MBR have a great phyco remediation potential for the treatment of sewage water. High-quality treated water was achieved which can be used for toilet flushing, gardening, civil construction etc. (*Chem. Eng. Technol.* **2016**, 39, 1629; *Chemical Industry Digest*, June, **2016**, 77; *Ind. J. Microbiol.* **2017**, 57, 241).

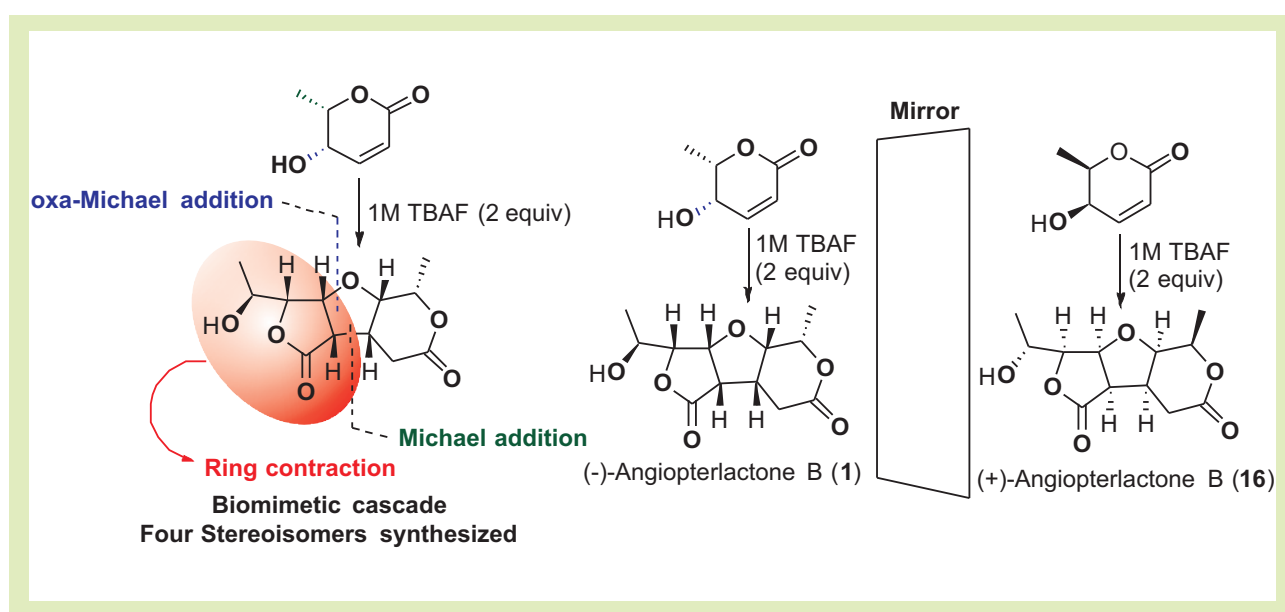
Healthcare

Natural products and methodology

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Biomimetic total synthesis of angiopterlactone B and other potential natural products: A one-pot biomimetic synthesis of (-)-angiopterlactone B and its enantiomer (+)-angiopterlactone B were accomplished via TBAF-catalyzed tandem ring contraction followed by oxa-Michael/Michael addition sequence. Comparison of specific optical rotations, absolute

configurations, and CD spectra of natural, synthesized (-)-angiopterlactone B and (+)-angiopterlactone B unequivocally proved that the isolated angiopterlactone B must be levorotatory. Synthesis of hitherto undiscovered natural products and analogues of angiopterlactone B demonstrated the versatility of this method (*Org. Lett.* **2017**, 19, 3564; Patent: IN 3557/DEL/2015; PCT Int. Appl. WO 2017077549 A1 20170511).



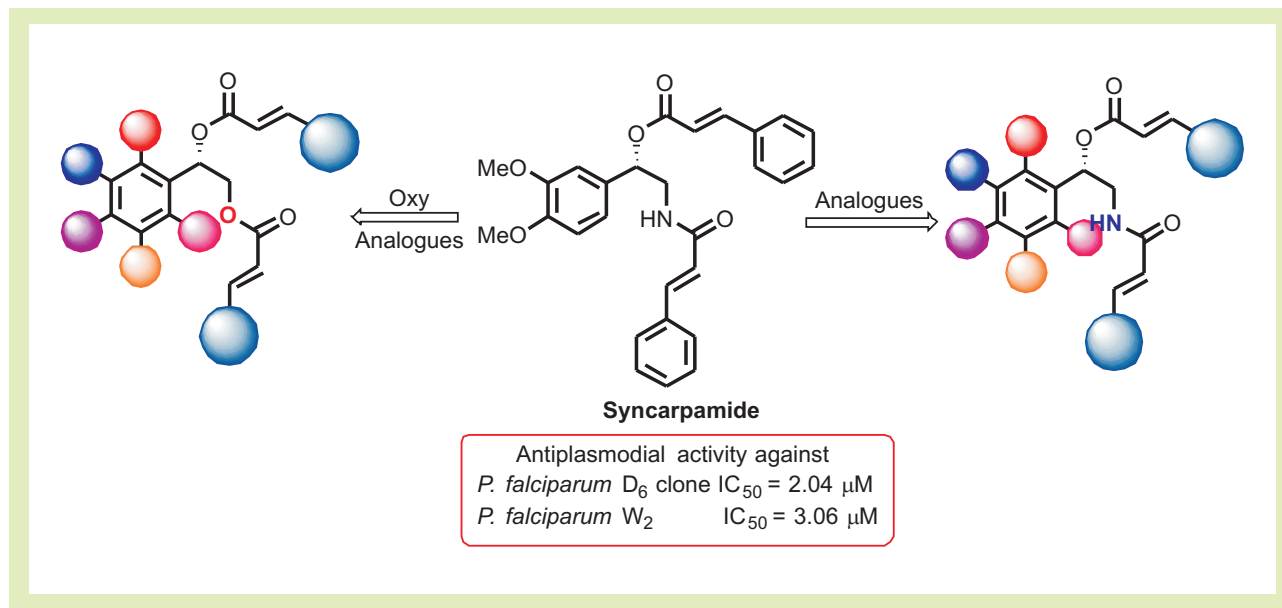
Norepinephrine alkaloids as antiplasmodial agents: Syncarpamide, a norepinephrine alkaloid isolated from the leaves of *Zanthoxylum syncarpum* exhibited promising antiplasmodial activities against *Plasmodium falciparum* with reported IC₅₀ values of 2.04 μM (D6 clone), 3.06 μM (W2 clone) and observed by the group 3.90 μM (3D7 clone) and 2.56 μM (K1 clone). Synthesis of syncarpamide and its enantiomer using Sharpless asymmetric dihydroxylation as a key step was accomplished. A library of 55 compounds which are analogues/ homologues of syncarpamide were synthesized to study structure-activity-relationship; further assayed in vitro against 3D7 and K1 strains of *P. falciparum* to evaluate their antiplasmodial activities. In order to study the effect of position of functional groups on antiplasmodial activity profile, a (S)-regioisomer of syncarpamide was synthesized; it turned out to be inactive against both the strains. The

in vitro antiplasmodial activity data of synthesized library suggested that the electron density and possibility of resonance in both the ester and amide side chains increased the antiplasmodial activity as compared to the parent natural product. The natural product syncarpamide and four analogues/ homologues out of the synthesized library of 55 were assayed in vivo assay against chloroquine-resistant *P. yoelii* (N-67) strain of *Plasmodium* (*Eur. J. Med. Chem.* **2017**, 138, 1089; Patent: IN 2014DE03005 A 20160831; PCT Int. Appl. WO 2016063301 A2 20160428).

Research & Development

Healthcare

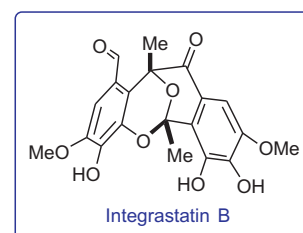
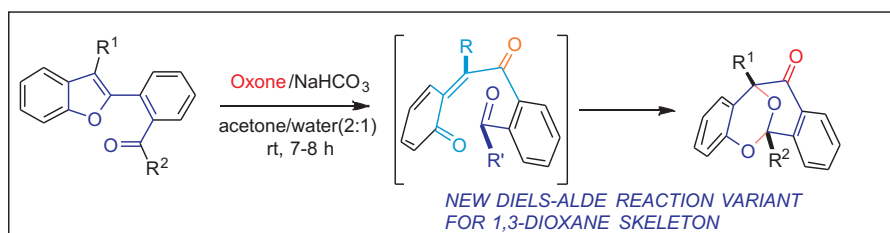
Natural products and methodology



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Total synthesis and new methodologies: The group focused on expanding the landscape of small molecules synthesis by employing a wide-range of transition metal complexes; developing new catalytic methods that are aided by the understanding of the reactivity/reaction paths, the orchestration of sequential reactions in one-pot; unravelling the capability of these new methods in forging a variety of complex natural products; and designing modular strategies that employ endless recombination of simple building blocks, thus providing simple solutions for accessing pharmaceutically relevant small molecules in large numbers and on large scales.

Total Synthesis: The first total synthesis of integrastatin B was achieved in six steps. The route utilized a unique oxidative dearomatization cascade of a benzofuran derivative to construct the central [6/6/6/6]-ring system. This reaction comprised the oxone-mediated oxidation of a benzofuran resulting in an ortho-quinonemethide that subsequently undergone an intramolecular [4+2]-cycloaddition with a suitably positioned carbonyl group. The simplicity and high yield (up to 97%) of this transformation allowed the synthesis of a large number of integrastatin analogues that were available for diverse biological assays. The tactical use of Pd-catalyzed C–H activation and C2-arylation of benzofurans was instrumental in accessing the key substrates and improved the overall practicality of this approach (Org. Lett. **2016**, 18, 612; 1458).

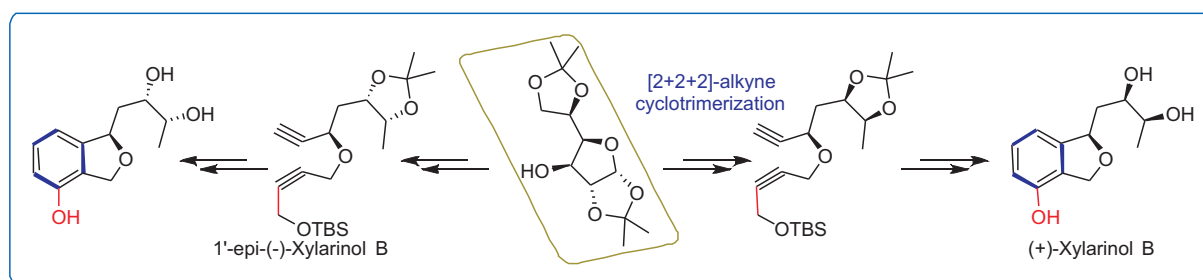


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Natural products and methodology

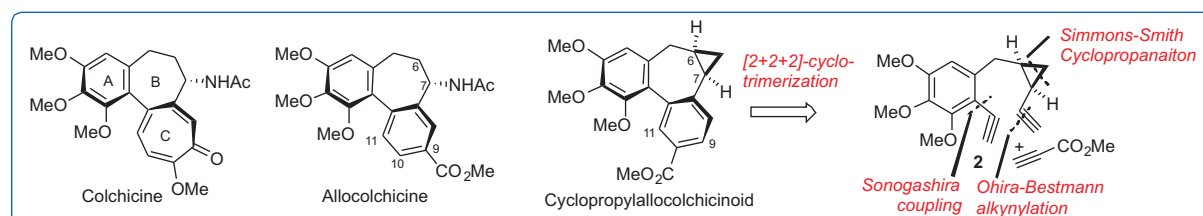
The total synthesis of two isomeric hexaketides isolated along with the sordarial having the proposed relative arabino- and ribo-configurations was executed. The Rh-catalyzed [2+2+2]-alkyne cyclotrimerization was employed as the key reaction to construct the central dihydroisobenzofuran core. The

absolute configuration of the xylarinol B hexaketide was established as L-arabino. This was the first natural product of this family having the absolute configuration fixed that can be extended in providing structural details of several of related hexaketides (*Asian J. Org. Chem.* **2016**, 5, 417).



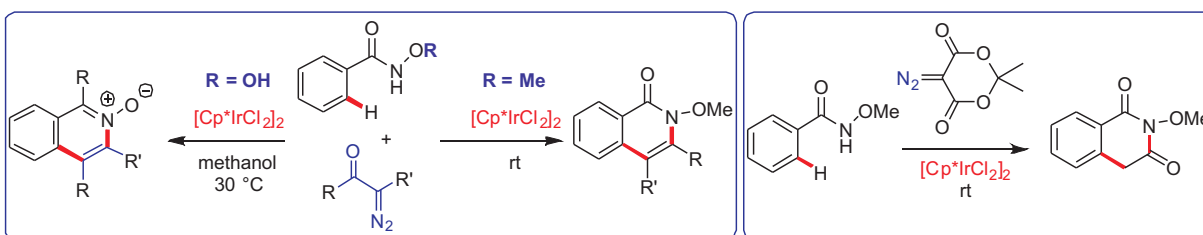
A short and efficient synthesis of cyclopropyl allocolchicinoid with potent tubulin binding affinity was as good as colchicines. It was reported by employing a cobalt-catalyzed [2+2+2] alkyne

cyclotrimerization as the final step. Its analogues having the functional group variations at C9 and/or C10 and C11 of ring C were also synthesized (*J. Org. Chem.* **2016**, 81, 3400).



New catalytic methodologies: In continuation on the C–H activation and functionalization of aromatic rings, a mild and efficient Ir(III)-catalyzed strategy was developed to access N-methoxy isoquinoline diones and N-methoxy isoquinolinones. The reaction proceeded efficiently in high yield at room

temperature without requirement of any additional oxidants or a base. When aryloxime was employed, an interesting dimeric iridacyclic complex allied through a bis-silver carboxylate bridge was isolated that efficiently catalyzed the reaction (*Org. Lett.* **2016**, 18, 292;2828).



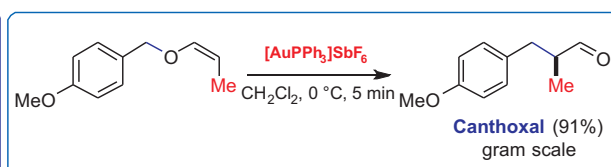
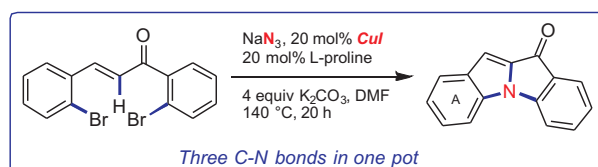
Research & Development

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In addition, a reaction cascade comprising of Cu-catalyzed SNAr with azide; nitrene C–H insertion and intramolecular Ullmann reaction with all three C–N bond formations in one-go. As a part of our on-going research program on gold-catalysis, gold-catalysed

[1,3] O-C rearrangement of the benzylvinyl ethers has been investigated. Further the reaction has been employed for the synthesis of canthoxal in gram scale in excellent yield with low catalyst loading (*Org. Chem. Front.* **2016**, 3, 43; 453).

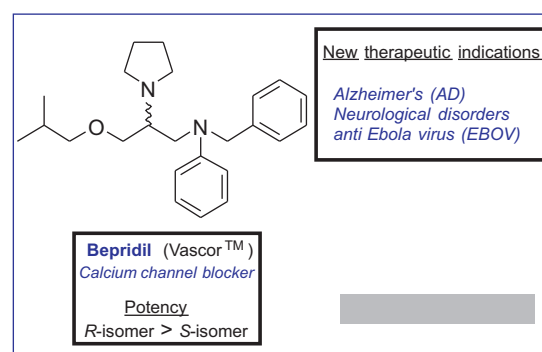


M. Muthukrishnan m.muthukrishnan@ncl.res.in

Asymmetric synthesis of biologically important compounds

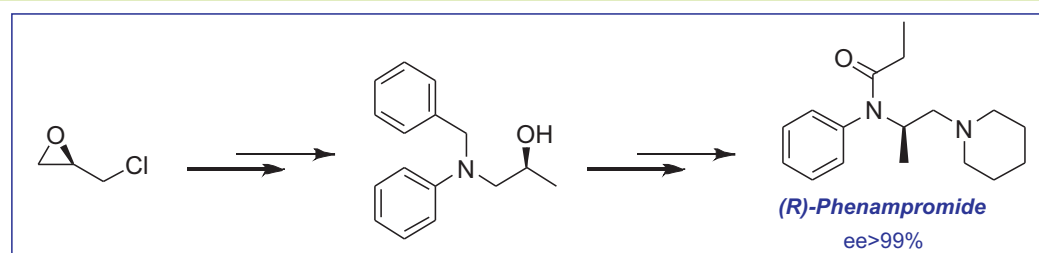
Enantioselective synthesis of both enantiomers of the calcium channel blocker bepridil: It was recognized that bepridil could be important in new therapeutic areas such as alzheimer's, antiviral, atrial fibrillation and in certain neurological disorders. Bepridil was identified as a potential lead molecule against Ebola virus disease by inhibiting a late stage of viral entry. Presumably, bepridil being an approved drug, repurposing of this may rapidly move to human testing and have a potential to become a frontline against Ebola virus infection. By understanding the significance of bepridil in many new therapeutic

indications, a short and efficient method was developed for the enantioselective preparation of both the enantiomers of bepridil for the first time in an overall yield about 18% and ee>98% (*New J. Chem.* **2017**, 41, 824).



An efficient synthesis of the opioid analgesic (R) phenampromide via an aziridinium ion: (R)-Phenampromide has greater analgesic potency than its (S)-enantiomer. Studies revealed that based on the structure of phenam-promide, U50, 488, a highly selective kappa opioid agonist was discovered. Few reports are available for the synthesis of the (R)-enantiomer of phenampromide, which mainly

involve resolution processes. An efficient new route for the synthesis of (R)-phenampromide was developed via aziridinium ring formation as the key step using simple commercially available starting materials. The final product was obtained with >99% enantiopurity. (*Tetrahedron Asymmetr.* **2017**, 28, 983).



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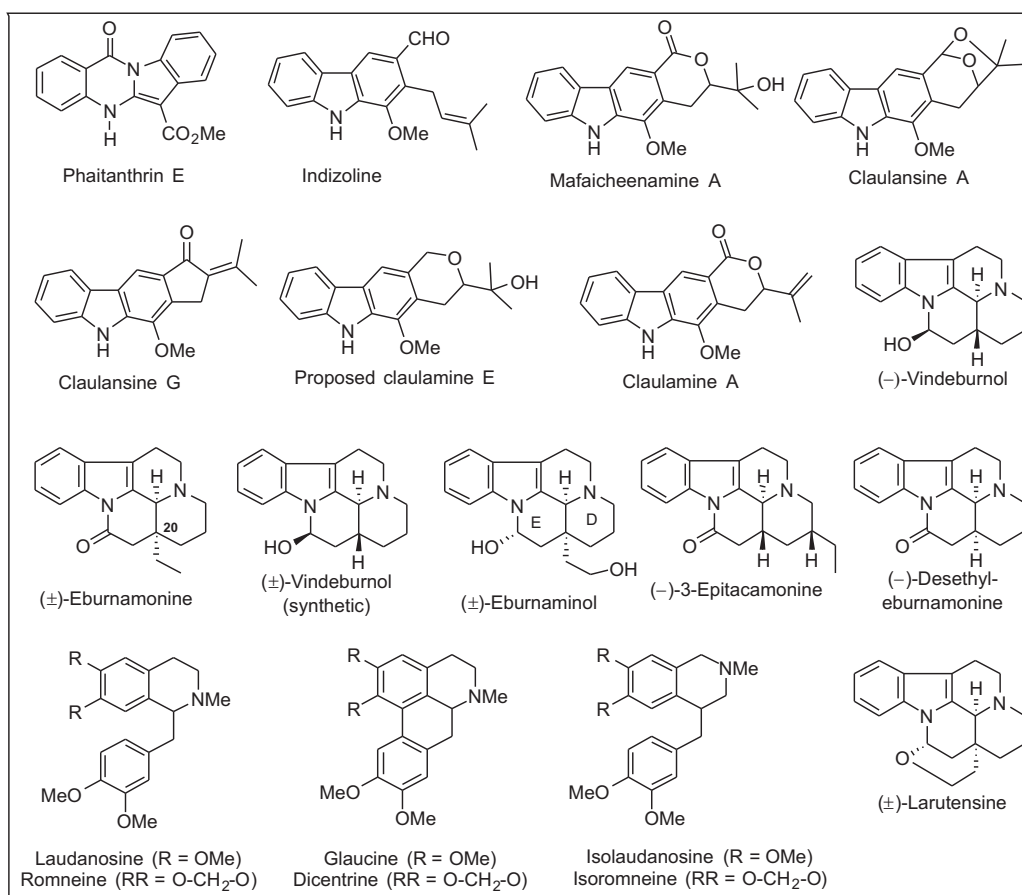
Narshinha P. Argade np.argade@ncl.res.in

Total synthesis of bioactive natural products

Total synthesis of recently isolated bioactive natural products:

The group was involved in 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 list of natural products synthesized during the past year included phaitanthrin E, (\pm)-eburnamonine, (\pm)-eburnaminol, (\pm)-vindeburnol, (\pm)-larutensine, laudanosine, romneine, glaucine, dicentrine and their unnatural analogues isolaudanosine and isoromneine, (-)-desethyleburnamonine, (-)-vindeburnol, (-)-3-epitacamonine,

indizoline, mafaicheenamine A, claulamine A, claulansine A, claulansine G and the proposed claulamine E. The key feature of this work was the spontaneous rearrangement of β -imino esters/ketones to the corresponding γ -amino α , β -unsaturated carbonyl systems, the use of acetoxy group from (\pm)-acetoxyglutarimide to induce the diastereoselectivity and also as a latent source of ketone carbonyl group, generation of two different types of benzylic carbanions and uncommon intramolecular aryl-aryl coupling reactions, substrate dependant reversal of the distereoselectivity in ester aldol reactions of hexahydroindolo [2,3-a] quinolizinsones, biogenetic collective total synthesis of carbazole alkaloids and remarkable cascade reaction leading to claulansine A (*Ind. J. Chem.* **2017**, 56B, 527; *Synthesis* **2017**, 49, 1655; 1849; *Org. Biomol. Chem.* **2016**, 14, 10394; *J. Org. Chem.* **2016**, 81, 5222).



Bioactive natural products synthesized

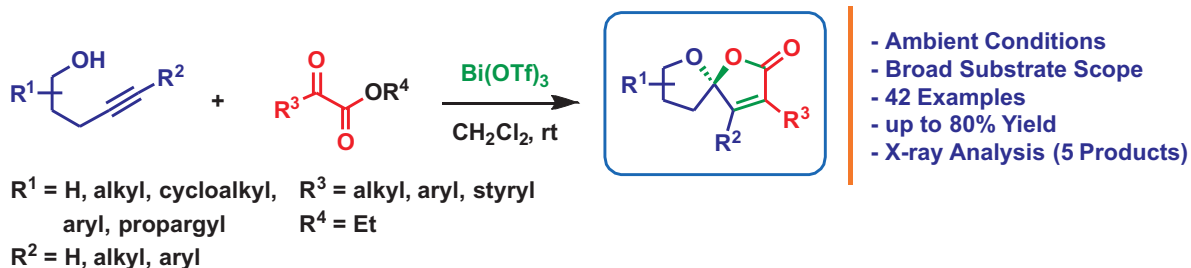
Natural products and methodology

Ravindar Kontham k.ravindar@ncl.res.in

Synthesis of novel oxygen-heterocycles using cascade annulation processes

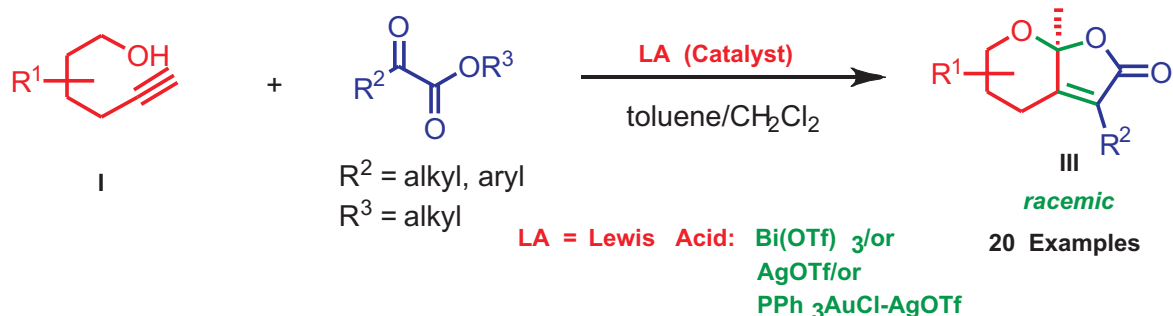
Lewis acid catalyzed cascade annulation of alkynols with α -ketoesters: A novel Lewis acid catalyzed intermolecular cascade annulation of alkynols with

α -ketoesters was developed. This simple and efficient cascade annulation proceeded through a 5-exo-dig cyclization of alkynols followed by annulation with α -ketoester to provide a wide variety of unsaturated γ -spiroketal γ -lactones (1,6-ioxaspiro[4.4]non-3-en-2-ones) related to many natural products (Chem. Commun. **2017**, 53, 6641).



Synthesis of furo [2,3-b] pyran-2-one via dual activation of soft nucleophiles and hard electrophiles: A novel and efficient synthetic methodology to construct these scaffolds were developed in an atom

and step economic way in light of interesting biological profile of natural products with furo[2,3-b] pyrans, and in combination with the emerging importance of cascade/domino reactions (Patent Appl: In 201711015471).



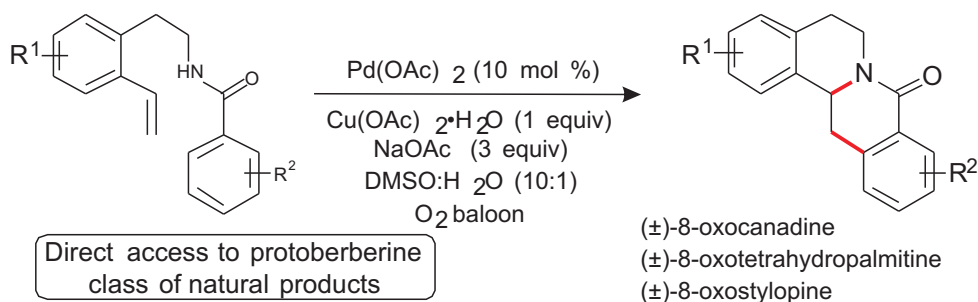
Santosh B. Mhaske sb.mhaske@ncl.res.in

Pd(II)-catalyzed intramolecular tandem olefin amidation/C-H activation protocol for the syntheses of the protoberberine class of natural products: Pd(II)-catalyzed intramolecular tandem olefin amidation-C-H activation protocol was developed for the synthesis of 8-oxoprotoberberine core. It was successfully

applied for the syntheses of (\pm)-8-oxocanadine, (\pm)-8-oxotetrahydropalmitine and (\pm)-8-oxostylophine, which was easily, converted to the respective protoberberine natural products. The short synthetic route demonstrated was useful for the synthesis of a large number of natural products and their analogues featuring protoberberine scaffold (Org. Lett. **2016**, 18, 3862).

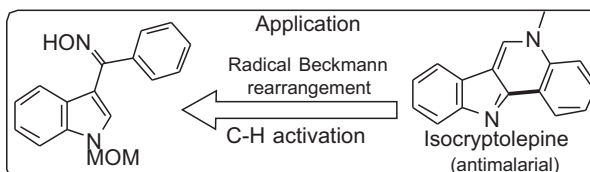
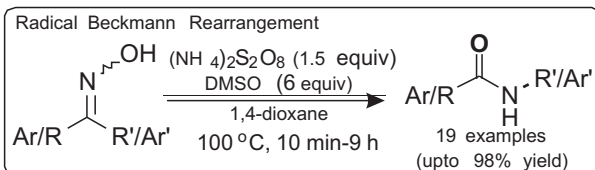
Healthcare

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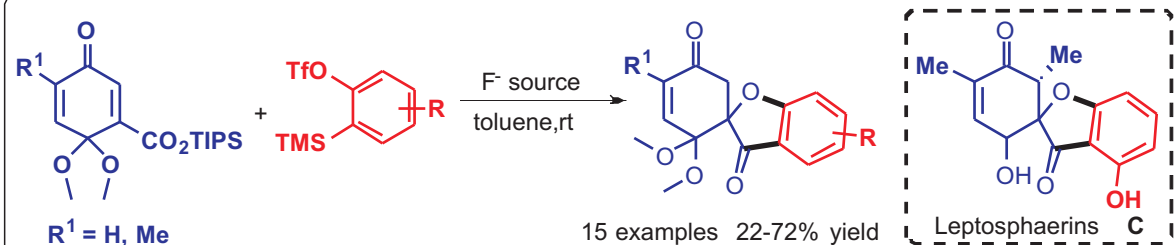
Total synthesis of antimalarial natural product isocryptolepine via C-H activation: The Beckmann rearrangement of ketoximes, mediated by ammonium persulfate-dimethyl sulfoxide as a reagent was achieved under neutral conditions. Based on the radical trapping and ^{18}O -labelling experiments, the transformation followed a mechanism involving a

radical pathway. The scope and generality of the developed protocol was demonstrated by nineteen examples. The developed protocol and Pd-catalyzed intramolecular double C-H activation were used as key steps in the formal total synthesis of antimalarial natural product isocryptolepine (*Org. Lett.* **2016**, *18*, 3450).



Diversity-oriented synthesis of spiroannulated benofuran-3-one scaffold of leptosphaerin C and congeners via aryne insertion: A concise synthesis of functionalized cyclohexenone-fused spirobenzofuran-3-ones under mild reaction condition was developed. The reaction proceeded via insertion of aryne into C-O

bond followed by a regioselective intramolecular conjugate addition. The use of silyl-protected acid was crucial for the transformation. This protocol was successfully applied for the synthesis of leptosphaerins C core and its novel analogues (*J. Org. Chem.* **2017**, *82*, 4875).

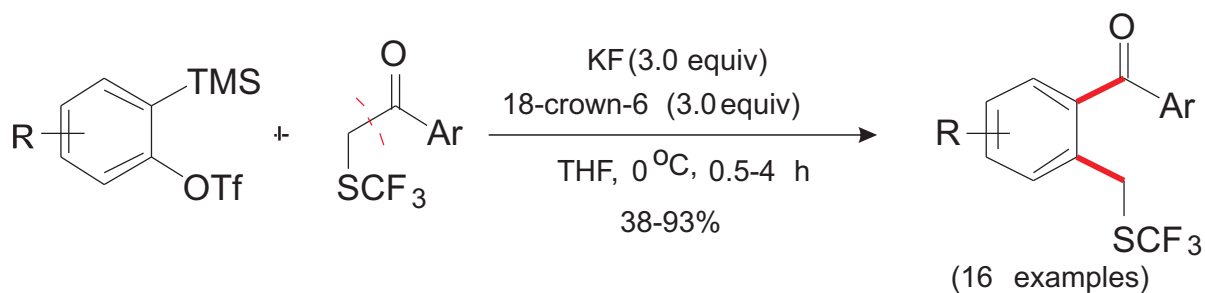


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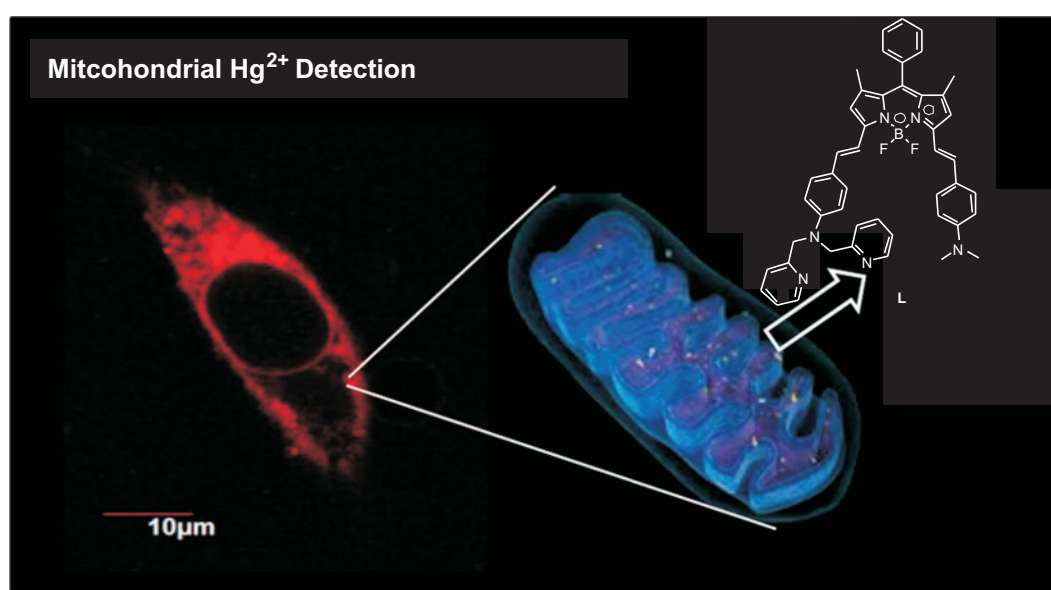
Synthesis of *o*-methyl trifluoromethyl sulfide substituted benzophenones via 1,2-difunctionalization of aryne by insertion into the C–C Bond: An efficient process for the preparation of valuable ortho-methyl trifluoromethyl sulfide substituted benzophenones was reported. The transition-metal free method

featured insertion of aryne in C–C σ -bond under a mild reaction condition for the first time to achieve ortho-difunctionalized arenes containing pharmaceutically important trifluoromethyl thio functional group. A wide substrate scope was demonstrated for the developed protocol (*Org. Lett.* **2017**, *19*, 2134).



A switch-on NIR probe for specific detection of Hg²⁺ ion in aqueous medium and in mitochondria: A new 4,4-difluoro-4-bora-3a,4a-diaza-s-indacene (BODIPY)-based probe molecule (L) was synthesized for specific binding to Hg²⁺ ion in physiological condition with an associated luminescence ON response in the near-IR region of the spectrum. Appropriate functionalization in the 5-position of each of two pyrrole moieties with styryl functionality in a BODIPY core helped us in achieving the extended conjugation and a facile intramolecular charge transfer transition with

a narrow energy gap for frontier orbitals. This accounted for a poor emission quantum yield for the probe molecule L. Binding to Hg²⁺ helped in interrupting the facile intramolecular charge transfer (ICT) process that was initially operational for L. This resulted in a hypsochromic shift of absorption band and a turn-on luminescence response with λ_{max} Ems of 650 nm on specific binding to Hg²⁺. The ability of the present reagent to specifically recognize Hg²⁺ in the mitochondrial region of the live Hct116 cells showed certain significance (*Inorg. Chem.* **2016**, *55*, 12052).



Research & Development

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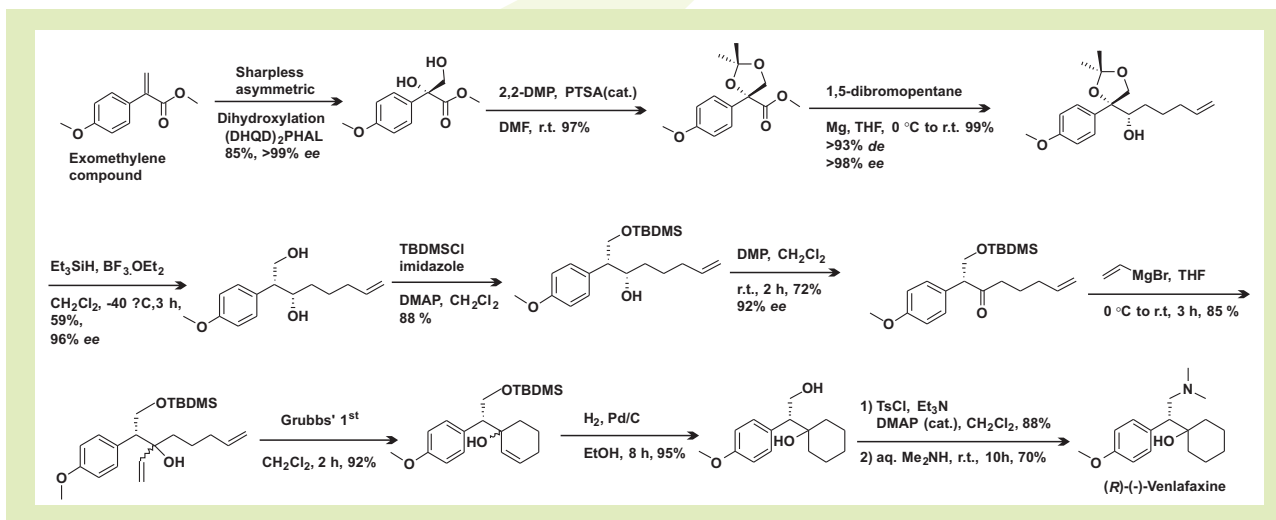
Synthesis and biological evaluation of new fluconazole β -lactam conjugates linked via 1,2,3-triazole: Novel 1,2,3-triazole-linked β -lactam-fluconazole conjugates 12(a-l) were designed and synthesized. The compounds showed potent antifungal activity against two pathogenic *Candida* strains; *Candida albicans* ATCC 24433 and *Candida albicans* ATCC 10231 with MIC values in the range of 0.0625–2 $\mu\text{g mL}^{-1}$. Compounds 12h, 12j and 12k showed promising antifungal activity against all the tested fungal pathogens except *C. neoformans* ATCC 34554 compared to fluconazole. Mechanistic

studies for active compounds revealed that the antifungal action was due to ergosterol inhibition. The molecular docking study revealed that all the fluconazole β -lactam conjugates 12(a-l) could snugly fit into the active site of lanosterol 14 α -demethylase (CYP51) with varying degrees of affinities. As anticipated, the binding energy for compound 12j ($-58.961 \text{ kcal mol}^{-1}$) was much smaller than that for fluconazole ($-52.92 \text{ kcal mol}^{-1}$). The synthesized compounds showed therapeutic potential for the control of candidemia (*New J. Chem.* **2017**, *41*, 470).

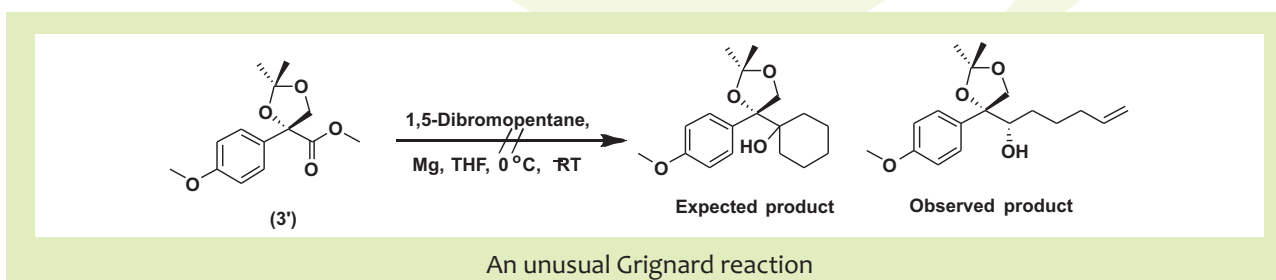
Subhash P. Chavan sp.chavan@ncl.res.in

Application of unusual grignard reaction for the stereoselective synthesis of antidepressant drug (R)-(-)-venlafaxine: Racemic as well as the asymmetric

synthesis of (R)-(-)-Venlafaxine was achieved involving sharpless asymmetric dihydroxylation reaction for chirality induction and unusual diastereoselective Grignard reaction for the installation of secondary alcohol (*Synthesis* **2017**, *49*, 1410).



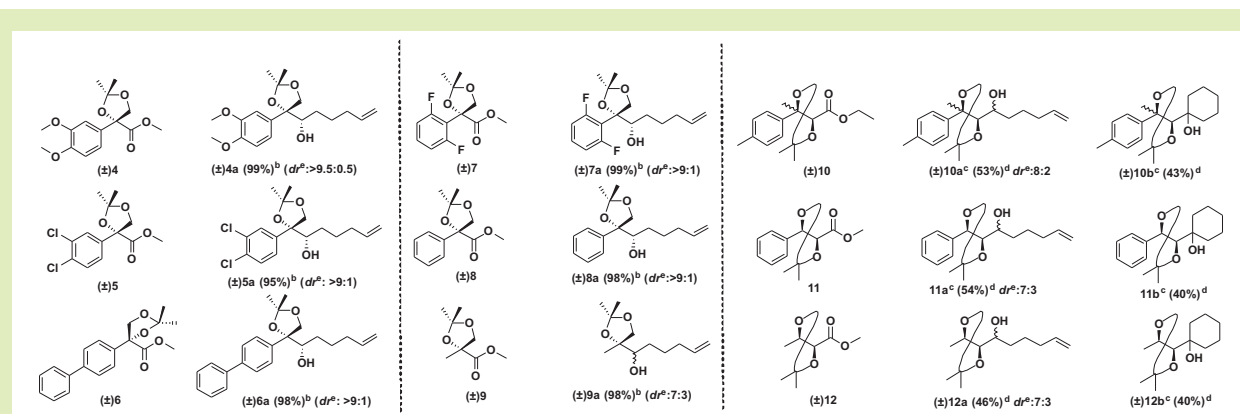
Unusual Grignard reaction and its application towards the synthesis of styryl lactones 7-*epi*-(+)-goniodiol and 8-*epi*-(-)-goniodiol: Styryllactones were shown to exhibit moderate to significant biological activity including antitumor, antifungal as well as antibiotic properties. Efforts were focused on the development of methodology for the synthesis of the (7-*epi*-(+)-goniodiol and 8-*epi*-(-)-goniodiol) because of their unique and intriguing structures and



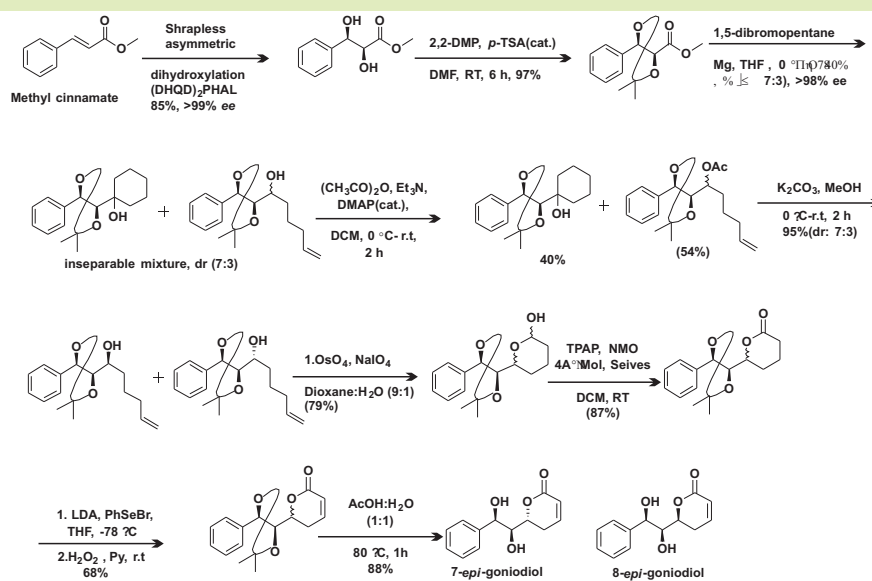
Research & Development

Natural products and methodology

the activity associated with it. More than fifty bioactive styryllactones with a large variety of basic structures were isolated from several species of the genus *Goniothalamus*.



Unusual Grignard reaction of acetone protected ester substrates



The unusual Grignard reaction furnishes long chain secondary alcohols possessing a terminal olefin, which are synthetically important intermediates. The diastereoselective synthesis of styryl lactones viz. 7-*epi*(+)-goniodiol and 8-*epi*(-)-goniodiol was achieved (RSC *adv.* 2016, 6, 50721).

Hybrids of thienopyrimidinones and thiouracils as anti-tubercular agents: A number of hybrid molecules containing thienopyrimidinones and thiouracil moieties were designed, synthesized and tested against *Mycobacterium tuberculosis* H37Ra wherein it was observed that the compounds 11-14 exhibited antitubercular activity in vitro (MIC 7.6-19.1 mg/mL, 12-35 mM) against dormant stage while the compound 15

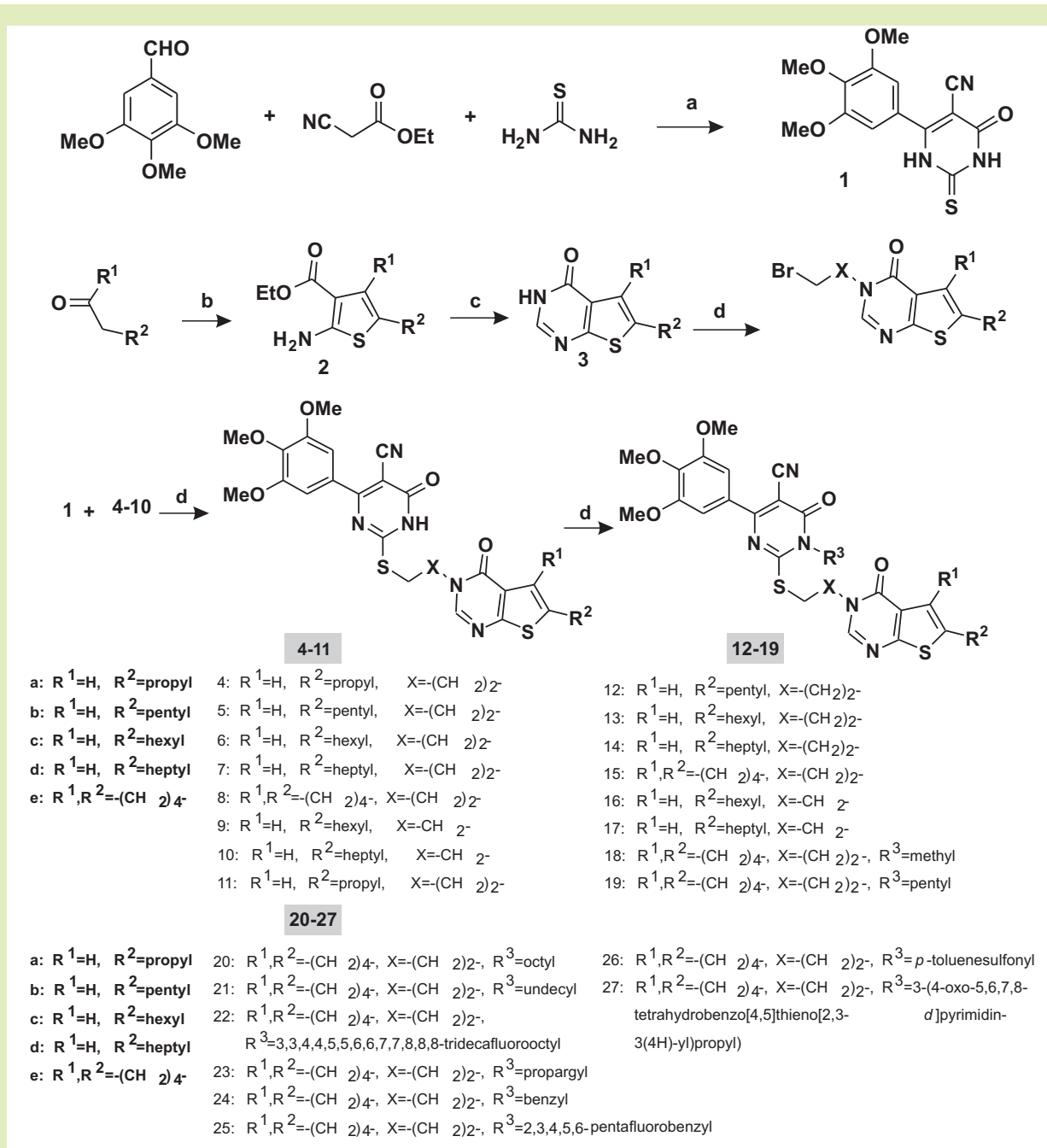
exhibited antitubercular activity in vitro against dormant (MIC 23.4 mg/mL, 41 mM) as well as active (MIC 25.4 mg/mL, 45 mM) stage. Structural modifications of the compound 15 were carried out to study the structure-activity relationship and it was observed that the compound 18 exhibited antitubercular activity comparable to the compound 15. Cytotoxicity studies revealed that these molecules

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were non-toxic. The docking study of the compound 15 showed that there was binding with the active site of mycobacterial pantothenate synthetase. Further docking studies led to the synthesis of the compounds 16 and 17 and the antitubercular activity screening results showed that these compounds have significant antitubercular activity. The compounds 15-18

(MIC 11e29 mg/mL, 19 -51 mM) can be used as starting points for further optimization. The synthetic strategies used in the present work have potential to prepare a large number of compounds for further refinement of structures and the present results will be very useful in the development of a new class of antimycobacterial agents.



Scheme: Reagents and conditions: a: K₂CO₃, DMF, 110°C, 3 h; b: Ethyl cyanoacetate sulphur, triethyl amine, DMF, 55°C, 12 h; c: Ammonium acetate formamide, 145°C, 12 h; d: Required halide, K₂CO₃, DMF, RT, 12 h.

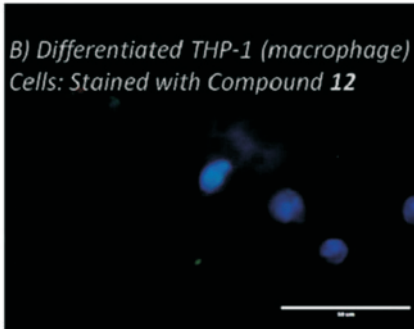
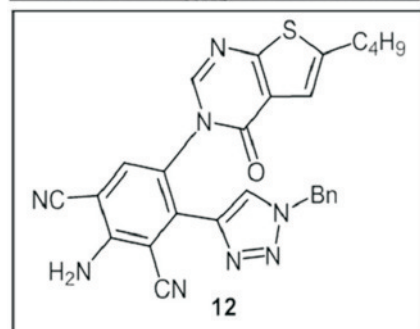
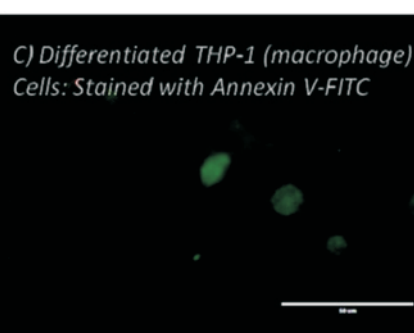
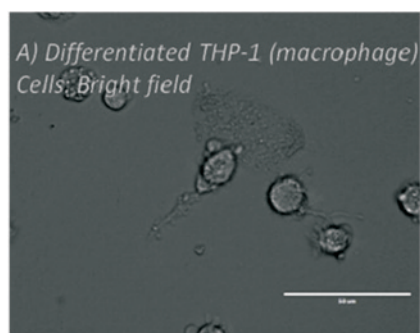
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Synthesis of hybrid molecules containing thiouracil and thienopyrimidinone moieties was achieved. The new result on *Mycobacterium tuberculosis* H37Ra and it was observed that some compounds exhibited antitubercular activity against dormant stage while one compound exhibited antitubercular activity against dormant as well as active stage. Structural modifications of same compound were carried out to study the structure-activity relationship and it was observed that good result. Cytotoxicity studies revealed that these molecules were non-toxic. The docking study of some compound showed that there is binding with the active site of mycobacterial pantothenate synthetase with the docking score of -5.863. Further derivatized the compounds were designed based on docking studies and their docking scores were found to be -7.949 and -8.666, respectively indicating the possibility of these compounds to be more active. The synthesis and antitubercular activity screening of this hybrid compounds and was carried out and it was found that these compounds were having potent antitubercular activity supporting the binding of these compounds with mycobacterial pantothenate synthetase. Hence, these compounds can be used as starting points for further optimization.

The synthetic strategies used in the present work have potential to prepare a large number of compounds for further refinement of structures and the present results will be very useful in the development of new class of antimycobacterial agents (*Eur. J. Med. Chem.* **2017**, *127*, 459).

Synthesis and cell imaging applications of fluorescent mono/di/tri-heterocyclyl-2,6-dicyanoanilines

Synthesis of 3,4,5-triheterocyclyl-2,6-dicyanoanilines starting from heterocyclic aldehydes and 1,2-diheterocycle-substituted ethanones was reported. 2,6-Dicyanoanilines with one or two heterocyclic substituents were also synthesized. It was found that some of these molecules have selective cell-staining properties useful for cell imaging applications. Some compounds were found to stain cytoplasm of the cells in contact but not the nucleus while one compound showed affinity to apoptotic cells resulting in blue fluorescence. The cell imaging results with same compound were similar to Annexin V-FITC, a known reagent containing recombinant Annexin V conjugated to green-fluorescent FITC dye, used for detection of apoptotic cells. These compounds were found to be non-cytotoxic and have potential application as cell imaging agents (*Bioorg. Med. Chem. Lett.* **2017**, *27*, 979).



Compound formula imaging applications and photo fluorescent property

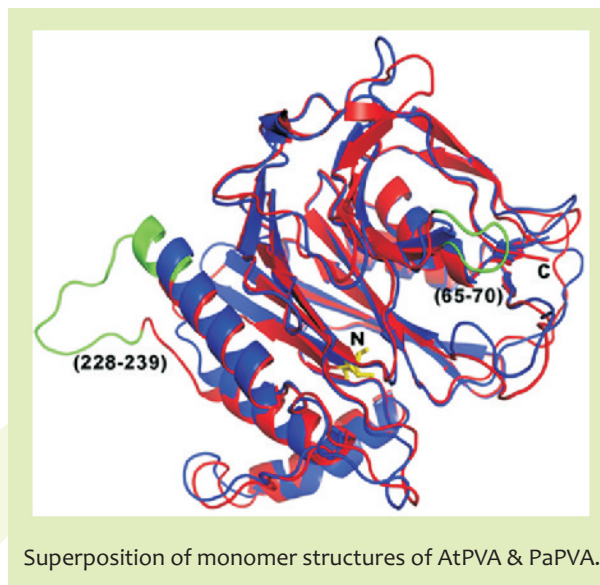
Healthcare

Chemical biology

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A highly active penicillin V acylase from *Pectobacterium atrosepticum*: Virulence pathways in gram-negative pathogenic bacteria were regulated by quorum sensing mechanisms through the production and sensing of N-acylhomoserine lactone (AHL) signal molecules. Enzymatic degradation of AHLs led to attenuation of virulence (quorum quenching) paved the way for the development of new anti-bacterials. Penicillin V acylases (PVAs) belong to the Ntn hydrolase super family, together with AHL acylases. PVA from Gram-negative bacterium *P. atrosepticum* was cloned and expressed in *E. coli* that attained high enzyme yield (250 mg/l) and maximum Pen V hydrolysis activity (434 IU/mg) was reported for PVAs so far. Disruption of quorum sensing in *Pseudomonas aeruginosa* by PVAs was studied and the potential for using these enzymes as therapeutic agents were discussed. The loop extensions in PaPVA are shown in green residue

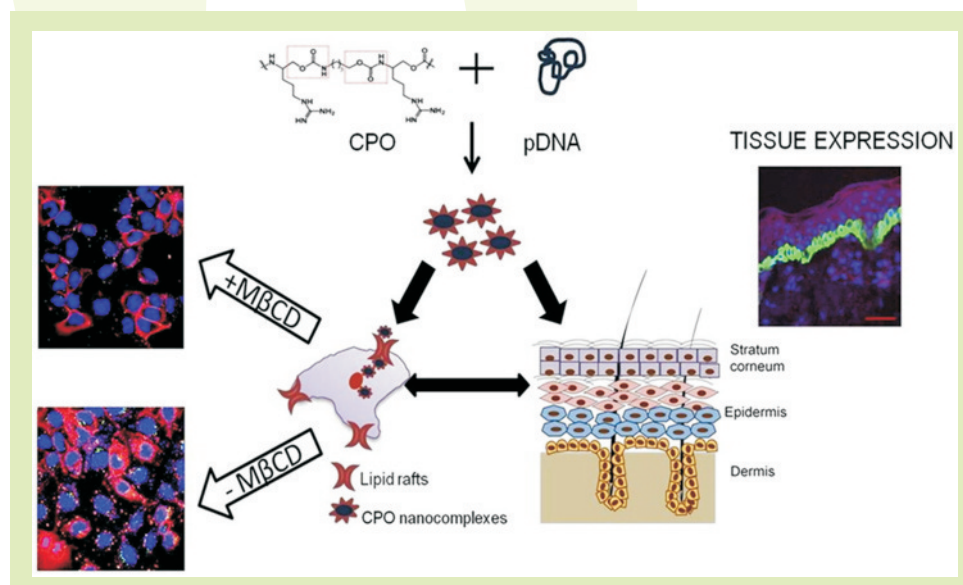
numbering according to PaPVA. N terminal cysteine (stick representation) is shown in yellow (Appl. Microbiol. Biot. 2017, 101, 2383).



Moneesha Fernandes m.dcosta@ncl.res.in

Efficient designed molecular transporters (r-x-r) 4-Carbamate for efficient non-invasive cargo delivery to skin: The (r-x-r) 4-carbamate-plasmid DNA complexes primarily utilize lipid raft-dependent pathway of cellular entry more than other pathways,

and this possibly facilitates their increased entry in the lipid rafts rich milieu of skin cells. The utility of oligomer (r-x-r) 4-carbamate as an efficient carrier for topical delivery of nucleic acids in skin tissue was demonstrated. This carrier can be utilized for safe, efficient, and non-invasive delivery of therapeutically relevant macromolecular hydrophilic cargo like nucleic acids to skin (Mol. Pharmaceut. 2016, 13, 1779).

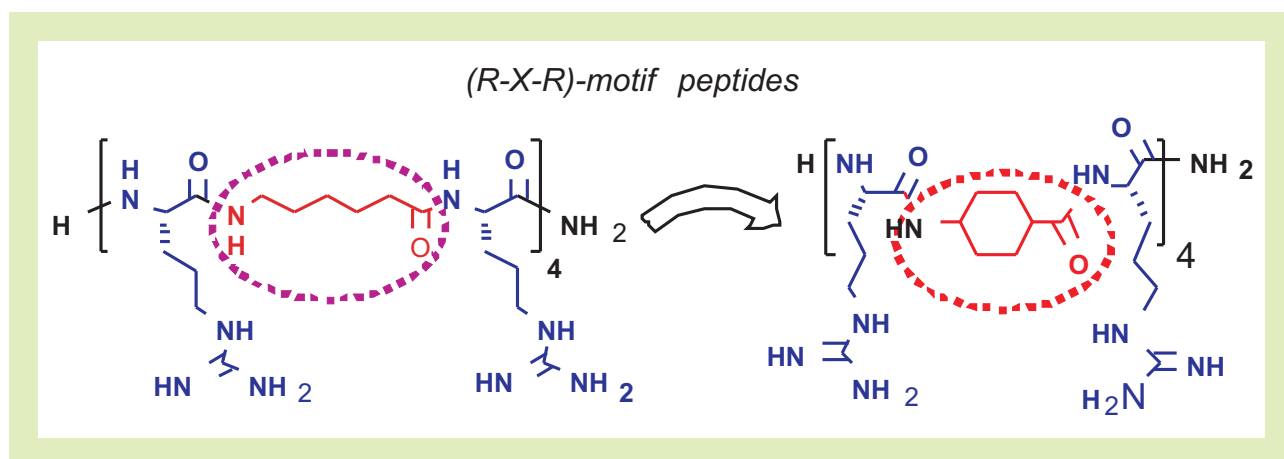


Research & Development

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Constrained cyclic 1,4-substituted cyclohexane-derived spacers in (R-X-R)-motif CPPs: Arginine-rich peptides having the (R-X-R)_n- motif are among the most effective cell-penetrating peptides. A several fold increase in the efficacy of such CPPs when the linear flexible spacer (-X-) in the (R-X-R) motif was replaced by

constrained cyclic 1,4-substituted cyclohexane-derived spacers was observed. The resulting CPPs were also more stable to proteolysis. Internalization of these oligomers in mammalian cell lines was found to be an energy-dependent process (*ChemMedChem*. 2017, 12, 1743).

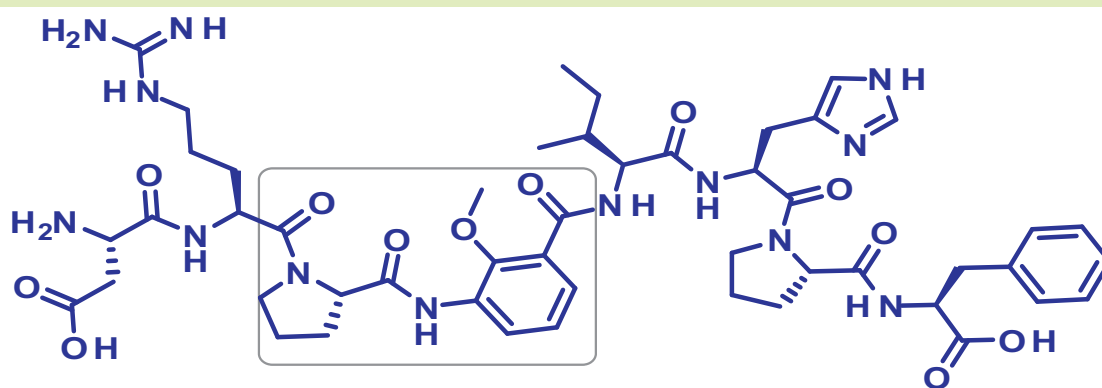


G. J. Sanjayan gj.sanjayan@ncl.res.in

De novo designed angiotensin II receptor agonists:

Novel Angiotensin II (AT₂) receptor agonists were developed recently based on the synthetic peptide scaffolds developed at CSIR-NCL. Solution-state NMR and CD studies suggested turn-like conformation in

Pro-Amb analogs. More importantly, Pro-Amb analogs were shown to act as strong AT₂ receptor agonists, which may have utility in treating cardiovascular diseases. AT₂ receptor has showed of developmental role having a potential to improve cognitive performance in Alzheimer's disease and other neurological cognitive disorders (*Chem. Commun.* 2016, 52,1645).



Pro-Amb-based AT₂ receptor agonist

α,β-Hybrid peptide vesicles for drug loading /unloading application: De-novo designed self-assembled peptides were successfully demonstrated for drug loading/unloading application. Urea-functionalized octapeptides underwent self-assembly through the directional hydrogen bonding interactions, forming vesicle in polar media.

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Chemical biology

Results of both fluorescence spectroscopy and microscopy revealed that the peptide vesicles were able to encapsulate and release the anticancer hydrophobic drug curcumin. These α,β -hybrid peptide vesicles may find application in cite-specific drug delivery. Moreover, the unnatural amino acid content such as anthranilic acid of the oligomer may have biological significance in imparting proteolytic stability to the supramolecular structures (*Chem. Commun.* **2016**, 52, 10771).

Highly stable triazine-based AADD-type self complementary quadruple hydrogen system: A new class of highly stable triazine-based AADD-type self

Mahesh Kulkarni/ D. S. Reddy

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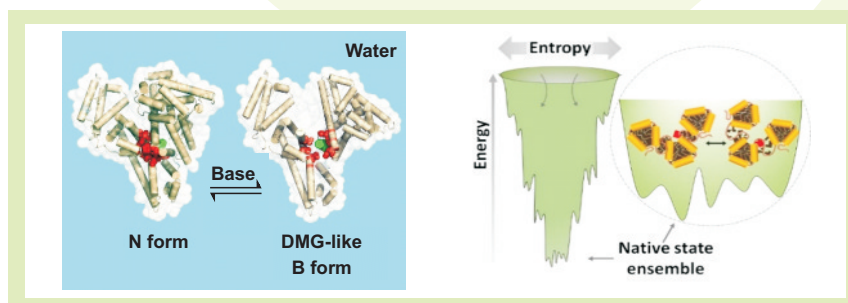
Molecules with O-acetyl group protect protein glycation by acetylating lysine residues: Pharmaceutical intervention for reduction of advanced glycation end products (AGEs) is considered as a therapeutic strategy to attenuate the pathogenesis of diabetes. Many molecules were reported to possess antiglycation activity, one such example is

complementary quadruple hydrogen system was developed successfully. It showed high K_{dim} value ($K_{dim} > 10^7 M^{-1}$ in $CDCl_3$). The system existed only as a single set of hydrogen-bonded molecular duplex – both in the solution- and solid-state and is thus devoid of the problem of prototropy-related issues. These strongly associating self-complementary motifs may have potential applications in the field of supramolecular chemistry wherein molecular duplexes of multiple protamers were not desired (*Chem. Eur. J.* **2016**, 23, 783).

acetylsalicylic acid (aspirin). It protects proteins from glycation by acetylating the lysine residues. The molecules containing free N-acetyl, O-acetyl and acetophenone groups were synthesized and screened. All the selected molecules in this study showed glycation inhibition but interestingly, only molecules with O-acetyl but not N-acetyl and acetophenone groups were capable of acetylating lysine residue (*RSC Adv.* **2016**, 6, 65572).

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Protein stability and folding: A protein present in human blood, human serum albumin, as a model system was studied employing a battery of spectroscopic methods, including site-specific fluorescence resonance energy transfer, time-resolved fluorescence, size exclusion chromatography, dynamic fluorescence quenching, red-edge excitation shift and circular dichroism spectroscopy. The group reported that Van der Waals forces contributed significantly to protein stability, in addition to the hydrophobic effect; the side-chain residues of proteins could be packed in multiple ways in the native state and hence the native state of proteins were conformationally and energetically heterogeneous; and that the base-induced unfolding of proteins begin with the formation of a dry molten globular intermediate state in which the structure was expanded and van der Waals interactions were disrupted without the hydration of the hydrophobic core (*J. Phys. Chem. Lett.* **2016**, 7, 173; *J. Phys. Chem. B.* **2017**, 121, 9336).

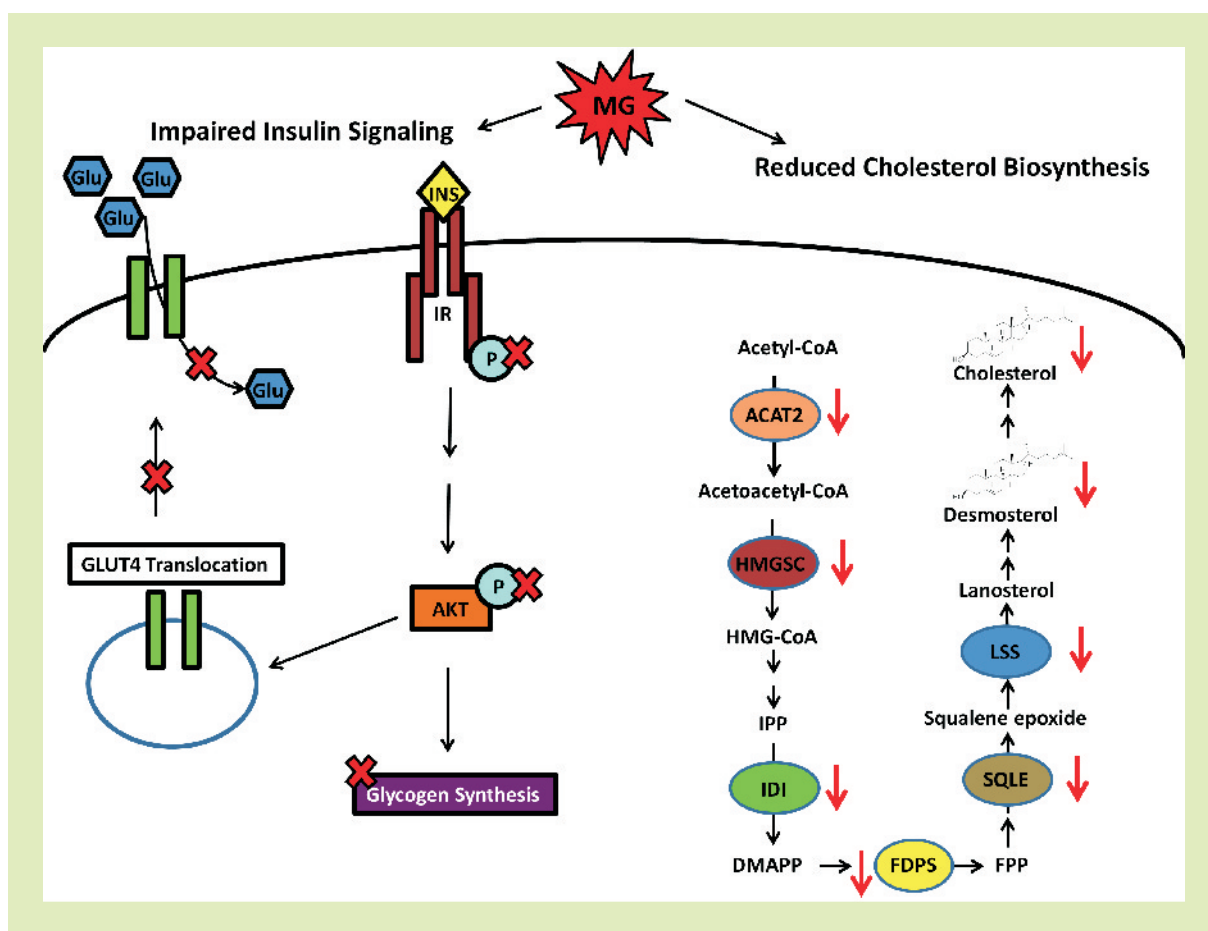


Chemical biology

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Methylglyoxal attenuates insulin signalling and down regulates cholesterol biosynthesis: The role of Methylglyoxal (MG) on insulin resistance was studied. The study suggested that MG impairs insulin signaling by inhibiting GLUT4 translocation leading to reduced glucose uptake. MG induced altered expression of

various proteins involved in stress response, protein folding and proteolysis, in proteomics analysis. Interestingly, aminoguanidine (AMG), a potent dicarbonyl scavenger, restored the deleterious effects of MG. It was reported for the first time that MG induces downregulation of enzymes involved in cholesterol biosynthesis. GC MS analysis of sterol metabolites corroborated the proteomic results (*Mol. BioSyst.* **2017**, *13*, 2338).

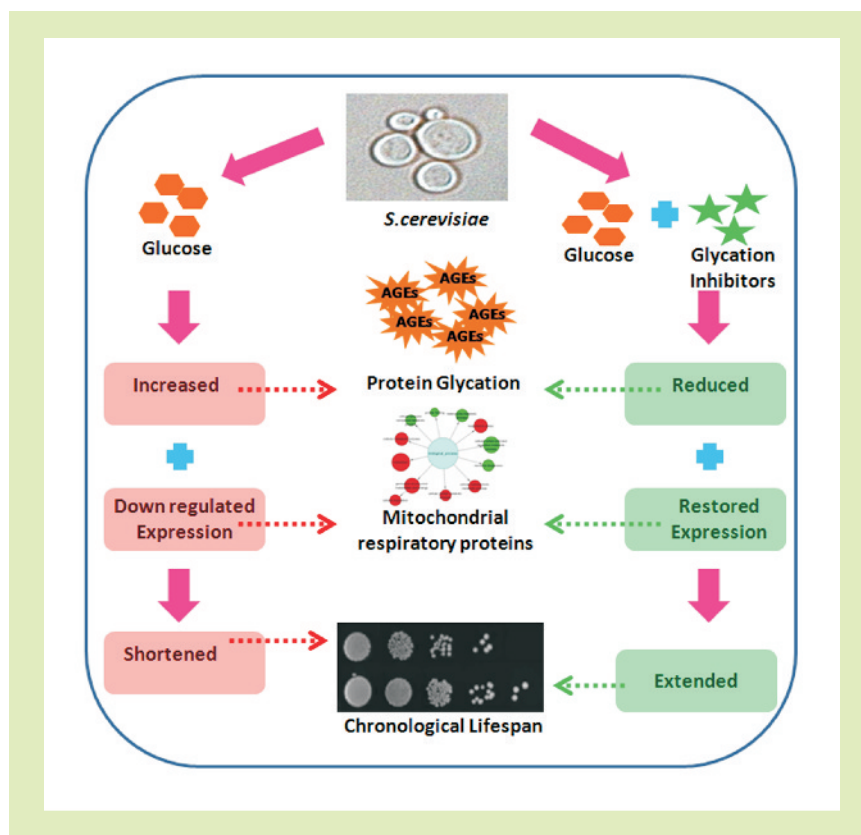


Glycation inhibitors extend yeast chronological lifespan: Advanced Glycation End products (AGEs) are implicated in aging process. Thus, reducing AGEs may help in attenuating the aging process. In this study using yeast system, it was showed that Aminoguanidine(AMG), a well-known glycation inhibitor, decreased the AGEs in non-calorie restriction (NR) and extended chronological lifespan (CLS) similar to that of calorie restriction (CR) condition. Proteomic analysis revealed that AMG back regulated the expression of

differentially expressed proteins especially those involved in mitochondrial respiration in NR condition. AMG induced back regulation of differentially expressed proteins was due to glycation inhibition that was demonstrated by using other inhibitor such as hydralazine and metformin (*J. Proteomics.* **2017**, *6*, 104).

Healthcare

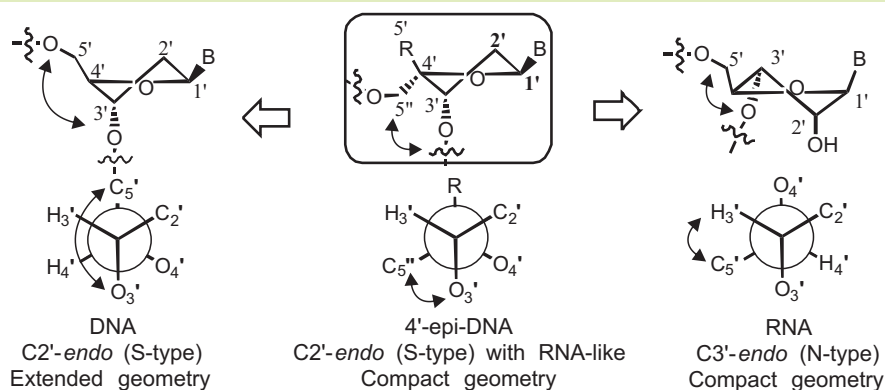
Chemical biology



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Nucleic acid analogues: C4'-Epi-DNA Synthesis of C4'-epi-DNA containing 3'→5'-linkages was reported for the first

time. Crystal structure study of the monomer indicated that though the dihedral angle $O3'-C3'-C4'-C5''$ in this case would be like in RNA, the sugar conformation would remain like that in DNA. The study of the effect of this backbone configuration in DNA with respect to its binding to cDNA and RNA was reported (*Nucleos.Nucleot. Nucl.* 2016, 35, 445).



2'-O-(2-Amino-3-methoxypropyl)-U-containing and serinol-capped RNA: miRNAs are highly conserved class of small ncRNAs whose involvement in human pathophysiology was extensively investigated. mi R

-21 is a well established oncogenic miRNA whose deregulation played a significant role in onset and progression of cancer. Potent inhibition of miR-21 was achieved by chemically modified 2'-O-methyl RNA

Research & Development

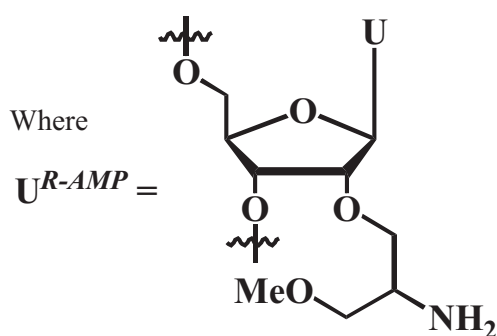
Healthcare

Chemical biology

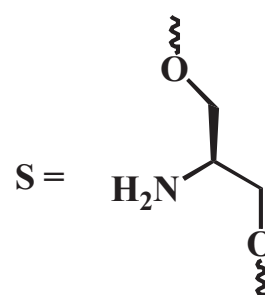
oligonucleotide. The serinol capping at 3' and 5'-ends and the interspersed 2'-O-(2-amino-3-methoxypropyl) uridine units enhanced the nuclease resistance and efficacy of 2'-O-methyl RNA for the inhibition of miR-21. It represents a simple and novel modification for developing oligo nucleotide-based therapeutics (*Nucleic Acid Ther.* **2016**, 26, 327).

AMO-1 sequence: uca aca uca guc uga uaa gcu a

AMO-2 sequence: SS U^{R-AMP} ca aca U^{R-AMP} ca guc U^{R-AMP} ga uag cu a SS



and

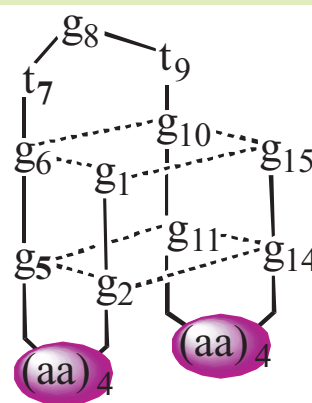


To preserve the duplex stability with target RNA and to enhance the stability against nucleases

To enhance the stability against nucleases

PNA G-quadruplex with amino acid loop residue replacements:

An uncharged PNA 15mer sequence formed unimolecular antiparallel G-quadruplex similar to that observed for DNA-TBA. Replacement of 'tt' loop regions by peptides which induced helices or turns were found to have unprecedented effect on the quadruplex topology and stability. This study opened up a completely new strategy of utilizing G-quadruplex formation to display the array of functional groups in three dimensional space thus creating a possibility of getting closer to the dream of designed peptides with three dimensional structures as observed in catalytic protein folds (*Tetrahedron* **2017**, 73, 1534).



Conformational, functional and in silico analysis of a serine protease from *Conidiobolus*: The commercial importance of *Conidiobolus* serine protease (CProt) in biopesticides, silk and leather industries made it an interesting candidate for structural investigations. Cprot is a beta sheet rich protein, found to be active over a wide pH range and up to 55 °C, also stable in organic solvents up to 50% (v/v) and DMSO for >24h and

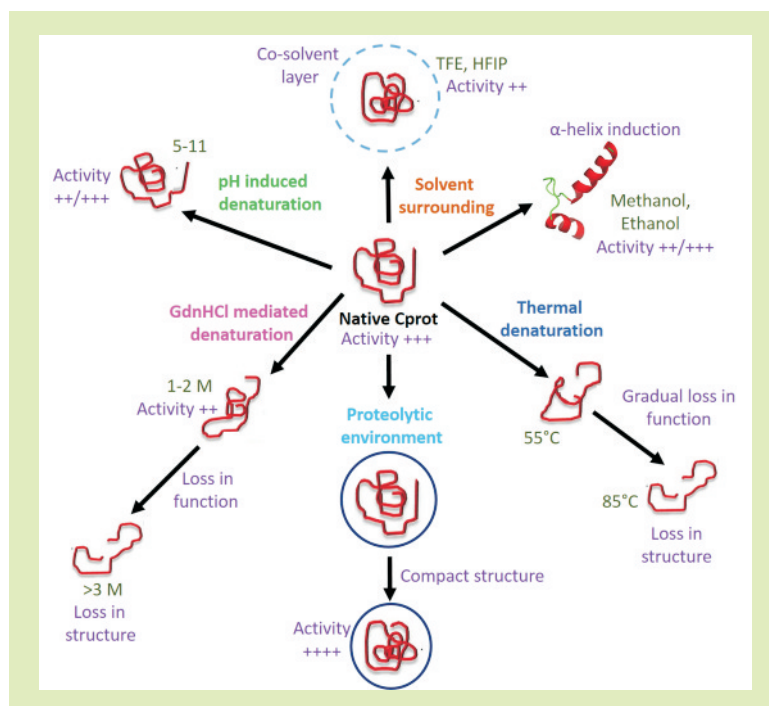
Sushama Gaikwad sm.gaikwad@ncl.res.in

in 2M guanidine hydrochloride for >12 h. Cprot was resistant to trypsin, chymotrypsin, proteinase K and fluorinated alcohols. Structural information was supported by the homology model revealing its similarity to PA clan. The results seemed to be useful in improving efficiency of the enzyme (*Int. J. Biol. Macromol.* **2017**, 98, 387).

Research & Development

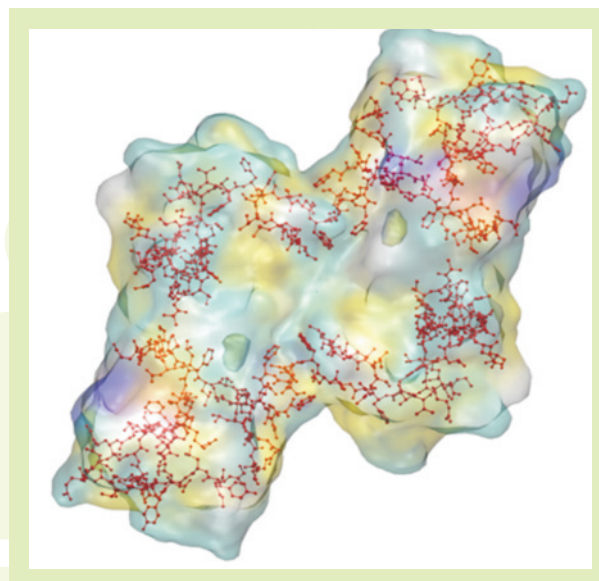
Healthcare

Chemical biology



Amaranthus caudatus lectin with polyproline II fold:

Polyproline II (PPII) fold was detected in the *Amaranthus caudatus* seed lectin (ACL) based on far UV circular dichroism spectrum, conformational transitions of the lectin, and a distinct isodichroic point in thermal denaturation. The lectin got aggregated at 60°C with instantaneous structural alterations. The aggregation-prone regions in ACL were predicted using online servers that were represented by Visual Molecular Dynamics tools. Nine conserved regions were identified as being 'hot-spots' for aggregation. MD simulation studies at 60°C revealed increase in radius of gyration. The polyproline II fold has been rarely detected in lectins, ACL being the second after the potato lectin (*J. Biomol. Struct. Dyn.* **2017** doi.org/10.1080/07391102.2017.1345328).

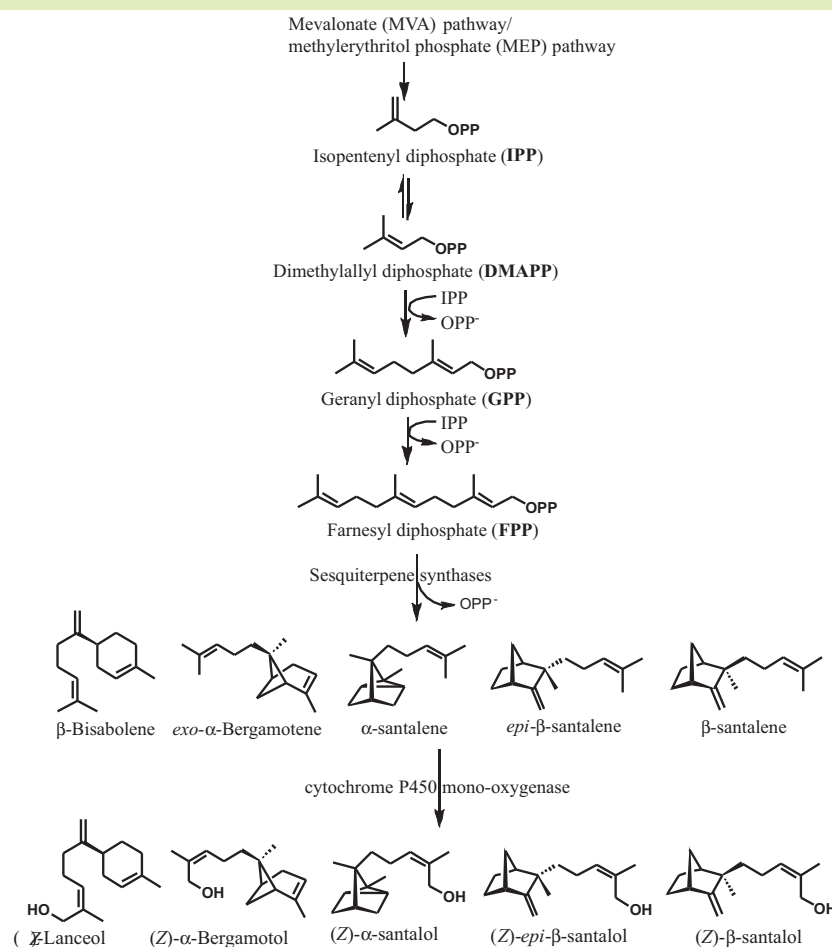


Chemical biology

Triterpenoid profiling and functional characterization of the initial genes involved in isoprenoid biosynthesis in neem: Neem tree (*Azadirachta indica*) is one of the richest sources of skeletally diverse triterpenoids called limonoids that are well-known for their broad-spectrum pharmacological and insecticidal properties. They are quantitatively profiled across various tissues. C-secotriterpenoids were observed in kernel as compared to the other tissues. Pericarp, flower and leaf contained mainly ring-intact triterpenoids. Transcriptome annotation led to the identification of the putative genes involved in isoprenoid biosynthesis. Two short-chain prenyltransferases, geranyl diphosphate synthase (AiGDS) and farnesyl diphosphate synthase (AiFDS) and squalene synthase (AiSQS) were cloned and functionally characterized. Furthermore, nine limonoids isolated/semi-synthesized from *A. indica* were screened for α -amylase inhibition which resulted in azadiradione and gedunin as lead molecules.

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Functional Characterization of Novel Sesquiterpene Synthases from Indian Sandalwood: Indian Sandalwood, *Santalum album* L. is highly valued for its fragrant heartwood oil and is dominated by a blend of sesquiterpenes. Transcriptome based approach in mining the putative genes aided in characterization of novel sesquiterpene synthases from Indian Sandalwood. Sesquiterpenes are formed through cyclization of farnesyl diphosphate (FPP), catalyzed by metal dependent terpenocyclases. This report describes the cloning and functional characterization of five genes, which encode two sesquisabinene synthases (SaSQS1, SaSQS2), bisabolene synthase (SaBS), santalene synthase (SaSS) and farnesyl diphosphate synthase (SaFDS). These results may pave the way for *in vivo* production of sandalwood sesquiterpenes in genetically tractable heterologous systems.



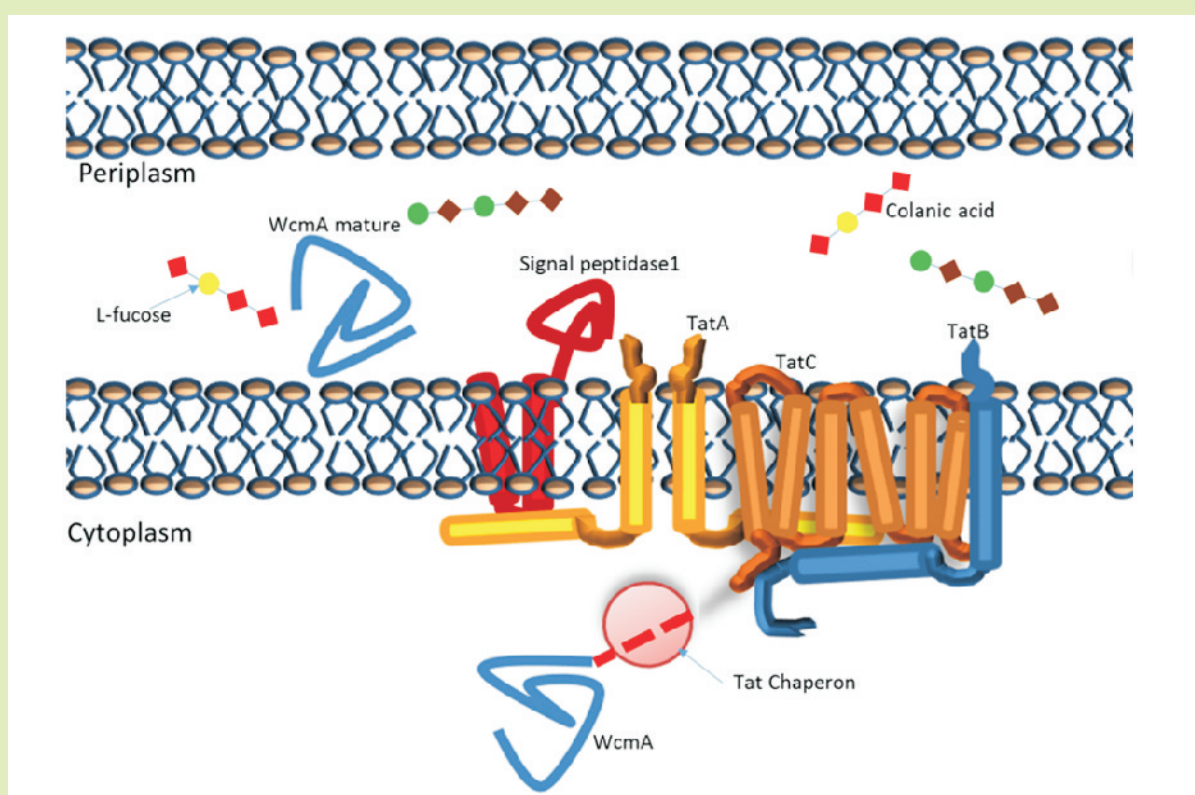
Healthcare

Screening methods and bioassays

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Evaluating a new high throughput twin arginine translocase assay in bacteria for therapeutic applications: A simple but efficient assay based on the quantification of the exopolysaccharide colanic acid was developed. Colanic acid contains a methylpentose (L-fucose) component, and its production is directly linked to the Tat pathway through the transport of enzymes

involved in polysaccharide biosynthesis was reported. Tat pathway involved in bacterial protein translocation and implicated in virulence and biosynthesis of exopolysaccharide colanic acid linked to Tat pathway. It reported the Colanic acid quantification as a specific and easy method to quantify Tat activity. The Assay can be used for high-throughput identification of Tat mutations and inhibitors (*Curr. Microbiol.* **2017**, 74, 1332).



Tat assay components and WcaM transport through the Tat pathway for colanic acid biosynthesis

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Hydralazine inhibits amyloid beta aggregation and glycation and ameliorates Ab1-42 induced neurotoxicity: It was shown that hydralazine, a potent glycation inhibitor inhibits Ab aggregation and fibril formation as evident by various biophysical assays such as fluorescence assays, atomic force microscopy, light

scattering assay circular dichroism. This is also corroborated with molecular dynamics simulations studies. This study suggested that hydralazine is a potential candidate for drug repositioning for the management of AD. However, it has to be re-engineered to reduce vasoactive effects and improve blood brain barrier permeability (*RSC Adv.* **2016**, 6, 108768).

Research & Development

Healthcare

Screening methods and bioassays

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Molecular typing of non-*Helicobacter pylori* bacteria isolated from dyspeptic cases: The diversity of non-*Helicobacter pylori* bacteria (*Ochrobactrum* spp.) was studied in urease-positive biopsies across three different geographical regions using molecular typing. About 62 *Ochrobactrum* isolates were recovered from patients ($n = 218$). *H. pylori* DNA was found in the majority of biopsies, which had variable degrees of *Ochrobactrum* sp. present. Based on phylogenetic analysis, the *Ochrobactrum* isolates were distributed into the *O. intermedium*, *O. anthropi* and *O. oryzae* groups. It is important to evaluate the commensal and

pathogenic nature of non-*H. pylori* bacteria (*J. Infect. Publ. Heal.* **2017**, *10*, 201).

Genome based insights into bacterial adaptation outside hosts: The group re-sequenced the gut bacterium *Ochrobactrum intermedium* M86 laboratory adapted strain and evaluated for gain and loss of genes. The strain lacked genes encoding transposase protein, insertion elements family, phage tail-protein. A 5 kb indel was detected in chromosome 2 was absent in original strain mapped with phage integrase gene of *Rhizobium* spp. and acquired and integrated through horizontal gene transfer indicating the gene loss and gene gain phenomenon in this genus (*Genomics Data* **2016**, *8*, 72).

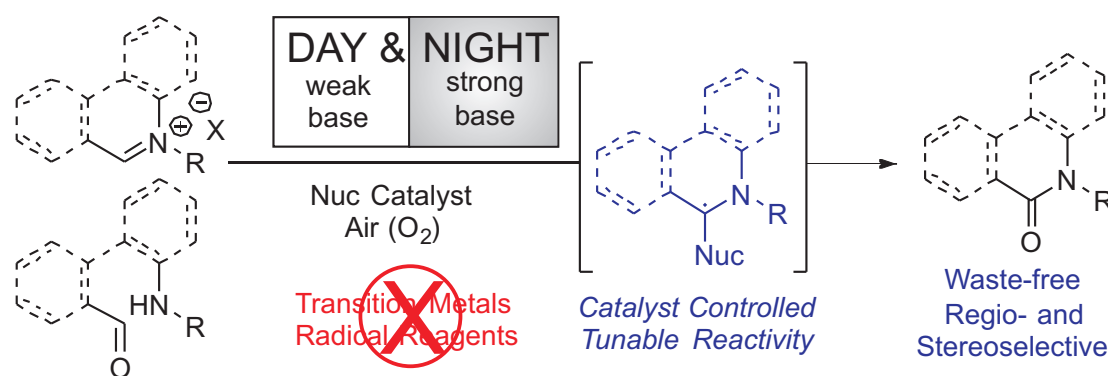
Synthesis of API

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New homogeneous catalytic methods for sustainable/green chemistry

A sustainable organocatalytic method for aerobic oxidation: A cheap and non-toxic nucleophilic catalyst-mediated aerobic oxidation of various types of iminium salts was reported via a novel catalyst-bound radical

intermediate whose tunable reactivity was successfully demonstrated, along with an unprecedented regiocontrol and kinetic resolution. This new mode of reactivity was extended for the oxidation of cyclic and acyclic iminium ions to lactam and amide, and has potential to be a general waste-free oxidative amidation method from aldehydes and amines (Provisional patent application filed # 201711008390).



Research & Development

Healthcare

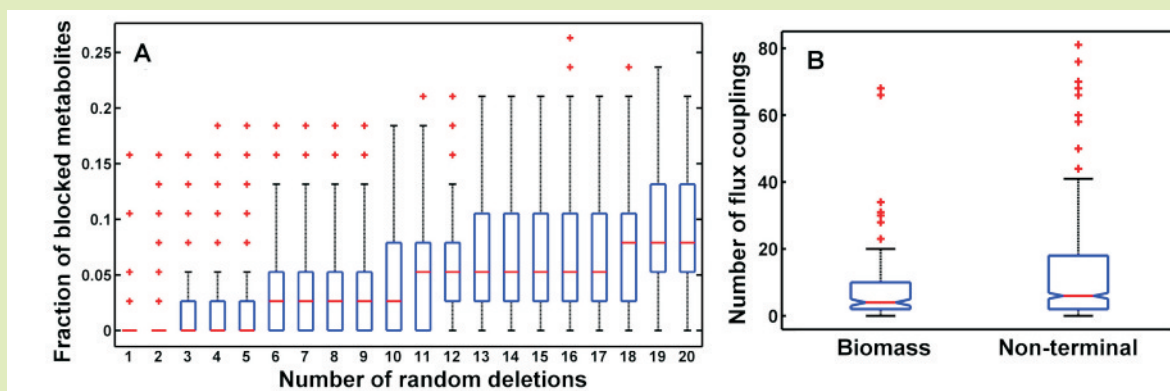
Mathematical modeling and big data analytics

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Modelling of biochemical processes to understand complexities of infectious diseases: Mathematical modeling, computational approaches and optimization techniques were used to understand the complexities of different biochemical pathways, their cross-talks and cellular interactions holistically. It helped to understand the progression of complex diseases and identify potential treatment strategies. It has brought out many potential drug targets to counteract and control the disorders, which constituted a basis for system level understanding and has potential application in pharmaceutical industry.

Metabolic adaptations of the *Leishmania* parasite a new insight for KalaAzar: The role of the underlying metabolic network structure in metabolic adaptation of *L. infantum* to the host environment was investigated. A new manually reconstructed genome-scale metabolic network model (iAS556) was proposed for the species *Leishmania infantum* JPCM5 (a well characterized *L. infantum* strain), consisting of 1260 reactions and 1160 metabolites. From the analysis and simulations, it was hypothesized that the

underlying reaction stoichiometry and reversibility present within the *L. infantum* metabolic network were adequate to explain these specific route selections, which remained conserved across developmental stages. The corresponding flux changes are governed only by the constraints on uptake of environmental metabolites. The analyses of the proposed *L. infantum* genome-scale constraint-based model revealed the simple organization of the *Leishmania* metabolome and its usage to achieve complex metabolic phenotype traits for optimal synthesis of essential metabolites under varying host environments. The *L. infantum* genome scale flux-coupled network structure was highly modular and assortative, thereby remaining robust to a random node failure. This model-based analysis provided many testable hypotheses to design suitable experiments for identification of adaptive strategies of *L. infantum* within the host. Further, it may help the human community to combat against this neglected, but deadly tropical parasitic infection and provide fresh impetus for further targeted studies in *Leishmania* metabolomics and drug discovery (*Sci. Rep-UK* 2017, 7, 10262.).



Robustness of *L. infantum* metabolic network to random deletion - A) Fraction of biomass metabolites that are totally blocked after a set of random deletions B) Comparison of flux couplings of biomass forming reactions with non-terminal reaction

Healthcare

Mathematical modeling and big data analytics

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Cholesterol-dependent conformational plasticity of GPCR dimers: The organization and function of the serotonin_{1A} receptor, the main target in clinical depression were shown to be cholesterol-dependent, although the molecular mechanism is not clear. An analysis of dimerization of the serotonin_{1A} receptor was performed to explore the molecular details of its

cholesterol-dependent association. A major finding was that the plasticity and flexibility of the receptor dimers increase with increased cholesterol concentration. In particular, a dimer interface formed by transmembrane helices I was found to be sensitive to cholesterol. These results represent an important step in characterizing the molecular interactions in GPCR organization with potential relevance to therapeutic interventions (*SciRep.* **2016**, 6, 31858).

Diagnostics and therapeutics

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Placental proteomics predicts potential markers of preeclampsia: Pre-eclampsia is a hypertensive disorder characterized by the new onset of hypertension and proteinuria during gestation. Placental proteomics was performed for normotensive and pre-eclamptic patients. Out of total of 2145 proteins in the placenta, 180 were differentially expressed (>1.3 fold, $p < 0.05$). Gene ontology enrichment analysis of biological process suggested that the differentially expressed proteins belonged to various physiological processes implicated in the pathophysiology of pre-eclampsia. MRM analysis of plasma showed an increase in apolipoproteins A-I and A-II in pre-eclamptic patients. The study provided a proteomic insight and identified potential biomarkers associated with pre-eclampsia pathogenesis (*J. Proteome Res.* **2017**, 16, 1050).

Tubulointerstitial nephritis antigen-like 1 protein is downregulated in the placenta of pre-eclamptic women: Tubulointerstitial nephritis antigen-like 1 protein (TINAGL1), is a matricellular protein, known to play role in cell adhesion and cell receptor interaction. Research related to TINAGL1 is limited to cell culture and animal models. Demonstration of TINAGL1 as a positive regulator of angiogenesis and its expression in the decidua of postimplantation mouse uterus, prompted to validate its expression in human placenta during impaired angiogenesis in pre-eclamptic condition. This is the first study reporting TINAGL1 to be present in human placenta and differentially expressed in pre-eclamptic condition. The functional role of TINAGL1 in association to human pregnancy needs to be explored further (*Clin. Proteom.* **2017**, 14, 8).

Shrikant Madhukar Ghike sm.ghike@ncl.res.in

Metabolic syndrome– A truly psychosomatic disorder? A global hypothesis: Exact cause of the metabolic syndrome [MS] is still unclear. Man has same fundamental needs to live as animals. Contrarily none of the animals needs to earn money. Today money has become the sole life essential need. Brain is also an organ of the human body with a unique thought process. Life is a flow of desires followed by logical actions. The person struggles to attain desired goals via the all static load but a perceived insurmountable threat can make his flow of life stalled to freeze him. Published data from varied branches of medical science indicates role of a few hormones in overall homeostasis. From the integration of observations from published data, it is hypothesized that a perceived trapped situation in life creates acute chaos of thoughts in brain, which results in acute imbalance of a few but major hormones, which in turn triggers MS, and implies psychosomatic roots of the disorder. In addition to measurable concentration of the individual hormones, their ratios can be used effectively as the diagnostic markers and can pave a better way in deciding a personalized holistic protocol with combination of counter regulatory medications (*Med. Hypotheses* **2016**, 97, 46).

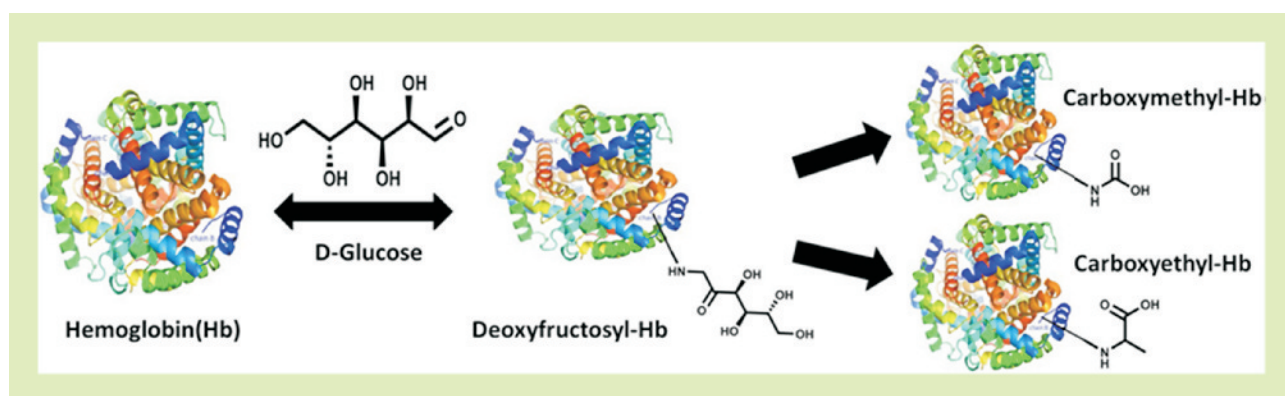
Healthcare

Diagnostics and Therapeutics

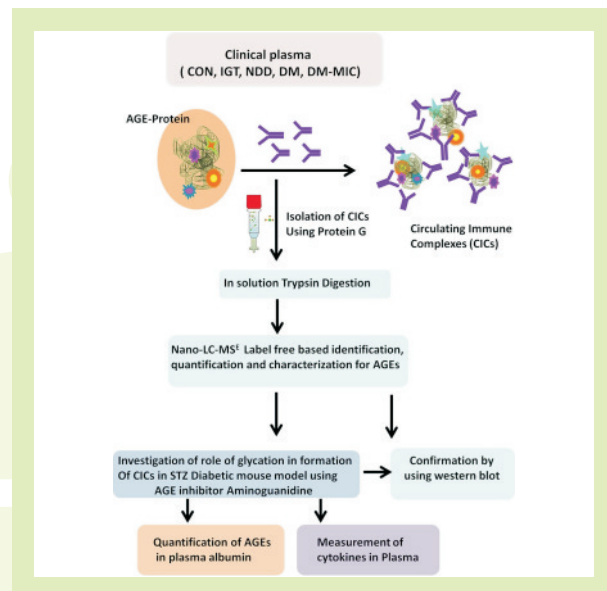
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Targeted quantification of N-1-(carboxymethyl) valine and N-1-(carboxyethyl) valine peptides of β -hemoglobin for better diagnosis in diabetes: N-1-(deoxyfructosyl) valine (DFV) β -hemoglobin (β -Hb), commonly referred as HbA_{1c}, is widely used diagnostic marker in diabetes, believed to provide glycemic status of preceding 90-120 days. However, during the lifespan

of hemoglobin (~120 days), the DFV- β -Hb, an early and reversible glycation product eventually may undergo irreversible advanced glycation modifications such as carboxymethylation or carboxyethylation. Hence, N-1-(carboxy-methyl) valine (CMV) and N-1-(carboxyethyl) valine (CEV) peptides of β -Hb were quantified that could be a useful parameter for assessing the severity of diabetes and may provide better alternative diagnostics (*Clin. Proteom.* **2016**, *13*, 7).



Elevated levels of albumin in circulating immune complexes in diabetic plasma: Advanced glycation end products (AGEs) elicit immune response and form complexes with immunoglobulins called circulating immune complexes (CICs) in diabetes. Proteomic analysis of CICs in clinical diabetic revealed elevated serum albumin in the CICs, which were also observed to be AGE modified. Aminoguanidine treated diabetic mice displayed decreased AGE modification of plasma albumin, accompanied by a reduced level of albumin in the CICs. In addition, elevated levels of proinflammatory cytokines such as IL-1 β , IL-2, and TNF- α were observed in diabetes, which were reduced with aminoguanidine treatment, suggesting the involvement of glycation in the immune response (*Mol. Cell Proteom.* **2016**, *15*, 2011).

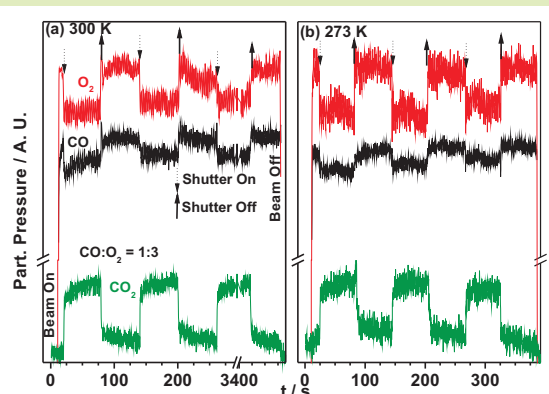
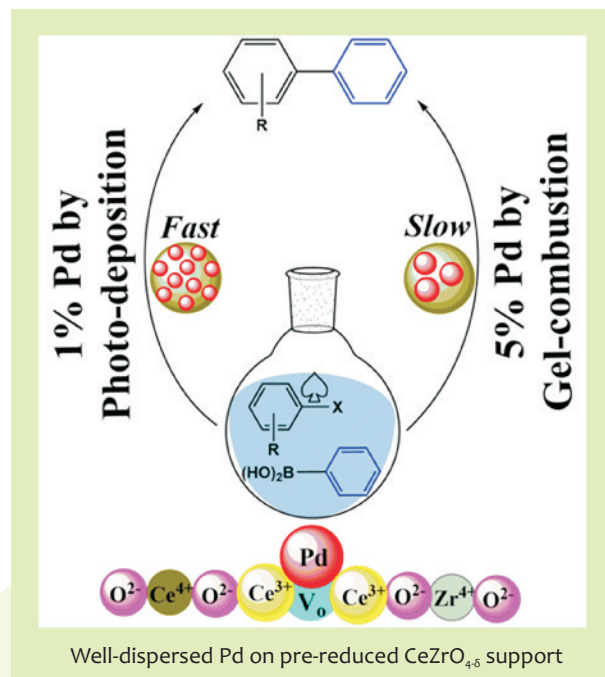


Catalysis

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Environmental catalysis

Ambient CO oxidation: Nanorod form of Co_3O_4 spinel was shown to oxidize CO at ambient temperatures in the literature. However, a simple surface oxidation of polycrystalline Co-metal surfaces with molecular oxygen led to Co_3O_4 spinel with random morphology. It showed to exhibit sustainable ambient CO oxidation activity even in the presence of up to 30 ppm moisture content in the reaction feed. Co oxidation by molecular oxygen, random morphology and tolerance towards moisture content up to 30 ppm made the present effort attractive and also provided further scope to improve the catalytic performance. The results complemented and broadened the ambient CO oxidation catalysis reported for Co_3O_4 nanorod (ChemistrySelect 2017, 2, 533).



CO oxidation reaction measured at (a) 300, and (b) 273 K

Fine chemical: Pd on redox $\text{CeZrO}_{4.5}$ catalysts was shown to be active for Suzuki coupling reaction in water-medium under reflux condition. 1 wt % Pd on pre-reduced $\text{CeZrO}_{4.5}$ support requires a mere 20 min. for 100% conversion of Suzuki coupling. Present work hints the possibility of achieving high conversion for Suzuki reaction with very small amount of Pd through better dispersion by taking advantage of redox support (ChemistrySelect 2016, 2, 2673).

Fundamental Mechanistic Studies in Catalysis

Bridging the material gap: An attempt has been made to bridge the material gap, exists between ideal single crystals and real world powder nanocatalyst employed in surface science and heterogeneous catalysis, respectively. Extremely different conditions most often lead to a “disconnect” between the findings from ideal and real world conditions. Simple wet chemical method has been applied to make $\text{Ce}_{1-x}\text{Zr}_x\text{O}_2$ ($x = 0-1$) (CZ) thin films with high surface quality. Porous nature of Ce-rich CZ compositions enhances O_2 adsorption and oxygen storage capacity (OSC), predominantly due to O-diffusion and redox nature, even at 400 K. A good correlation exists between O_2 adsorption measurements made on CZ films for oxygen adsorption, and OSC, and ambient pressure CO oxidation on powder form of CZ; this demonstrates the large potential to bridge the material gap (Catal. Struct. React. 2016, 2, 1).

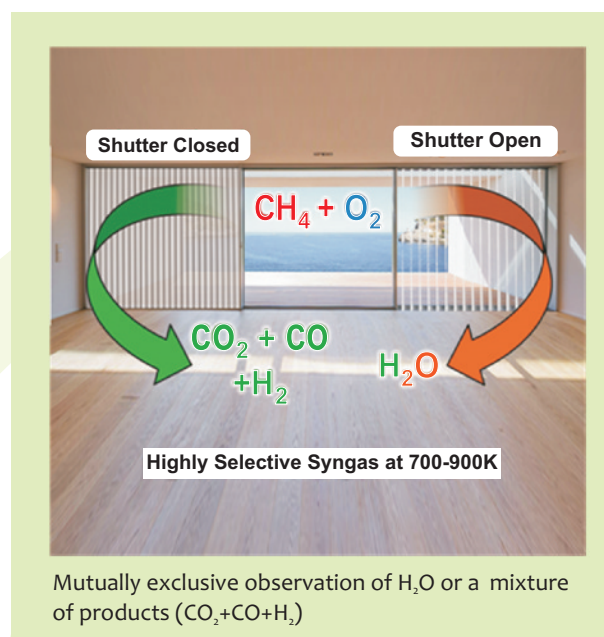
Sustainable Chemical Industry

Catalysis



C-H activation of methane: Selective conversion of methane to oxygenates, such as formaldehyde, syngas is important to exploit natural gas reserves. Formaldehyde is the simplest aldehyde which is an important precursor for many useful chemical compounds. Similarly with syngas, many hydrocarbon products are possible. The direct and selective oxidation of methane to oxygenates is very difficult process as it requires high temperature (~1000 K and above) for the activation of C-H bond. In the past few decades many efforts have been made to prepare

active catalysts for methane to oxygenates with molecular oxygen. In the present work, ceria-zirconia and Mn-doped ceria-zirconia are shown to produce syngas and formaldehyde, respectively, from methane and oxygen. Molecular beam methods also provide information about the mechanism of methane activation (*ChemCatChem*; 2016, 8, 2296, 3650).

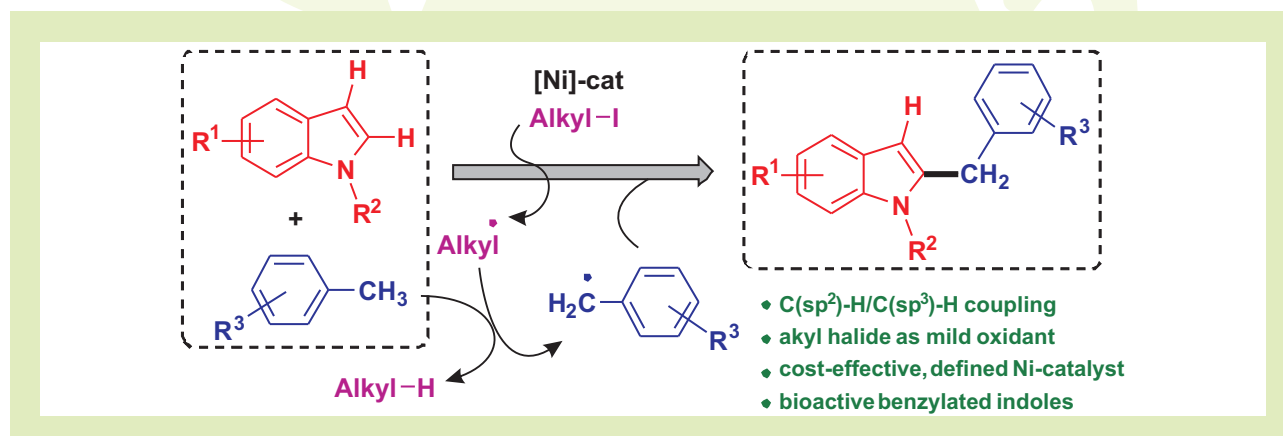


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Unified strategies for the nickel-catalyzed C-H bond functionalization

Nickel-catalyzed C(sp²)-H/C(sp³)-H coupling of indoles with toluene derivatives: A nickel-catalyzed method

for the regioselective C-2 benzylation of indoles was demonstrated via C(sp²)-H/C(sp³)-H oxidative coupling of indoles with toluene derivatives using 2-iodobutane as an oxidant. The method allowed coupling of diverse indoles with various toluene derivatives (*ACS Catal.* 2017, 7, 4202).



Research & Development

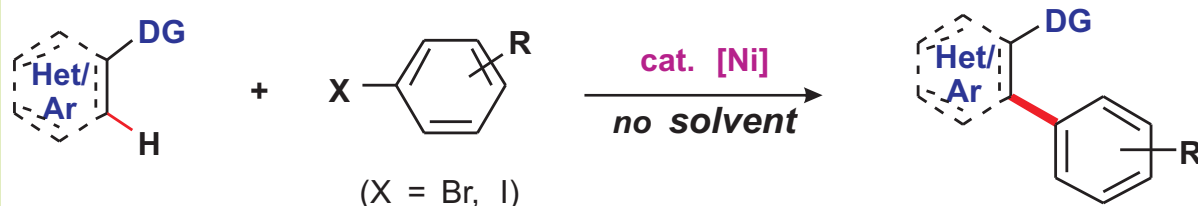


Sustainable Chemical Industry

Catalysis

Solvent-free nickel-catalyzed C-H arylation of arenes and heteroarenes: An efficient solvent-free nickel-catalyzed method for the C-H bond arylation of arenes and indoles was described that proceeded expeditiously *via* chelation-assistance. The reaction was

highly selective for mono-arylation. It tolerated sensitive and structurally diverse functionalities, such as halides, ethers, amines, indole, pyrrole and carbazole (*ChemSusChem* **2017**, 10, 2242).



- ♦ **Expeditious and solvent-free**
- ♦ **Selective mono-arylation**
- ♦ **Cost-effective, defined Ni-catalyst**
- ♦ **Arenes and indoles**

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Multifunctional catalyst for sustainable process development

Tandem synthesis of glycidol via transesterification of glycerol: Glycidol (GD) is a raw material for polyglycerols, glycidyl ethers and pharmaceuticals, as well as in perfumes and cosmetics, detergents, paints, de-emulsifiers, plastic modifier, surfactant and fire retardant. It is a substituent for epichlorohydrin which eliminates HCl generation. BaO in combination with lanthanides particularly, Ba-Ce (1-1) was found to be the best catalyst for glycerol transesterification to GC followed by its decarboxylation to give glycidol (80%). The strong basicity alone with the presence of oxygen vacancies in ceria lattice played an important role in decarboxylation step to adsorb CO₂ liberated in the decarboxylation step (*ACS Sustain. Chem. Eng.* **2017**, 5, 1763).

Tandem hydrogenation and aldolization of furfural without external hydrogen: Single pot CTH of furfural to furfuryl alcohol without external hydrogen and simultaneous aldolization of carbonyl compounds with furfural was achieved over non-noble metal oxides with bifunctional sites. Basic sites of MgO responsible for abstraction of proton showed complete conversion of furfural to give furfuryl alcohol and C8 monomer in a ratio of 3:1, respectively, later it altered to 1:1 by

an excellent activity with complete conversion and selectivity (>99%) to GVL in presence of IPA as H-donor (*Catal. Lett.* **2016**, 146, 1611; Patent: US 9527826 B2).

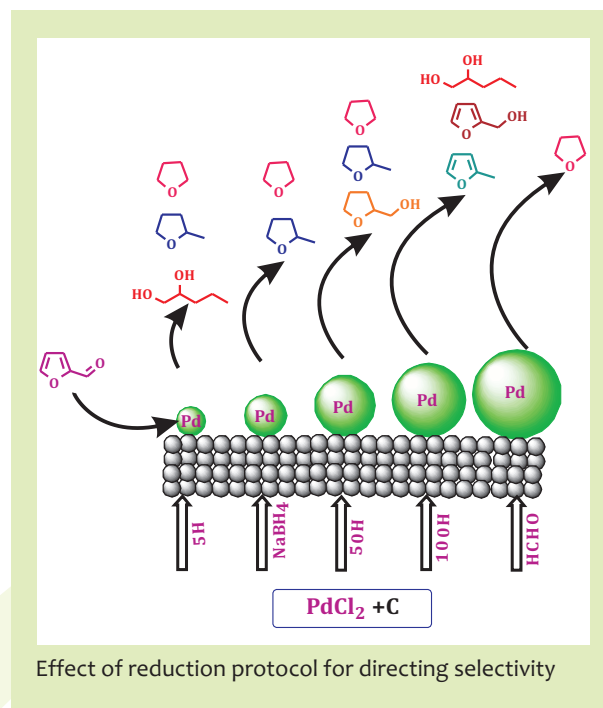
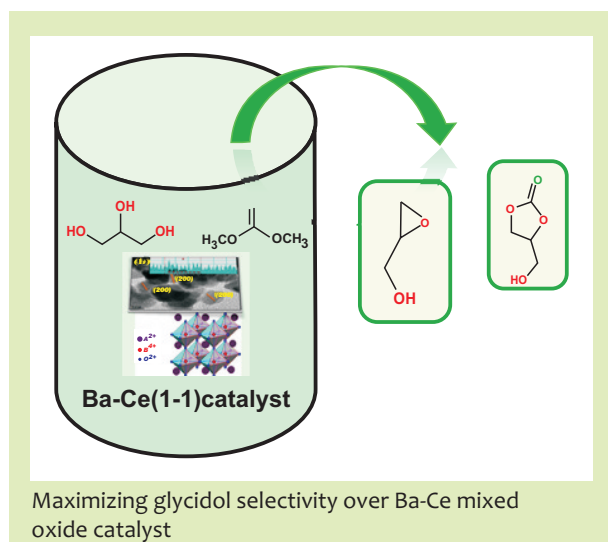
Selectivity tuning of diols and propanol in glycerol hydrogenolysis: The structural differences of the support materials affecting the dispersion and particle size of the Ru directly influenced the activity and product selectivities in glycerol hydrogenolysis. Added phosphotungstic acid led to the formation of 1,3-propadiol and enhanced 1-propanol selectivity, the later by hydrogenation of 1,2-PDO mediated by carbonium ion under acidic conditions. In absence of an acid additive (PTA), glycerol conversion increased from 44 to 58% for AC supported Ru, with major selectivities to the C-O and C-C bond cleavage products without any formation of 1,3-PDO and excessive hydrogenolysis product, 1-propanol was minimum to < 2%. This confirmed that the addition of acid additive (PTA) suppressed the C-C cleavage facilitating the formation of 1,3-PDO and 1-propanol (*Appl. Catal. B-Environ.* **2017**, 204, 134).

Effect of reduction protocol of Pd catalysts on product distribution in furfural hydrogenation: Particle size variation of Pd/C catalyst achieved using various chemical reducing agents and 5-100% molecular hydrogen led to product selectivity tuning in the single step hydrogenation of FFR. Pentanediol formation was favoured at 180 °C and 100 psi H₂ pressure while ring hydrogenation and decarbonylation occurred at higher

Sustainable Chemical Industry

Catalysis

temperature and H₂ pressure. Thus, integration of catalyst characteristics with the process conditions afforded to tune the selectivities in a multiproduct hydrogenation of furfural (*ChemistrySelect*, 2017, 2, 24).

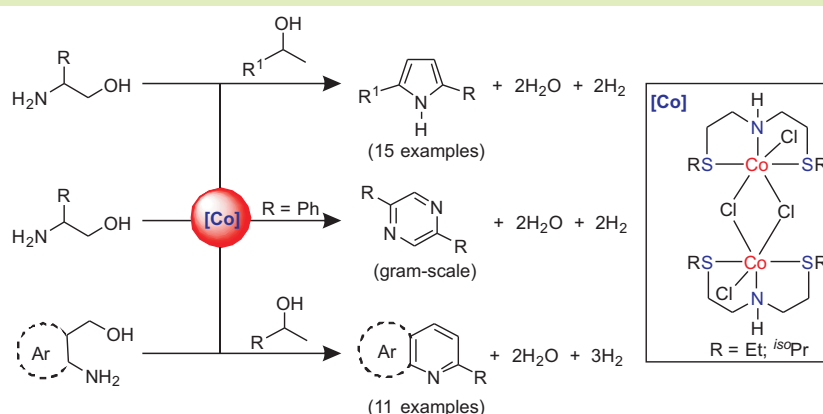


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Acceptorless dehydrogenation and hydrogen-atom transfer related reactions

Molecularly-defined homogeneous catalysts: The replacement of noble metals with base metals for similar or better reactivity is one of the promising approaches in homogeneous catalysis. However, the search for an efficient catalytic system based on base-metal catalysts for sustainable chemical transformations is extremely rare due to the challenge of working with paramagnetic materials (mostly

kinetically labile) and also due to underdeveloped mechanistic studies. Our group reported the first example of a new, molecularly defined SNS-cobalt(II) catalyst for the acceptorless dehydrogenative coupling (ADC) of unprotected amino alcohols with secondary alcohols leading to pyrrole and pyridine derivatives. This reaction proceeded with high step-economy via a sequence of acceptorless dehydrogenation (AD), condensation and annulation steps that efficiently led to the selective C–N and C–C bond formations, thereby releasing hydrogen gas and water as the sole by-products (*Catal. Sci. Technol.* 2017, 7, 3177).



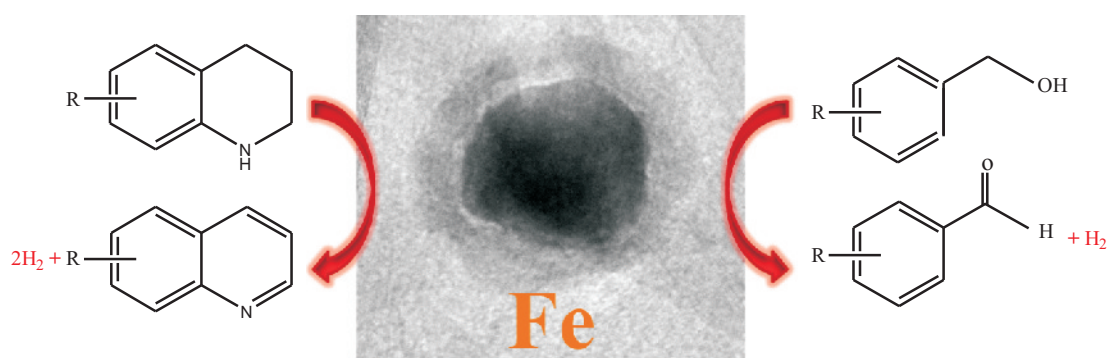
Research & Development

Sustainable Chemical Industry

Catalysis

Heterogeneous catalysis: The key research objective was to convert homogeneous catalytic reactions into heterogeneous versions (replacement of precious metal catalysts by first-row transition elements) through the attachment of catalytic sites on stable supports. Our approach involved a thermal decomposition of a molecular complex of a metal on a carbon support to obtain supported robust nanocatalyst and have designed several environmentally benign catalytic reactions, in particular acceptorless

dehydrogenation and related reactions based on developed nanocatalysts. No report had described a reusable iron-based heterogeneous catalyst for oxidant-free and acceptorless dehydrogenation reactions. It replaced expensive noble metal catalysts with an inexpensive, benign, and sustainable nanoscale iron catalyst for the efficient acceptorless dehydrogenation of N-heterocycles and alcohols with liberation of hydrogen gas (*Nature Commun.* **2017**, DOI: 10.1038/s41467-017-01603-3).



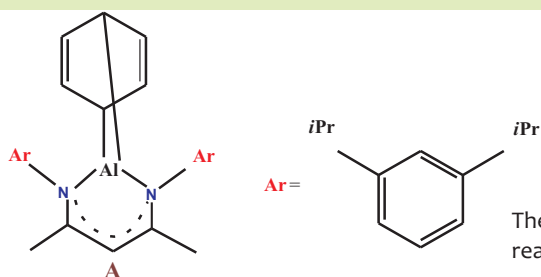
Iron-based nanocatalyst for the acceptorless dehydrogenation reactions

Kumar Vanka k.vanka@ncl.res.in

Computational studies of small molecule activation by main group complexes

Explicit catalytic role of solvent in low valent aluminum chemistry: The single site activation of strong σ bonds remains a significant challenge in main group chemistry, with only a few cases reported to date. The experiments done with Al^I complexes hold major significance as they too were seen to activate a variety of strong σ bonds. The current computational studies with density functional theory (DFT) revealed the interesting reason for this: it is seen that

an explicit aromatic solvent molecule acted as a catalyst by converting the Al^I complex to Al^{III} during the process. Different cases of σ bond activation by Al^I complexes were investigated and the efficiency for the H-X (X=H, NHtBu, PPh₂) bond activation in the presence of an explicit benzene solvent molecule was seen to be orders of magnitude higher than in its absence. The current work therefore revealed the chemistry of Al^I complexes to be richer and more complex than realized to date, and showed it to be dependent on metal-solvent co-operativity, the first known example of its kind in main group chemistry (*Chem. Eur. J.* **2017**, 23, 13957).



The optimized geometry of the complex "A" formed by reaction of the $Al(I)$ complex with benzene

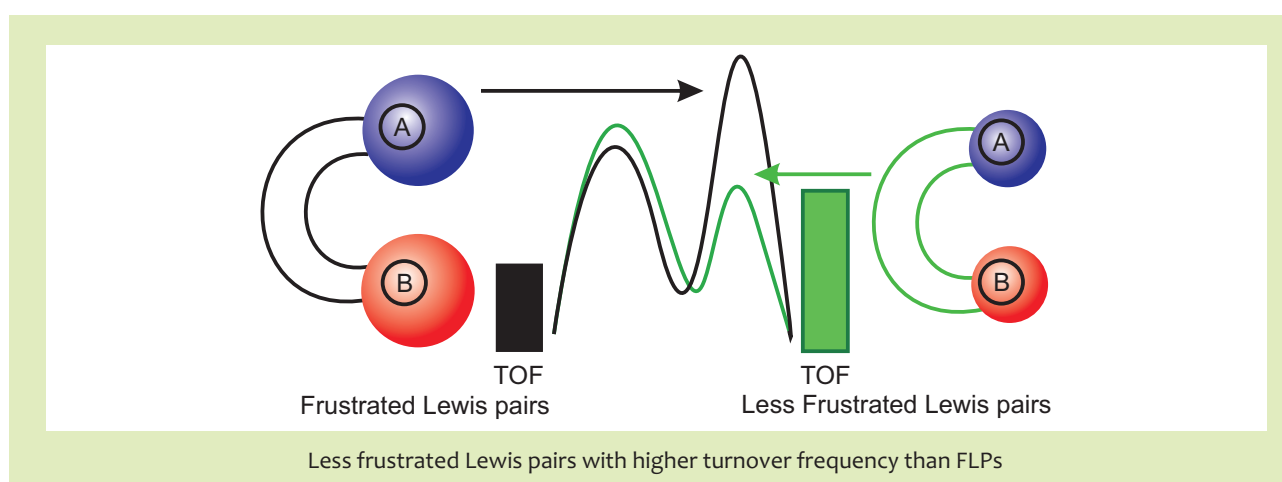
Research & Development

Sustainable Chemical Industry

Catalysis

Theoretical insights into frustrated lewis pairs for hydrogenation catalysis: A wide variety of FLP based systems can catalyze the hydrogenation of a range of different substrates, including imines, enamines, ketones, alkynes and alkenes. However, FLP based hydrogenation catalysts are yet to match the efficiency of their transition metal counterparts. The current investigation addresses this issue, and revealed an important aspect of FLPs that can be exploited to improve their efficiency. What is shown is that the more sterically hindered the FLP catalyst, the lower is

its turnover frequency (TOF). Full quantum chemical calculations with DFT for a family of different, experimentally known hydrogenation FLP catalysts showed that in every case, superior FLP catalysts can be designed by reducing the frustration (by reducing the steric demand and acid/base strength) in the FLP. However, since lowering the sterics without reduction in the frustration can result in unwanted side reactions what became clear is that the design of the most efficient FLP catalysts depended on tuning the system so that both the sterics and the frustration were reduced appropriately (ChemCatChem 2017, 9, 3013).



Mathematical and computational modeling

Kavita Joshi k.joshi@ncl.res.in

Unraveling role of oxygen in ethylene oxidation on Ag surface: Ethylene oxide is one of the most produced organic chemicals and Global Industry Analyst (GIA) has forecasted consumption of ethylene oxide to exceed 27 million tons by 2017. Thus, ethene epoxidation on silver surface to produce ethylene oxide (EtO) is one of the most important reactions. This reaction is a classic example of kinetically controlled reaction as thermodynamic equilibrium leads to total oxidation of ethene into CO and H₂O. The driving force in research is to increase selectivity towards formation of EtO. We have investigated role of surface and subsurface oxygen in this reaction in order to unravel the reaction mechanism.

Understanding reactivity at nanoscale: Catalytic properties of clusters have been investigated extensively through experiments as well as simulations. In recent years, clusters as catalyst has been explored extensively and their importance as catalyst has realized beyond doubts. However, an explicit correlation between size - structure - reactivity has to be established yet. We have investigated clusters to understand their reactivity as a function of size, structure and temperature with a goal to built a predictive model of reactivity at nanoscale. Specifically we are investigating dissociation of N₂ on Al clusters at elevated temperatures.

Research & Development

Sustainable Chemical Industry

Process intensification and engineering

Sanjay P. Kamble sp.kamble@ncl.res.in

A process for the synthesis of bio-lubricants using heterogeneous catalyst: A cost effective process was developed for the synthesis of bio-lubricants with very low acid value by direct esterification of polyol with carboxylic acid using metal-doped on zeolite 13-X catalyst. The salient feature of the process is that it is solvent free and requires less reaction time as

compared with conventional route. Catalyst can be easily separated because of its heterogeneous property; it can be reused in many cycles. The esterification was performed under reduced vacuum in reactive distillation mode of operation so the reaction time was considerably reduced. The colorless quality bio-lubricants were produced having acid value below 0.01 and desired viscosity value was achieved as required for industrial applications (Patent Appl.: IN 201711001598).

Process development and scale-up

A process for the preparation of tertiary butyl phenol: There is a need to develop eco-friendly, cost effective route for the synthesis of tertiary butyl phenols. In this work an eco-friendly catalytic process was developed for the synthesis of Tertiary butyl phenol where homogenous catalyst was used for the reaction.

The major merits of this developed process are i) for isolation of reaction product, a viable simple extraction method was established ii) the developed process led to higher selectivity towards *p*-TBP and 2,4-DTBP based on reaction conditions (Patent Appl.: IN 201611035582).

Agriculture, Food and Nutrition

Crop protection

Chickpea-fusarium interaction transcriptome reveals differential modulation of plant defense strategies:

The transcriptomes of wilt-susceptible and wilt-resistant cultivars were investigated under both *Fusarium oxysporum* f.sp. *ciceri* (Foc) challenged and unchallenged conditions using LongSAGE, that revealed several known and novel genes with differential or unique expression patterns contributing to lignification, hormonal homeostasis, plant defense signaling, etc. Similarly, several Foc genes required for its survival and growth expressed only in the susceptible cultivar. This study revealed a rich resource for functional characterization of plant defense genes and their use in breeding wilt-resistant varieties. It also provided pathogen targets to facilitate development of novel control strategies (*Sci. Rep-UK* 2017, 7, 7746).

Colonization and expression of pathogenicity related genes in *Fusarium oxysporum*: The Foc was transformed using GFP and used it to characterize pathogen progression and colonization in wilt-susceptible and wilt-resistant cultivars using confocal microscopy. The qPCR was employed to estimate pathogen load across various tissues of chickpea cultivars during the disease. The expression of several pathogen virulence genes analyzed using qRT-PCR showed characteristic expression in wilt-susceptible cultivar. It was concluded that the pathogen defeats defense of the susceptible cultivar to colonize it. However, due to its efficient defense mechanism, pathogen proliferation was severely restricted in the resistant cultivar (*Plos One* 2016, DOI: 10.1371/journal.pone.0156490).

Functional food and nutrition

V. Koteswara Rao v.koteswara@ncl.res.in

Effect of antioxidants of culinary herbs and spices for the management of mycotoxins: Plant derived antioxidants were explored to mitigate the ill effects of the mycotoxins and to suppress mycotoxin contamination in foods using *C. zeylanicum*, *C. longa*, *A. sativum*, *M. spicata* and *N. sativa* and their chemical constituents (*ISMP* 2017, 46, 8).

Production of thermostable lipase by *Thermomyces lanuginosus*: A thermophilic fungus, *Thermomyces lanuginosus* NCIM-1394 (HE984155) was isolated that showed high lipase production at pH 6.5 and at 50°C (*J. Basic Applied Sci.* 2017, 6, 1).

Microbial synthesis of mammalian metabolites of spironolactone by *Thermomyces lanuginosus*: Spironolactone and its major metabolite, canrenone are mineralocorticoid receptor antagonists. The thermophilic fungus *Thermomyces lanuginosus* NCIM-1394 (HE984155) transformed 75% of the steroidal drug, spironolactone to canrenone. This strain transformed SPI into four metabolites viz. 7- α -thio-SPI (M_1), active metabolite canrenone (M_2), 7- α thiomethyl SPI (M_3) and 6 β -OH-7 α -thiomethyl SPI (M_4). The study demonstrated the potential of *T. lanuginosus* in the synthesis of metabolites of spironolactone similar to mammals in an ecofriendly and economical way. This fungus showed the potential to use as a model organism for studying drug metabolism and also in synthesizing huge quantity of metabolites for pharmacological studies.

Industrial production of penicillin V by *Penicillium chrysogenum*: The screening of the fungi *P. chrysogenum* was undergone successfully and got five high-yielding strains. Further, optimization and strain improvement is under process.

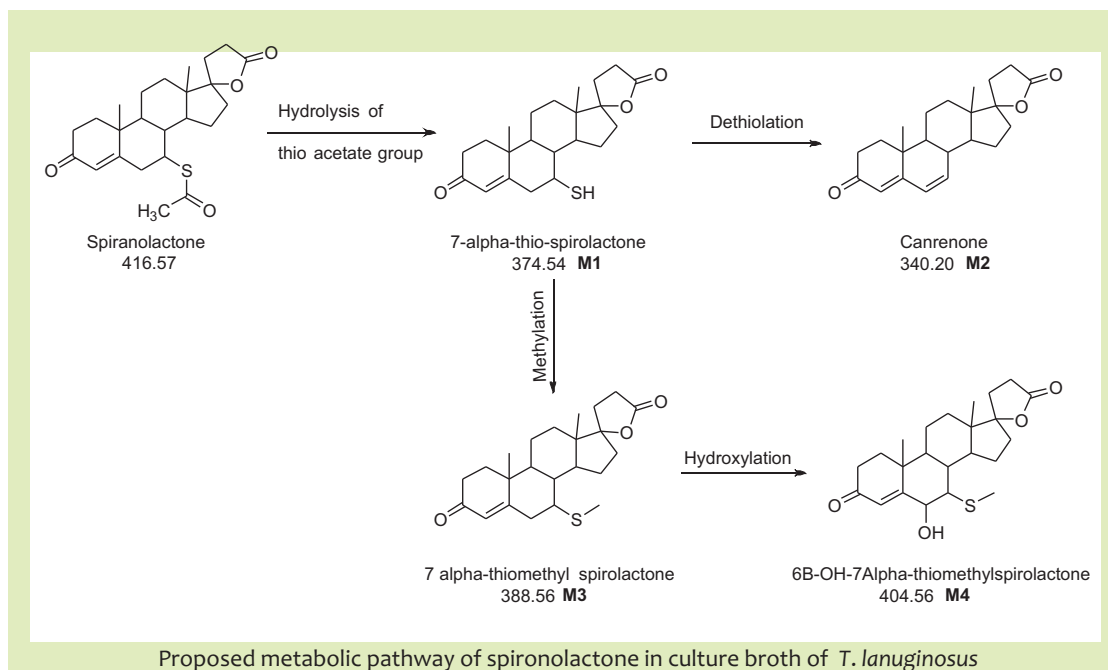
Mycosynthesis of gold nanoparticles and their biomedical applications: The non-toxic gold nanoparticles (AuNPs) were synthesized by *Penicillium rubens* and evaluated for antifungal and mycotoxin, Ochratoxin A production. Biosynthesised AuNPs showed particle size in the range of 3.84–12.14 nm. The AuNPs demonstrated significant antifungal activity

Agriculture, Food and Nutrition

Functional food and nutrition

against *P. verrucosum* and complete inhibition was observed at 70 µg/ml. Further, the AuNPs were evaluated against HeLa cell line for the cervical cancer

and it showed growth inhibition (GI) at 46.97µg/ml. These AuNPs showed applications in management of fungal toxins in processed food and to treat cancers.



Plant secondary metabolites and pathway analysis

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

Insights in to alphonso flavor biogenesis and delayed ripening: The isolation and characterization of 9-lipoxygenase and epoxide hydrolase 2 genes was undergone that provided molecular insight into lactone biosynthesis in mango fruit (*Mangifera indica* L.). Further, transcriptional analysis of different stages was performed that provided transitions during fruit development and ripening that explained distinct aroma and shelf life characteristics of Alphonso mango fruits (*Phytochemistry* **2017**, 138, 65; *Sci. Rep.-UK* **2017**, 7, 8711).

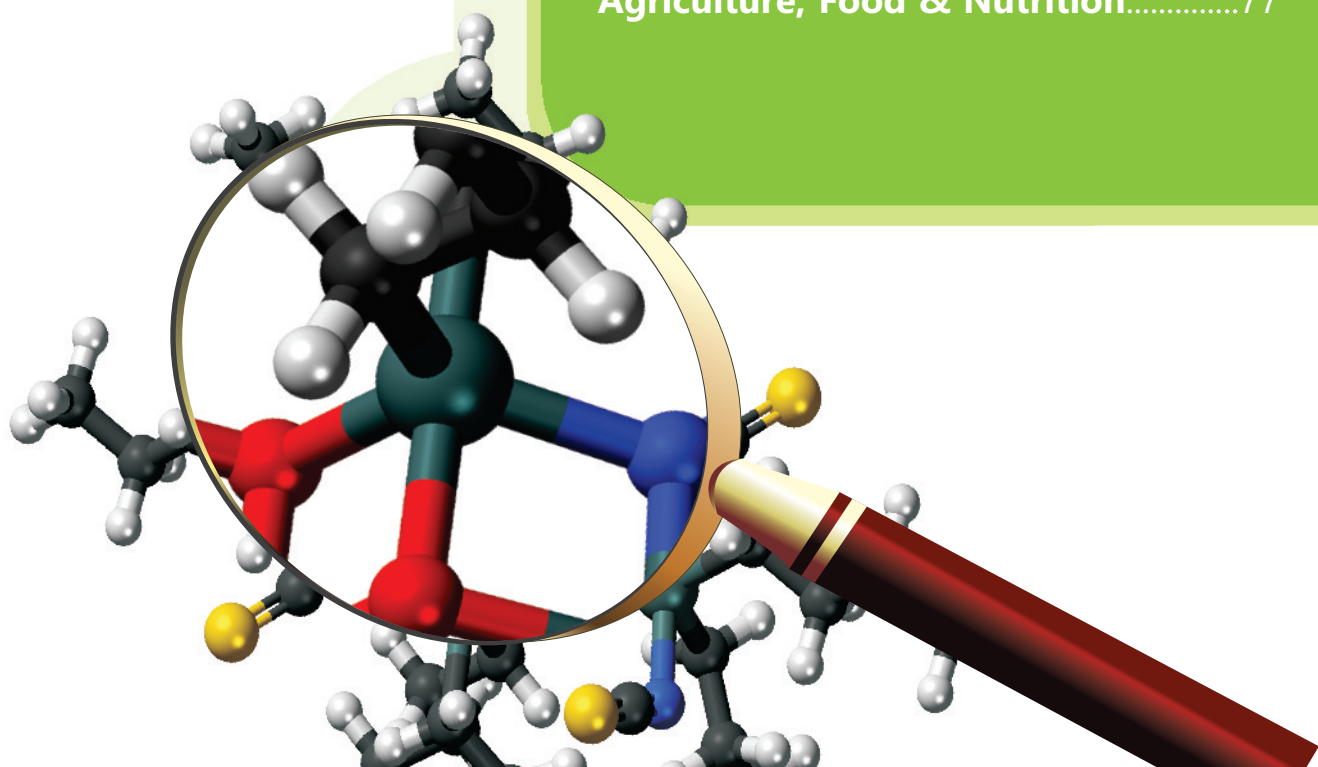
Plant cholesterol biosynthetic pathway in tomato: Integrating tomato transcript and protein co-expression data revealed candidate genes putatively associated with cholesterol biosynthesis. A combination of functional assays including gene silencing, examination of recombinant enzyme activity and yeast mutant complementation suggested the cholesterol

pathway comprises 12 enzymes acting in 10 steps. This work has contributed to this project going on at Weizmann Institute of Science, Israel collaboration initiated during the visit under Raman Research Fellowship program (*Nat. Plants* **2016**, 3, 16205).

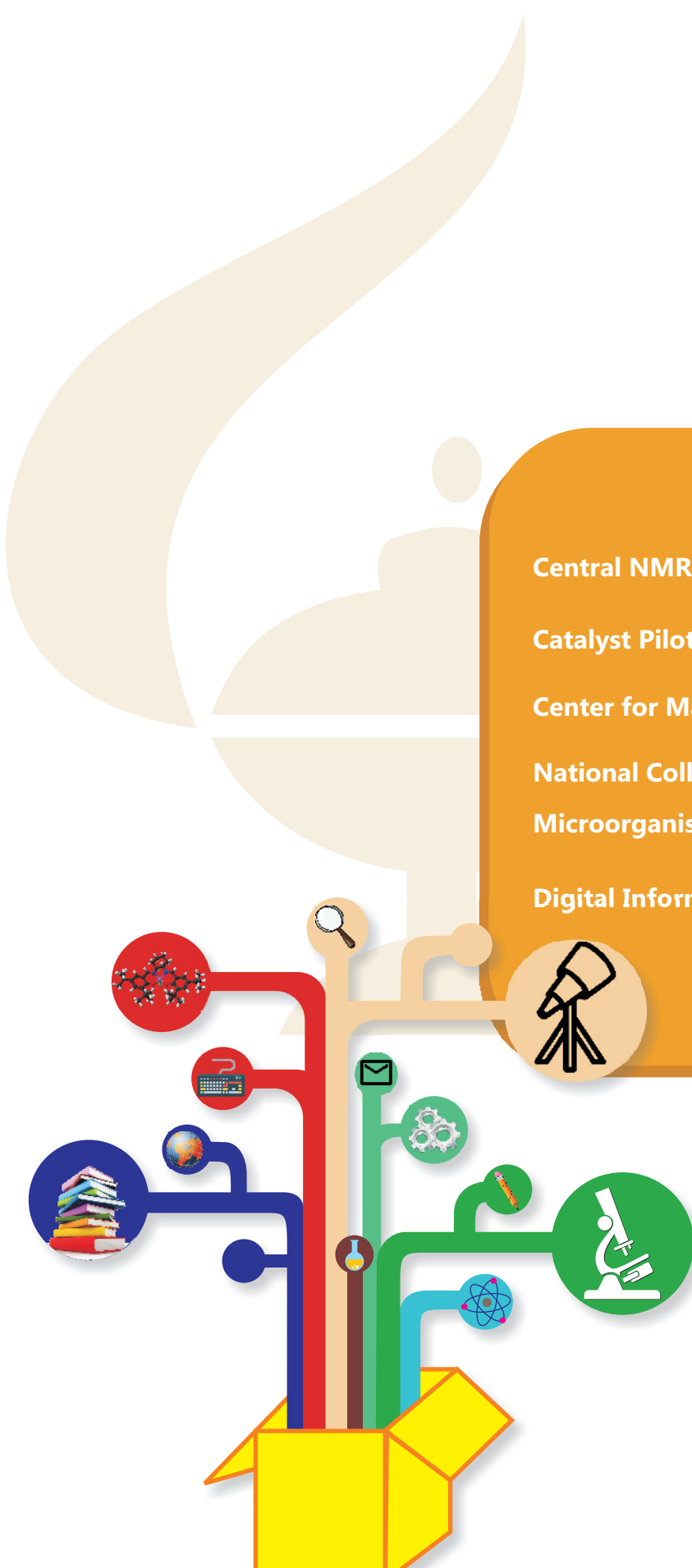
Functional characterization secondary metabolic pathway enzymes from *Ocimum* species: The β-caryophyllene synthase gene was isolated from *Ocimum kilimandscharicum* Gürke. The deduced amino acid sequence revealed 50-70% similarity with known sesquiterpene synthases from angiosperms. Recombinant OkBCS converted farnesyl diphosphate to β-caryophyllene as a major product (94%) and 6% α-humulene. Further comparative analysis of eugenol synthase from four different *Ocimum* species provided clues on eugenol accumulation (*Biochem. Bioph. Res. Co.* **2016**, 473, 265; *BBA Proteins Proteomics* **2016**, 1864, 1539).



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Resource Centers

Central NMR Facility

The Central NMR Facility 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 Bruker Avance 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 capable for solution state and solid state NMR research activities. Center also plays an integral part in the basic and applied research activities of the Laboratory.

During the year, the NMR Facility analyzed about 46000 samples in solution state and 900 samples in solid state including about 400 samples from industries, other R&D and academic institutes generating the ECF of ₹ 55.20 lakhs.

Catalyst Pilot Plant

Catalyst Pilot Plant (CPP) is well equipped with all the catalyst scale-up facilities such as wide range of batch reactors from 250 mL to 1000 L capacity along with other wet and dry processing units required for filtration; centrifugation; drying; calcinations and formulation of the catalyst. These wide ranges of reactors are also suitable for translating batch process from Laboratory scale to Pilot Plant scale. It also houses the micro-fixed bed reactors for the performance evaluation of the catalysts in various reactions of academic and industrial importance.

The work for Industrial client on 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. In another activity, new catalyst development and process optimization for converting biomass derived C₅ sugars to valuable chemicals such as 5-HMF; Levulinic acid; Ethoxymethyl furfural; furfural; levulinic esters in single or one step is a continuous activity under Department of Biotechnology sponsored project. CPP also made an attempt to prepare and supply the catalysts for the R & D purpose at client's end. Moreover, the activities in the following research areas are focused:

- Heterogenization of heteropolyacid as a catalyst in polar medium
- One step pretreatment of biomass with selective extraction of lignin by liquid ammonia/steam explosion and acid treatment
- Catalytic epoxidation of renewable feedstocks for CSIR-CNR Bilateral Exchange Programme (2016-2018)

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 microscope (TEM), X-ray photoelectron spectroscope (XPS), High Resolution Mass Spectrometer (HRMS), Maldi-TOF 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 Twenty thousand samples were analysed of which about Two percent comprised of industrial samples. This generated some amount of ECF for the laboratory.

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National Collection of Industrial Microorganisms

National Collection of Industrial Microorganisms (NCIM) facility is dedicated to the isolation, identification, collection, preservation and distribution of authentic microbial strains to industries and academia for biotechnological applications. It is also one of the unit generating significant revenues in recent times utilizing microbiology and biotechnological interventions to preserve Indian microbial wealth and diversity.

It generated of cash flow of ₹ 275 Lakhs through the supply of 9000 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 and VITEK. Standardized certification of analysis (COA) of microbial cultures was undergone and it was sent along with each culture. Various postgraduate students from universities and academic institutions were trained under skill development workshops. Latest catalog of microbial strains was made available in the form of hard copy and online version. The deposit forms and sequencing forms were updated as per global standards.

Digital Information Resource Center

The center upgraded existing 'Tier-II' type 'Data Center' of 400 Sq. Ft. to 880 Sq. Ft. located at the newly constructed 'Convergence' building. It can now accommodate HPC clusters worth ~100 TF and storage

worth 500 TB capacities. The center completed all the activities related to the establishment of LAN connectivity in the newly constructed NRM Building. The center migrated existing Microsoft exchange



based E-mailing system to central 'E-mailing system' located at NIC, New Delhi. The center revamped the entire NCL guest house Wi-Fi by deploying about ten wireless devices of higher strength. The center also deployed IP based surveillance system in the guest house, by installing about seven, indoor as well as outdoor IP based cameras. The center upgraded its E-training cell by installing Twenty-four number of latest, state-of-the-art, all-in-one Desktop PCs. The center manages two dedicated Internet leased lines in order to fulfill all the Internet requirements of the lab.

The center manages AMC for more than 1000 desktops, laptops, printers and other computer peripherals in the lab. The center looks after the web based 'Access Control and Time Management' system while maintaining more than sixty biometric readers as well as four boom barriers and four turn styles. The center installed four visitor management kiosk machines. The center laid about 2 km redundant single mode fiber cable from DIRC to more than 70% hub centers in the lab and also provided about 50 new LAN points at various locations.



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S & T Support Services

Publication and Science Communication

Publication and Science Communication (PSC) Unit is a channel that communicates between the laboratory and its stakeholders. It uses the facilities like web, print, electronic media and social media. It takes care of the video conference facility, external and internal websites; prepares annual reports and brochures. The unit communicates the impact making work from the

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

CSIR-NCL has developed Hollow Fiber Membrane based ultra filtration water purification technology for purifying water. It removes pathogenic species from drinking water at low pressures (ex. Tap water).

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.

CSIR-NCL has licensed this technology to companies based in Pune and Kanpur. Under this program, CSIR-NCL deployed fifty water filtration units having capacity of 500 LPH in Hospitals, Government Schools, Ashram Shalas, Major Bus Stands, Railway Stations, Municipal Corporation run schools, etc.

CSIR-NCL has also deployed fifteen oxygen enrichment units mainly in primary health centers of Thane/ Palghar districts and in government hospitals in Pune.



Engineering Services Unit

Engineering Services Unit (ESU) is using modern techniques like online job card system, ERP system, E-mail system and latest software related to CAD etc to cope up with increasing responsibilities. ESU has also introduced efficient systems particularly in electrical and air- conditioning area, which are not only energy saving but also more reliable with long life.

The engineering support included providing civil engineering setup and maintenance of buildings. Setting up electrical source for equipments, making setup of Lab furniture, fume hoods, exhaust systems, air-conditioning, providing basic services like water, electricity, vacuum, compressed air, gas lines etc. ESU also makes arrangement of liquid nitrogen & glass blowing services for scientific purposes. The activities related to construction works, electrical power setup provision, maintaining major A/C plants, procurement

of Liquid Nitrogen etc. is managed by outsourcing. Major Engineering setup of workshop unit, Pump house unit, Electrical substations etc. is maintained by sectional staff.

CSIR-NCL Colony has a setup of about 545 staff quarters. Common centers like Community hall, Guest house, students' hostels, Dispensary etc. Maintenance of all these installations is taken care by ESU. ESU takes care of required engineering back up for all the Seminars related to Electrical, Air-Conditioning, and Civil Engineering Services.

Civil Engineering Section added a major facility of filtered drinking water by erecting clean water bottled filter plant by using CSIR-NCL technology for entire laboratory.



वित्त एवं लेखा

1	निधि की उपयोगिता 2016.17	
	सीएसआईआर अनुदान राशी	
	परियोजनाएँ	(रु. लाख में)
	नेटवर्क (सी/एफ सहित)	2904.744
	गैर-नेटवर्क	15451.23
	NMITLI परियोजनाएँ	243.183
	ईएमआर एवं वैज्ञानिक पूल	900.008
	प्रयोगशाला आरक्षित निधि	133.218
	बाहरी वित्तपोषित परियोजनाएँ	2335.980
	विविध जमा राशि	13.258
	बाहरी निकायों की ओर से भुगतान	336.306
	प्रायोजित सम्मेलनों/संगोष्ठियों हेतु अमानत	27.397
		कुल 22345.324
2	प्रयोगशाला आरक्षित निधि का अर्जन	(रु. लाख में)
	वर्ष के दौरान अतिरिक्त निधि (सीएसआईआर के अलावा) के निवेश पर अर्जित ब्याज के माध्यम से प्रयोगशाला आरक्षित निधि का अर्जन	248.656
	अन्य लेखाशीर्षों से	610.045
		कुल 858.701
3	31.3.2017 को अतिरिक्त निधि का निवेश (रु. लाख में)	1300.000
4	आपत्ति-पुस्तिका मर्दों का निपटारा	
	वर्ष के दौरान किए गए समायोजन	
	निजी	1001.804
	यात्रा भत्ता /छुट्टी यात्रा खियायत	54.825
	स्थानीय	71.457
		कुल 1128.086
		कुल मर्दे 470
5	निम्न लिखित प्रकार के वाउचर तैयार किए गए	
	भुगतान	16488
	प्राप्त राशि	4548
	टी.ई.	266
		कुल 21302

Finance & Accounts

1.	Funds Utilization 2016-17	(₹ in lakh)
	CSIR Grant	
	Projects	2904.744
	Non Projects	15451.23
	NMITLI Projects	243.183
	EMR & Scientist Pool	900.008
	Laboratory Reserve	133.218
	Externally Funded Projects	2335.980
	Misc. Deposits	13.258
	Payment on behalf of outside bodies	336.306
	Deposits for Sponsored conf. / seminars	27.397
	Total	22345.324
2.	Generation of Lab Reserve	(₹ in lakh)
	Through earning of interest on investment of surplus funds (other than CSIR) during the year	248.656
	From other heads	610.045
	Total	858.701
3.	Investment of surplus funds as on 31.3.2017 (Rs. in lakh)	1300.000
4.	Clearance of OB items	
	Adj. made during the year 2016-17	(₹ in lakh)
	Private	1001.804
	TA/LTC	54.825
	Local	71.457
	Total	1128.086
	No. of items	470
5.	Following types of vouchers were generated	
	Payment	16488
	Receipt	4548
	TE	266
	Total	21302

भंडार एवं क्रय

भंडार एवं क्रय: उपलब्धियां

मद	संख्या		मूल्य (₹ करोड़ में)	
	2015.16	2016.17	2015.16	2016.17
कुल प्राप्त एवं निष्पादित मांगपत्रा	2547	2427	49.53	51.93
कुल दिए गए ऑर्डर (आयातित)	385	144	27.80	30.21
कुल दिए गए ऑर्डर (स्वदेशी : ऑनलाइन आरसी ऑर्डर सहित)	2173	2283	22.01	21.72
स्थानीय खरीद; ऑनलाइन आरसी ऑर्डर सहित)	7300	4229	11.11	10.22
वित्तीय वर्ष के दौरान समायोजित बकाया शेष			20.83	15.99
वित्तीय वर्ष 2015.16 के दौरान सीमा शुल्क से छूट प्राप्त राशि का उपयोग			13.54	0.41

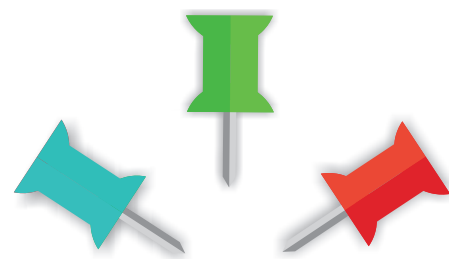
Stores & Purchase

Stores & Purchase : Accomplishments

Item	Numbers		Value (₹ In Crores)	
	2015-16	2016-17	2015-16	2016-17
Total indents received and Processed	2547	2427	49.53	51.93
Total orders placed (imported)	385	144	27.80	30.21
Total orders placed (indigenous : including on line RC orders)	2173	2283	22.01	21.72
Local purchases (including On-line RC)	7300	4229	11.11	10.22
OBs adjusted during the financial year 2015-16			20.83	15.99
Utilization of Custom Duty Exemption during			13.54	0.41



Patents Granted: Foreign & Indian.....	92
PhD Theses.....	99
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Annexures

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 Kunjkrishnan 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 Balaran	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 Balaran	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 ₂	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 α -aryloxy α' -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	Chandrashekar 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 ₂ O to TiO ₂ by TiCl ₄ 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

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 ₂ -C ₁₀ 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

Ph.D. Theses

Academy of Scientific and Innovative Research (AcSIR)

Author	Title	Guide(s)
Ghatak, Kamalika	Activation of small molecules via organometallic pincer catalysts and small rhodium cluster (pure and doped): a density functional theory approach	Pal, Sourav
Prasad, Pragati K.	Asymmetric synthesis of bioactive molecules and development of synthetic methodologies involving c-c, c-o and c-n bond formation via cu(i) and iodine catalysis	Sudalai, Arumugam
Venkataramasubramanian, V.	Asymmetric synthesis of bioactive molecules and development of synthetic methodologies via Enamine catalysis	Sudalai, Arumugam
Mhashal, Anil R.	ATP induced conformational flexibility in PcrA helicase and properties of lipid membrane in presence of nanoparticles and surface : molecular simulation	Roy, Sudip
Khivasara, Mamata B.	Biomass to lactic acid: microbial cellulases and their application in cellulosic lactic acid production	Gokhale, D. V.
Pathak, Himadri	Calculation of properties using relativistic coupled cluster theory for atoms and molecules	Vaval, Nayana
Mallick, Arjit	Chemical and electrochemical properties of Ca(II) and Mg (II) based lightweight metal organic framework (LWMOF) materials	Banerjee, Rahul
Pal, Amrita	Computational investigations of small molecule activation	Vanka, Kumar
Mane, Manoj Vasisht	Computational studies, using density functional theory of proton transfer through polymer electrolyte membrane in fuel cells as well as of hydrogenation and dehydrogenation reaction using frustrated lewis pairs	Vanka, Kumar
Kuriakose, Nishamol	Density functional theory (DFT) studies of the homogeneous activation of small molecules using transition metal and main group based compounds.	Vanka, Kumar
Bhaskar, Anand	Design and synthesis of metal organic framework (MOF) - polymer composite membranes for gas separation	Kharul, Ulhas K.
Kolhe, N. B.	Design and synthesis of novel π -conjugated molecules and polymers based on naphthalene and perylene diimides and their application in organic electronics	Asha, S. K.
Mane, S.	Design, synthesis, characterization, and applications of functional, porous, and crosslinked polymers	Badiger, M. V.

Ph.D. Theses

Academy of Scientific and Innovative Research (AcSIR)...cont'd

Author	Title	Guide(s)
Kadam, Shantanu	Development o kinetic Monte Carlo methods for the stochastic simulation of chemical system	Vanka, Kumar
Singh, Ajeet	Development of MALDI-TOF MS methods for quantitative small molecules analysis	Panchagnula, Venkateswarlu
Reddi, Rambabu N.	Enantioselective synthesis of bioactive molecules and development of synthetic methodologies involving N -heterocyclic carbene and iodine catalysis of alkenes and aldehydes	Sudalai, Arumugam
Badadhe, Satish S.	Engineered nanostructures of binary and ternary metal oxide for gas and humidity sensing application	Shelke, Manjusha V.
Tathod, A. P.	Exploration of the effects of supports, metals and promoters on the catalytic conversion of biomass derived monoand polysaccharidesin to sugar alcohols	Dhepe, Paresh L.
Pahari, Swagata	Exploring membrane materials for high temperature fuel cell application from Quantum chemical calculations and molecular simulation	Roy, Sudip
Kumar , Asheesh	Gas hydrate studies for carbon dioxide capture and methane recovery	Kumar, Rajnish
Dalal, Sayli	Investigation of conformational and functional relationship of selected serine proteases at molecular level	Kadoo, Narendra Y.
Rewar, Anita K.	Investigation towards applicability of polybenzimidazole (PBI) based polymeric ionic liquids (PILS) for gas permeation and fuel cells	Kharul, Ulhas K.
Soumya, B. N.	Layered solid state compounds for photocatalytic water splitting	Nandini Devi, R.
Saha, Subhadeep	Low-molecular weight amino acid based supramolecular metallo-gels for photo and electrochemical applications	Banerjee, Rahul
Dhavale, Vishal M.	Low-platinum and platinum-free electrocatalysts for energy applications	Kurungot, Sreekumar
Venugopal, Edakkal	Organisation of colloids and polymers with nonionic surfactant assemblies	Bhat, Suresh
Shaligram, Sayali V.	Polymeric ionic liquids based on asymmetrically N-substituted polybenzimidazoles for gas permeation studies	Kharul, Ulhas K.
Chatterjee, Prathit	Protein thermal stability, conformational dynamics and solvent properties : insights with atomistic molecular dynamics simulations	Sengupta, N.
Reddy, G. U.	Recognition and sensing of biologically and environmentally significant analytes	Das, Amitava

Ph.D. Theses

Academy of Scientific and Innovative Research (AcSIR)...cont'd

Author	Title	Guide(s)
More, P. M.	Selective catalytic reduction of nox by hydrocarbon using bimetallic ag-au supported on alumina catalyst	Umbarkar, Shubhangi B.
Unnikrishnan, P.	Solid oxide catalysis for making dimethyl carbonate	Srinivas, Darbha
Baby, Bindhu	Solid-state NMR investigations of materials with magnetoplumbite and perovskite structures	Ajithkumar, T. G.
Govind Raj K.	Studies on magnetic and electrical properties of disordered carbon	Joy, Pattayil A.
Vadhadiya, Paresh M.	Studies toward the total synthesis of (+)-stagonolide D, mangiferaelactone, cytospolide E and sinenside A	Ramana, Chepuri V.
Joshi, Sayali, P.	Study of molecular response properties within extended coupled cluster framework	Vaval, Nayana
Gupta, Preeti	Study of negative magnetisation exchange bias and magnetisation switching in rare earth chromites	Poddar, Pankaj
Nepak, Devadutta	Supported gold catalysts for selective oxidation and hydrogenation reaction	Srinivas, Darbha
Bihag, A. M.	Supported nanostructured materials with enhanced electrode-electrolyte interface for high performance supercapacitors and dye sensitized solar cell counter electrodes	Kurungot, Sreekumar
Rajesh, T.	Synthesis and characterization of noble metal doped structured oxides for water gas shift reaction and co oxidation	Nandini Devi, R.
Jayaprabha, K. N.	Synthesis and studies on surface functionalised magnetite nanoparticles for biomedical applications	Joy, Pattayil A.
Das, Subhadip	Thermodynamic and kinetic stability of pure and mixed gas hydrate through molecular dynamics simulation	Rajnish
Rout, J. K.	Total synthesis of naturally occurring sacidumlignans A, B, D, and stereoselective synthesis of C-Disaccharides	Ramana, Chepuri V.
Roy, Kanak	Toward bridging the pressure gap between real world catalysis and ideal surface science conditions using ambient pressure photoelectron spectroscopy and molecular beam instrument	Gopinath, Chinnakonda S.
Jose, Jaya C.	Conformational dynamics and solvent interactions of amyloidogenic peptides in biologically relevant environments : insights with molecules dynamics simulations	Sengupta, N.

Ph.D. Theses

Savitribai Phule Pune University

Author	Title	Guide(s)
Kulkarni, Shuklangi A.	Biochemical and molecular studies of chitin deacetylase from <i>Metarhizium</i> species	Deshpande, M. V.
Sebastian, Joby	Catalytic Activity Study of Double-Metal Cyanide Complexes for Biodegradable Polymers Synthesis	Srinivas, Darbha
Lucas, Nishita	Conversion of carbohydrate biomass to value added chemicals	Satyanarayana, C. V. V.
Jedhe, G.	Design, synthesis and biophysical evaluation of novel angiotensin ii and combretastatin analogs comprising hydrogen bonding directed scaffolds	Sanjayan, Gangadhar J.
Ramesh, V. R.	Desymmetrization approach for the synthesis of 1,3-disubstituted isoindolines and conduramine analogues	Pandey, Ganesh
Bhagwat, R. M.	DNA barcoding of some forest tree species of western ghats	Giri, Ashok P.
Dhanalakshmi, M.	Electrospinning of biocompatible and biodegradable polymers and their application in scaffold tissue engineering	Lele, A. K.
Reddy, Bontha Narasimha	Enantioselective synthesis of bioactive molecules employing proline catalyzed aminoxylation, sharpless asymmetric epoxidation and oxidative aromatization of 1,4-dihydropyridines	Singh, R. P.
Show, Krishanu	Enantioselective synthesis of hydroxylated pyrans, pyrrolidine alkaloid and lactones using asymmetric dihydroxylation, hydrolytic kinetic resolution and organocatalytic aldol reaction	Kumar, Pradeep
Bhosale, R. K.	Engineered metal oxide and chalcogenide nanomaterials for sensitized solar cells and solar photoelectrochemical water splitting	Ogale, Satishchandra B.
Singh, Pradeep Kumar	Formation of fluorescent bio-molecular assemblies by UV laser treatment and solution phase molecular interactions	Prabhune, Asmita A.
Bhattacharya, D.	Formulation and implementation of transition dipole moment and electric response properties using multi-reference methods	Pal, Sourav
Panigrahi, Priyabrata	In silico structure-function, specificity and stability studies of n-terminal nucleophile hydrolase enzymes	Suresh, Cheravakattu Gopalan
Shukla, S.	Ionic liquids: measuring thermosolvatochromism and hammett acidity function and understanding kinetics of organic reactions	Kumar, Anil
Singh, Anshu	Kinetic and mechanistic investigations of 1,3-dipolar cycloaddition and other C-C bond forming reactions in water and ionic liquids	Kumar, Anil
Nanda, Raju	NMR self-diffusion coefficients, NMR relaxation and	Kumar, Anil

Ph.D. Theses

Savitribai Phule Pune University...cont'd

Author	Title	Guide(s)
Unni, Sreekuttan	Platinum-free electrocatalysts based on graphene and carbon nanohorn for polymer electrolyte membrane fuel cell cathode	Kurungot, Sreekumar
Kumar, Yashwant	Proteomic and metabolomic analysis of chickpea fusarium oxysporum interactions	Gupta, Vidya S.
Santhakumari, B.	Proteomic profiling of <i>Dunaliella</i> SP. for identification of salt tolerant genes	Kulkarni, Mahesh J.
Ambal, S. R.	Solar light harvesting by ZnO based materials	Gopinath, Chinnakonda S.
Batwal, R. U.	Studies on chemical and chemoenzymatic total synthesis of bioactive natural products	Argade, Narshinha P.
Mondal, Pravat	Studies on synthesis of bioactive alkaloids from cyclic anhydrides and derivatives	Argade, Narshinha P.
More, Atul	Studies toward the total synthesis of iontegrastatins A/B, allocolchicine and xylarinol B	Ramana, Chepuri V.
Varada, Manojkumar	Synthesis and biophysical evaluation of cyclohexenyl nucleic acids and its analogues	Kumar, Vaijayanti A.
Chhatre, S. Y.	Synthesis and chemical modification of poly(phenylene vinylene) and polystyrene systems for energy applications	Wadgaonkar, Prakash P.
Negi, Sanjay Singh	Synthesis characterization and catalytic application of disordered mesoporous materials for oxidation reactions	Gopinath, Chinnakonda S.
Senthilkumar, T.	Synthesis of novel polyfluorenes for biosensor applications	Asha, S. K.
Beeran, Senthilkumar	Synthesis of small molecule PIP3 antagonists as potential anticancer agents and metal-catalyzed C-H oxidation of cyclotri veratrylene derivatives	Ramana, Chepuri V.
Kumari, S.	Synthesis, functionalization and catalytic application of porous hybrid materials	Gupte, S. S.
Pawar, K.	Synthetic studies towards (-)-venlafaxine, (+)-deoxoprosophylline, 3-hydroxy pipercolic acid, 1-deoxyojirimycin, α -lipoic acid and development of synthetic methodology Theoretical investigation on structure and reactivity	Chavan, Subhash P.
Das, Susanta	properties of molecule and metal clusters: a conceptual dft and ab initio molecular dynamics approach	Pal, Sourav
Janakiram, V.	Total syntheses of (+)-Cylindricine C, D, E and (-)-Lepadiformine A by development of a non-biogenetic tandem rearrangement	Pandey, Ganesh
Bokil-Kulkarni, P.	Tuning the PNA backbone conformation : synthesis and biophysical studies of Dialkyl substituted peptide nucleic acids	Ganesh, Krishna N.

Network Projects

Title	Project Leader
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

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

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

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

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

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

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



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 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।





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