ANNUAL
REPORT
2014-15

वैज्ञानिक तथा औद्योगिक अनुसंधान परिषद

CSIR-National Chemical Laboratory

वार्षिक प्रतिवेदन 2014 - 15

सीएसआईआर-राष्ट्रीय रसायनिक प्रयोगशाला

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Cover Page, layout & Printed by
Typographica Press Services
Pune

सीएसआईआर – राष्ट्रीय रासायनिक प्रयोगशाला

CSIR - National Chemical Laboratory

वार्षिक प्रतिवेदन 2014 - 15

With Best Compliments from •

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CONTENT

PERFORMANCE INDICATORS

Research & Development Reports

CONTENT

RESOURCE CENTERS

S & T SUPPORT SERVICES

ANNEXURES

निदेशक की कलम से...

वर्ष 2014–15 के लिए सीएसआईआर–राष्ट्रीय रासायनिक प्रयोगशाला का वार्षिक प्रतिवेदन प्रस्तुत करते हुए मुझे अत्यंत हर्ष हो रहा है। वार्षिक प्रतिवेदन हमारी प्रयोगशाला की अनुसंधान संबंधी उपलब्धियों तथा हमारे प्रदर्शन के कई मापदंडों को दर्शाता है। हमारी प्रयोगशाला के प्रदर्शन में प्रतिवर्ष निरंतर सुधार आ रहे हैं। पिछले कुछ वर्षों में विशेष रूप से, हमारे प्रकाशनों के साथ ही एकस्व (पेटेंट) प्रस्तुत करने में विशेष बढ़ोतरी देखी गई है , जो प्रगति का प्रतीक है। इस वर्ष भी प्रकाशन और एकस्व (पेटेंट) की संख्या बढ़ी है। हमने उद्योगों के साथ हमारे सहयोग को मजबूत किया है, जिसका परिणाम अनुकूलित प्रौद्योगिकी हस्तांतरण के रूप में सबके सामने है। इसके अलावा वर्ष 2014–15 के दौरान हमारी बाहरी नकद आय में भी बढ़ोतरी हुई है। मैं इस प्रयोगशाला को गौरवशाली बनाने के लिए सभी स्टाफ सदस्यों को बधाई देता हूँ।

वर्ष के दौरान बहुत से महत्वपूर्ण कार्यक्रमों का आयोजन हमारे द्वारा किया गया। सीएसआईआर–एनसीएल में विश्व के प्रख्यात वैज्ञानिकों के विभिन्न व्याख्यान इस दौरान आयोजित हुए। भारतीय अभियांत्रिकी, विज्ञान तथा प्रौद्योगिकी संस्थान के अध्यक्ष डॉ. के. राधाकृष्णन ने राष्ट्रीय विज्ञान दिवस के उपलक्ष्य में “Recent strides in Indian Space mission” पर व्याख्यान प्रस्तुत किया। डॉ. ए. वी. रामा राव, Avra Laboratories Pvt. Ltd. द्वारा ग्लोबल एलुमिनी सम्मेलन, जिसे अत्यंत उत्साहपूर्वक मनाया गया, में डॉ. के. अंजी रेड्डी स्मृति द्वितीय व्याख्यान प्रस्तुत किया गया। प्रो. सुधीर कुमार सोपोरी, जवाहरलाल नेहरू वि.वि. द्वारा एनसीएल–स्थापना दिवस समारोह में 'An Insight into Plant Life: Perception, feelings and survival strategies' नामक व्याख्यान प्रस्तुत किया गया।

प्रो. के. एन. गणेश, निदेशक आईसर द्वारा सीएसआईआर–स्थापना दिवस समारोह में Travails of a chemist at crossroads: A life in CSIR and beyond' पर व्याख्यान प्रस्तुत किया गया। प्रो. एंथोनी के. चीथम, यूनिवर्सिटी ऑफ केंब्रिज, ट्रिनिटी कॉलेज, यू.के. के फेलो द्वारा 'Recent developments in Metal Organic Frameworks' विषय पर प्रो. जे. डबल्यू. मेकबेन स्मृति व्याख्यान दिया गया। डॉ. टी. रामासामी, विज्ञान तथा प्रौद्योगिकी विभाग द्वारा राष्ट्रीय प्रौद्योगिकी दिवस पर “Changing India in Global S&T Landscape” विषय पर व्याख्यान दिया गया।

इस अवधि में प्रयोगशाला के द्वारा आर. ए. माशेलकर प्रतिभा व्याख्यानों के अलावा विभिन्न सम्मेलनों, संगोष्ठियों, कार्यशालाओं का भी आयोजन किया गया। अनुसंधान संबंधी गतिविधियों को बढ़ावा देने की दृष्टि से विभिन्न कार्यशालाएं और संगोष्ठियां आयोजित की गई। इन सभी कार्यक्रमों में हमारे विद्यार्थियों ने सक्रिय रूप से प्रतिभागिता की। जैसे कि:–रसायन शास्त्र में राष्ट्रीय संगोष्ठी CRSI, थियोरिटिकल केमिस्ट्री पर संगोष्ठी, Structural and Inorganic Chemistry पर आयोजित अंतर्राष्ट्रीय संगोष्ठी, Recent Advances in Polymer Science पर आयोजित अंतर्राष्ट्रीय सम्मेलन, Catalysis for Sustainable & Environmental Chemistry पर आयोजित इंडो–फ्रेंच बाइलेट्रल संगोष्ठी, Organic Photovoltaics for Solar Energy conversion पर आयोजित कार्यशाला तथा ICC & HSE Solutions, मुंबई द्वारा “Chemical burns management- Stopping incidents from becoming accidents” पर आयोजित अर्धदिवसीय संगोष्ठी।

रिसर्च स्कालर्स सम्मेलन का आयोजन जुलाई में किया गया, जिसे भारत के भूतपूर्व राष्ट्रपति स्वर्गीय माननीय डॉ. ए. पी. जे. कलाम द्वारा संबोधित किया गया। उनके अभिभाषण को सुनने के लिए विद्यार्थियों तथा स्टाफ सदस्यों द्वारा इस कार्यक्रम में अत्यंत उत्साहपूर्वक प्रतिभागिता की गई!

हमने प्रौद्योगिकी विकास करने तथा उसे उद्योग जगत को हस्तांतरित करने के अपने प्रयास जारी रखे हैं। पिछले वर्ष में हमने उद्योग जगत में विभिन्न प्रक्रियाओं के परिचालन हेतु कई प्रौद्योगिकियों/तकनीकी जानकारियों के उपयोग की अनुमति प्रदान की। प्रौद्योगिकी और प्रक्रियाओं के व्यवसायीकरण में scaled up preparation, modification and characterization of molecular sieves, development of a 2.7 V, 400 F supercapacitor for auto applications using in-house synthesized porous conducting carbon, process development for p-aminophenol (PAP) from nitrobenzene, hydrothermal conversion of lipid oils, evaluation of catalyst acidity and activity, perfluoropolyethers (PFPE) terminated with reactive functional groups and PFPE tetraol- based gels, synthesis of impurities, batch to continuous transformation of process step involving ethylene oxide, development of modeling framework for underground coal gasification, direct synthesis of dimethyl carbonate (DMC) from CO_2 and methanol, basic engineering package (BEG) for PAP plant- phase II इत्यादि प्रक्रियाएं सम्मिलित हैं।

इस प्रतिवेदन में वर्ष 2014–15 के दौरान हमारे द्वारा विभिन्न क्षेत्रों में किए गए अनुसंधान एवं विकास कार्यों की जानकारी तथा समीक्षा प्रस्तुत की गई है। निश्चित रूप से हम रासायनिक अभियांत्रिकी और जैव विज्ञान सहित रासायनिक और संबंद्ध विज्ञान के व्यापक क्षेत्र में अपार संभावनाओं को देखेंगे। प्रकाशनों की गुणवत्ता में अनुसंधान की गहराई भी स्पष्ट रूप से परिलक्षित है। हमारे बहुत से सहयोगियों ने विभिन्न सम्मान तथा पुरस्कार प्राप्त किए है, जिसके द्वारा प्रयोगशाला की प्रतिष्ठा बढ़ी है, इसके लिए मैं उन सबको बधाई देता हूँ।

अन्त में मैं प्रयोगशाला के सभी स्टाफ सदस्यों तथा सीएसआईआर–एनसीएल की अनुसंधान परिषद एवं प्रबन्ध परिषद के सदस्यों, सीएसआईआर,नई दिल्ली के महानिदेशक तथा स्टाफ की सहायता तथा सहयोग के लिए अपना आभार प्रकट करता हूँ। मैं अपने विभिन्न हितधारकों द्वारा दिए गए सहयोग के लिए भी अपनी कृतज्ञता प्रगट करता हूँ। उनका परामर्श और सहयोग हमारी उपलब्धियों के लिए हमेशा सहायक हुआ है। निश्चित रूप से हममें उनका दृढ़ विश्वास हमें अनुसंधान तथा विकास क्षेत्र में अग्रणी बनने के लिए कड़ी मेहनत करने की उर्जा प्रदान करेगा।

सौरव पाल

(सौरव पाल)

From the Director's Desk...

It is my pleasure to present the Annual Report of CSIR-National Chemical Laboratory for the year 2014-15. The report has highlighted the achievements in the field of research and displayed several parameters of performance of the laboratory. The performance of the laboratory has been continuously improving year by year. A significant increase in the number of publications and patents is seen which is considered as a sign of progress. This year also the numbers are improved. The association with the industries has been strengthened that resulted in the optimized technology transfer. Moreover, a significant growth in the external cash earnings was noticed for the year 2014-15. I take this opportunity to congratulate all the staff for making the laboratory feel proud.

Several important events took place during the year. Various talks by eminent scientists from across the world were organized at CSIR-NCL. Dr. K. Radhakrishnan, Chairman, Indian Institutes of Engineering Science and Technology delivered the National Science Day Lecture on "Recent strides in Indian Space mission". Dr. A. V. Rama Rao, Avra Laboratories Pvt. Ltd. delivered the second Dr. K. Anji Reddy Memorial Lecture on the occasion of NCL Global Alumni Meet which was organized with full enthusiasm. Prof. Sudhir Kumar Sopory, Jawaharlal Nehru University gave the NCL Foundation Day lecture on 'An Insight into Plant Life: Perception, feelings and survival strategies'.

Professor K. N. Ganesh, IISER, Pune spoke on 'Travails of a chemist at crossroads: A life in CSIR and beyond' on the occasion of the CSIR Foundation Day. Professor Anthony K. Cheetham, Fellow of Trinity College, University of Cambridge, UK delivered the Prof. J. W. McBain Memorial Lecture on Recent developments in Metal Organic Frameworks. Dr. T. Ramasami, Department of Science & Technology delivered the National Technology Day Lecture on "Changing India in Global S&T Landscape".

The laboratory hosted several symposia, conferences, workshops besides R. A. Mashelkar Endowment Lectures. Several workshops and symposia were organized to support the research activities. The students participated actively in such events. Events like the CRSI National Symposium in Chemistry, the Theoretical Chemistry Symposium, International Conference on Structural and Inorganic Chemistry, International Meet on the Recent Advances in Polymer Science, Indo-French Bilateral Symposium on Catalysis for Sustainable & Environmental Chemistry, a workshop on Organic Photovoltaics for Solar Energy conversion and a Half-day Seminar on "Chemical burns management- Stopping incidents from becoming accidents' by ICC & HSE Solutions, Mumbai.

The Research Scholars Meet was held in July which was addressed by Late Honourable Dr. A. P. J. Abdul Kalam, Former President of India. Many students attended the program with great zeal to hear his address.

The laboratory has continued the efforts to develop the technologies and transfer it to the industries. In last year it has licensed many technologies / know how for various processes. The technologies and processes commercialized included the scaled up preparation, modification and characterization of molecular sieves, development of a 2.7 V, 400 F supercapacitor for auto applications using in-house synthesized porous conducting carbon, process development for p-aminophenol (PAP) from nitrobenzene, hydrothermal conversion of lipid oils, evaluation of catalyst acidity and activity, perfluoropolyethers (PFPE) terminated with reactive functional groups and PFPE tetraol- based gels, synthesis of impurities, batch to continuous transformation of process step involving ethylene oxide, development of modeling framework for underground coal gasification, direct synthesis of dimethyl carbonate (DMC) from CO_2 and methanol, basic engineering package (BEG) for PAP plant- phase II.

The Annual Report highlights the research that took place in 2014-15 in different areas and hopefully provides an overview of the research and development that laboratory has carried. You will notice a very good breadth in broad area of chemical and allied sciences including chemical engineering and biosciences. The depth of the research is also evident in the quality of publications by the laboratory. Many of our colleagues received the distinctions and laureates that have brought the prestige to the laboratory. I congratulate all of them.

I acknowledge the support and co-operation of all staff, members of Research Council and Management Council of CSIR-NCL, DG-CSIR and Staff of CSIR, New Delhi. I also acknowledge our various stakeholders. Their advice and cooperation was always helpful in our endeavor. Their confidence in us will certainly provide us the energy to work hard to lead in the field of Research and Development.

Sourav

(Sourav Pal)

Vision, Mission & Guiding Principles & Values

Vision

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

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

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

Mission

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

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

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

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

Guiding Principles & Values

To be deeply committed to the success of our stakeholders

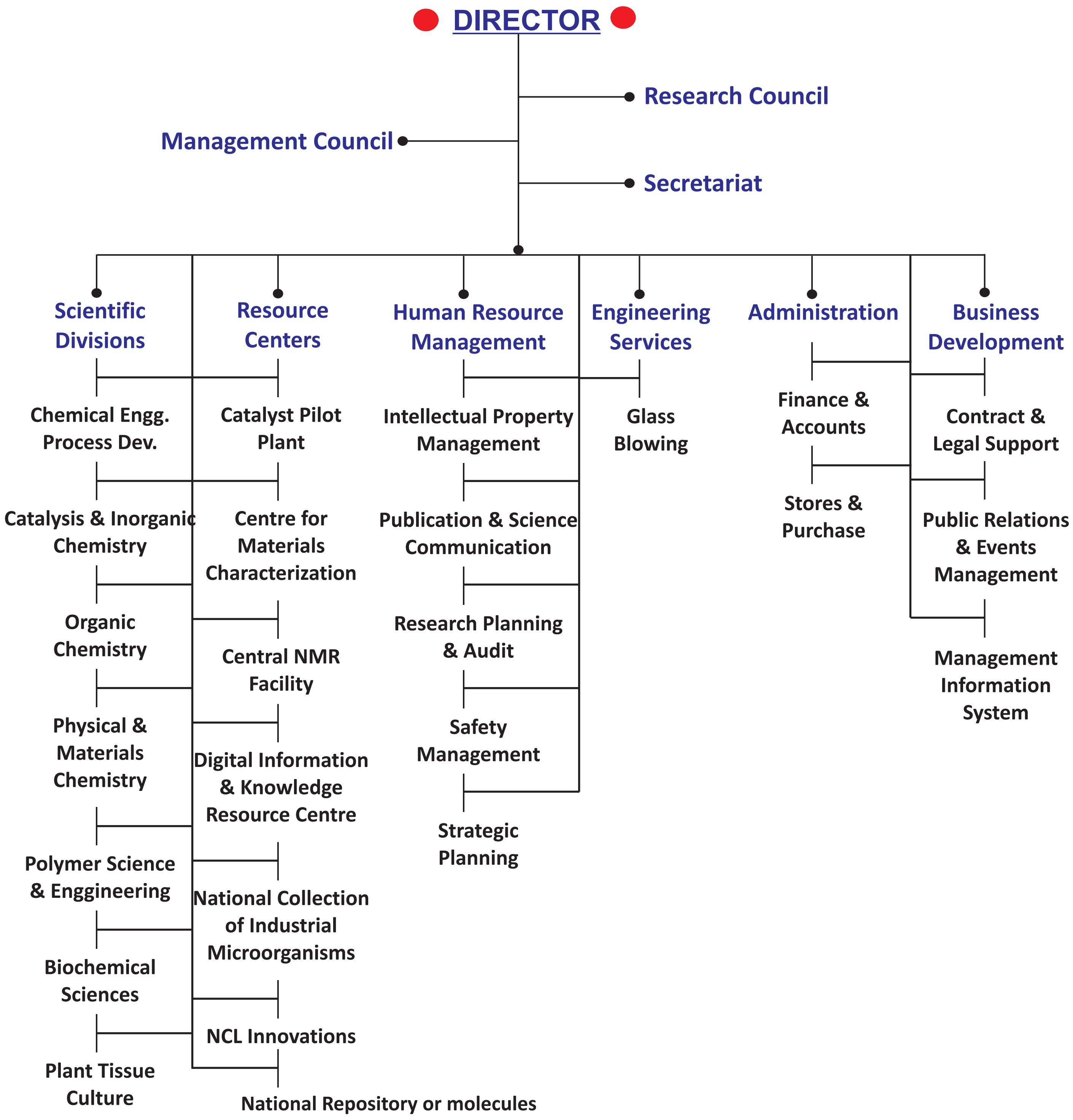
To create and sustain a self - driven and self - managed learning organization with a high degree of internal and external transparency

To encourage a culture of collective and principle-centred leadership

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

To nurture the highest standards of integrity and ethical conduct

Organisation Chart



Research Areas

Catalysis

- Heterogeneous Catalysis
- Organometallic Chemistry
- Surface Science

Biochemical Sciences

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

Organic Chemistry

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

Polymer Science & Engineering

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

Physical & Materials Chemistry

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

Chemical Engineering Science

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

CSIR-NCL serves to various sectors such as

- Chemicals & Petrochemicals
- Materials
- Water
- Healthcare
- Sustainable Environment
- Agriculture
- Fuel Cell

Centers of Excellence

- Micro reactor Engineering
- Scientific Computing
- Solar Energy
- Surface Science
- Sustainable Polymer Industry through Research Innovation and Training

Research Council

Chairperson

Prof. D. D. Sarma
Solid State & Structural Chemistry
Indian Institute of Science
Bengaluru

External Members

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Department of Organic Chemistry
Indian Institute of Science
Bengaluru

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Tata Institute of Fundamental Research
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Indian Institute of Technology
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(DG Nominee)
Director
CSIR-IICT, Hyderabad

Dr. S. K. Deshpande
(Invited Member)
DSIR, New Delhi

Dr. Rajesh S. Gokhale (Sister Laboratory)
Director,
CSIR- IGIB, Delhi

Dr. Suresh Das(Cluster Director)
Director,
CSIR –NIIST, Thiruvananthapuram

Director

Dr. Sourav Pal
Director
CSIR – NCL, Pune

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Head or his nominee
Planning & Performance Division
Council of Scientific and Industrial Research
New Delhi

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Dr. G. S. Grover
CSIR-NCL, Pune

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Chairperson

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Director
CSIR- National Chemical Laboratory
Pune

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Dr. V. V. Ranade
CSIR-NCL, Pune

Mr. G. Prabhakaran
CSIR-NCL, Pune

Dr. B. D. Kulkarni
CSIR-NCL, Pune

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Dr. (Ms) A. A. Prabhune
CSIR – NCL,
Pune

Representative Sister Laboratory

Dr. S. R. Wate
Director
CSIR-NEERI, Nagpur

Member Secretary

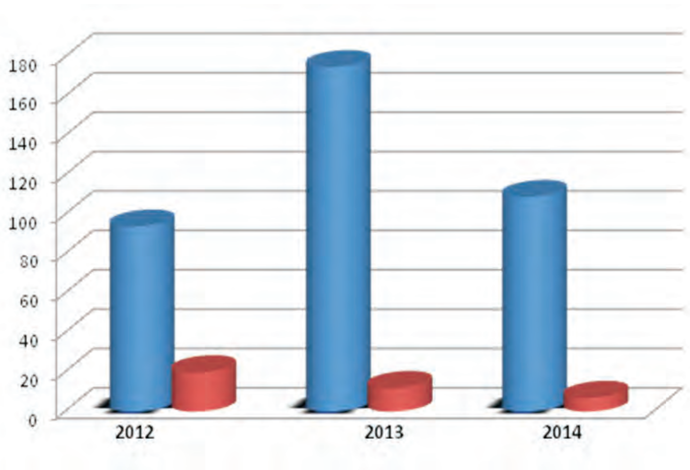
Prema Balakrishnan
Controller of Administration, CSIR-NCL

Performance Indicators

Technology Performance Indicators

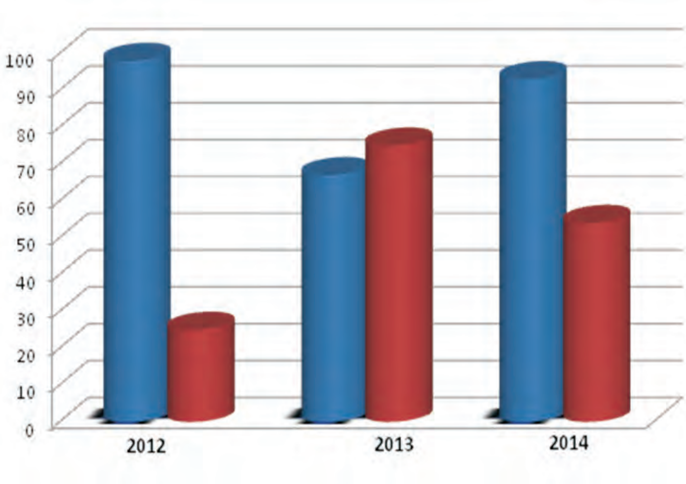
Indian Patents: Filed & Granted

Year	2012	2013	2014
Filed	86	173	103
Granted	19	10	7



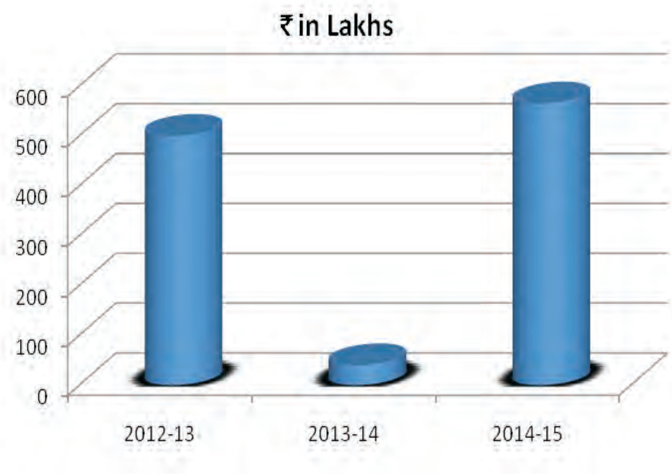
Foreign Patents: Filed & Granted

Year	2012	2013	2014
Filed	96	67	90
Granted	22	72	51



Premia/Royalty Earnings

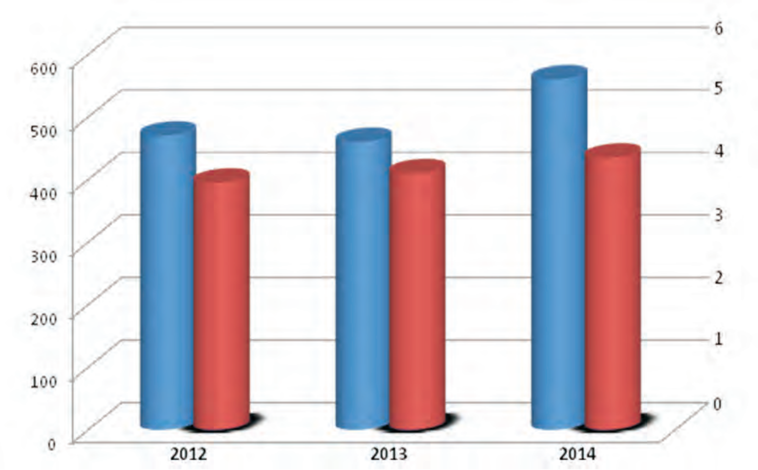
Year	₹ in Lakhs
2012–13	480.96
2013–14	16.85
2014–15	539.45



Science Performance Indicators

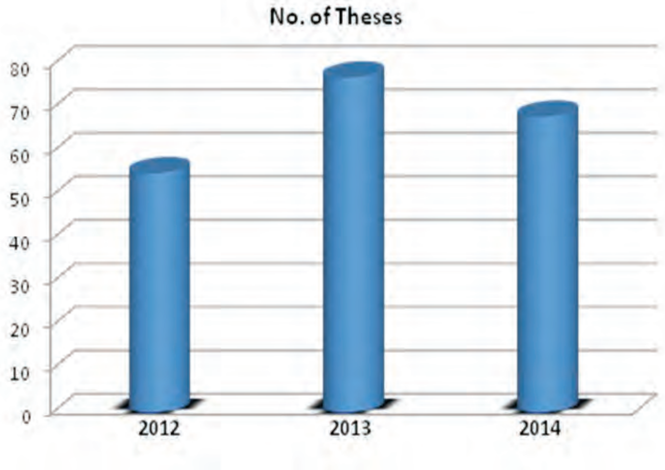
Research Output: Publications

Year	2012	2013	2014
Total Papers	444	442	540
Average Impact Factor	3.58	3.88	4.07



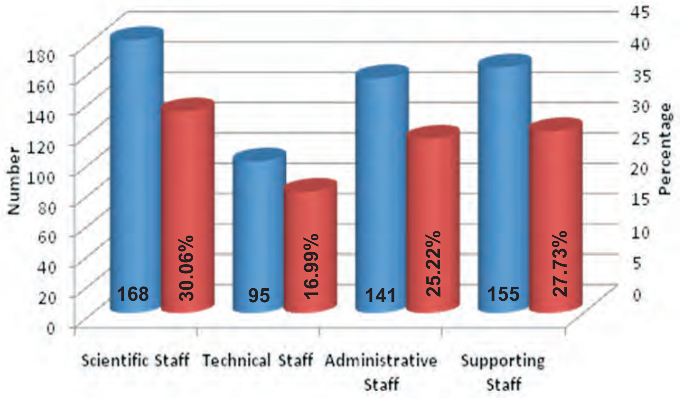
Ph.D. Theses

Year	2012	2013	2014
No. of Theses	52	73	68

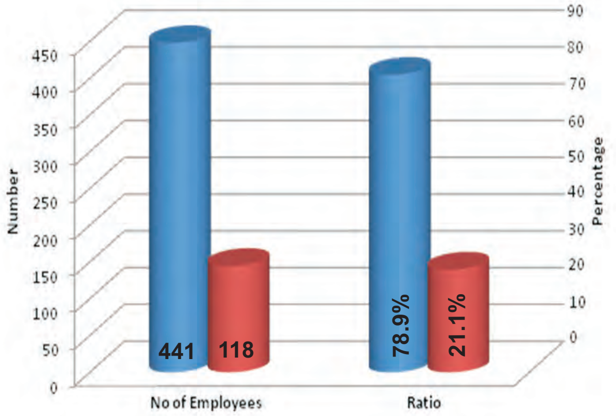


Human Resource Indicators (As on March 31, 2015)

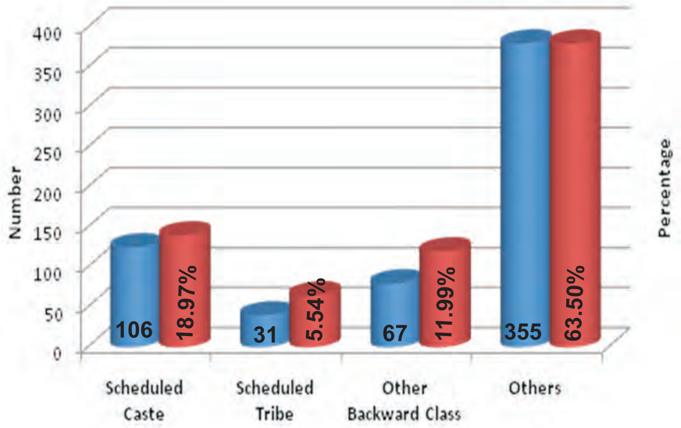
Total Staff: 559



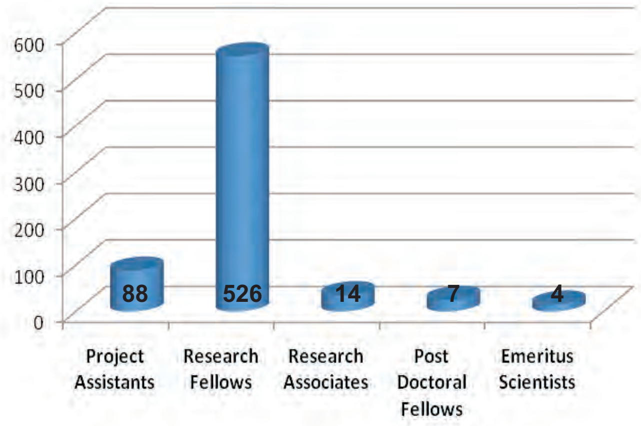
Male & Female Employees



Sc, ST, OBC & Others

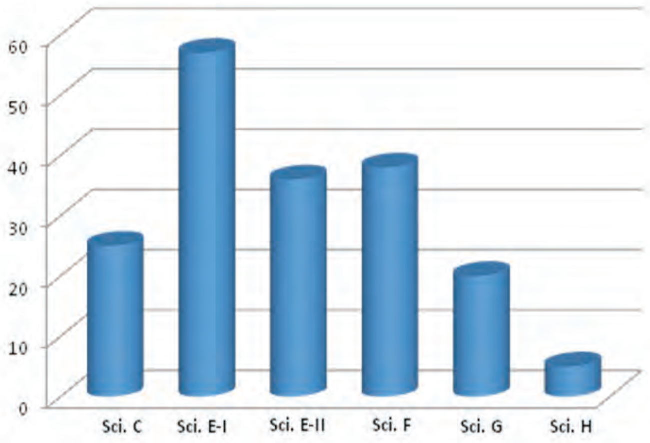


Research Fellows, Project Assistants & Others



Scientific Staff Distribution

Grade	Nos
Sci.B/Trainee Scientist	–
Sci.C/Scientist	24
Sci.E – I/Sr. Scientist	54
Sci.E – II/Principal Scientist	34
Sci.F/Sr. Principal Scientist	36
Sci.G/Chief Scientist	18
Sci.H /Outstanding Scientist	02
Total	**168**



We Welcome

Dr. Leelavati Narlikar
(10.07.2014)

Mathematical and computational modeling, Theory and Computational Science

- Wellcome Trust-DBT India Alliance Fellow, CSIR-NCL (2012-2014)
- Ramanujan Fellow, CSIR-NCL (2010-2011)
- Research Associate, Centre for Modeling and Simulation, University of Pune (2009-2010)
- Post-Doctoral Visiting Fellow, National Institutes of Health, USA (2008-2009)
- Ph. D., Duke University USA (2008)

Applications of Density Functional Theory to investigate atomic clusters, Reactions at surfaces and bulk properties, Born-Oppenheimer Molecular Dynamics

- Quick Hire Fellow, CSIR-NCL, Pune (2010-2013)
- Post-Doctoral Research Fellow/ Lecturer/ Research Associate, Department of Physics, and Centre for Modeling and Simulation, University of Pune (2005-2009)
- Post-Doctoral Research Fellow, CEA-Grenoble, France (2004-05)

Dr. Kavita Joshi
(10.07.2014)

Dr. Utpal Das
(24.07.2014)

Asymmetric Organocatalysis, Multicomponent Reactions, New Synthetic Methodologies

- Post-Doctoral Fellow, National Taiwan Normal University, Taiwan (2011-2014)
- Post-Doctoral Research Fellow, Université de Bourgogne, Dijon, France (2009-2010)
- Ph. D., University of Hyderabad (2009)

We Welcome...cont'd

Dr. Kontham Ravindar
(16.09.2014)

Total Synthesis of Biologically Active Natural Products and Medicinal Chemistry

- Senior Research Scientist, Toronto Research Chemicals Inc., Toronto, Canada (2013-2014)
- Post-Doctoral Research Fellow, Université Laval, Québec (Québec), Canada (2010-2013)
- Post-Doctoral Research Fellow, Université De Sherbrooke, Sherbrooke, Québec, Canada (2008-2010)
- Ph. D., Kakatiya University (CSIR – Indian Institute of Chemical Technology, Hyderabad (2003-2008)

Dr. Kadhiravan Shanmuganathan
(28.08.2014)

Nanofiber and Nanocomposites, Biopolymer and Bio-derived Materials

- Post-Doctoral Research Fellow, The University of Texas, Austin, USA (2010-2014)
- Ph. D., Macromolecular Science and Engineering, Case Western Reserve University, USA (2010)
- M. S., University of Massachusetts Dartmouth, USA (2006)
- B. Tech., Anna University, Chennai (1999)

We Welcome...cont'd

Functional pi-Assemblies, Organic Electronics, Stimuli Responsive Smart Materials

- Marie Curie-AUL Incoming Postdoctoral Fellow, University of Namur, Belgium (2012-2014)
- Post-Doctoral Research Fellow, National Institute for Materials Science, Japan (2010-2012)
- Post-Doctoral Research Fellow, Max Planck Institute of Colloids and Interfaces, Germany (2009-2010)
- Ph. D., CSIR-NIIST, Trivandrum (2004-2009)

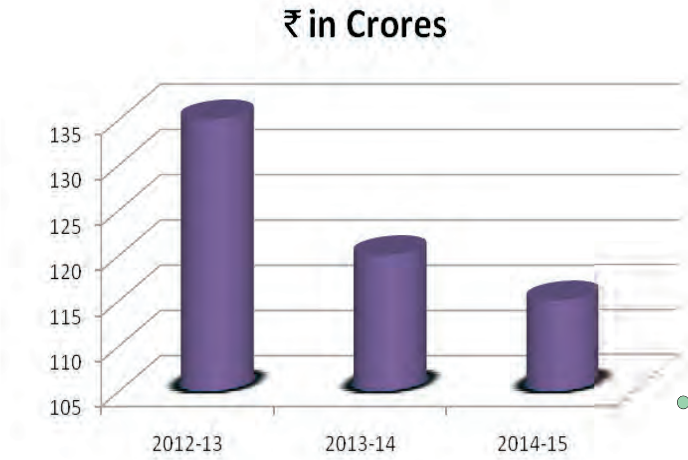
Dr. Santhosh Babu Sukumaran
(01.09.2014)

Dr. Pradip Maity
(03.03.2015)

Synthetic and Physical Organic Chemistry, Medicinal Chemistry

- Post-Doctoral Research Fellow, UT Southwestern Medical Centre at Dallas, USA (2011-2015)
- Ph. D., Florida Atlantic University, USA (2006-2011)
- M. Sc., Indian Institute of Technology, Kanpur (2003)

Financial Performance Indicators

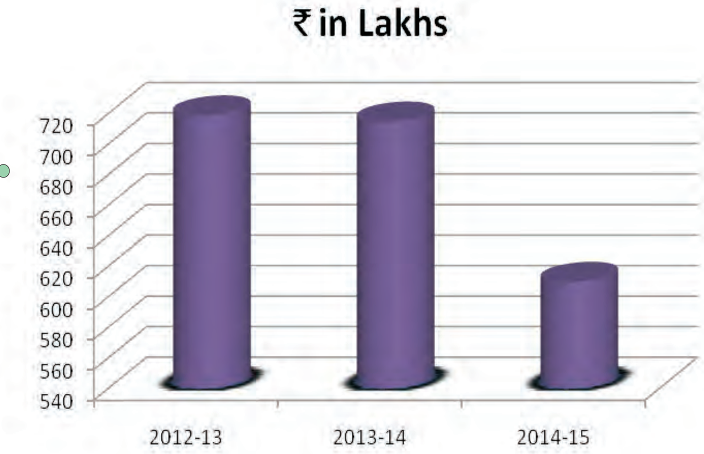


CSIR budget

Year	₹ in Crores
2012-13	131.72 (CSIR Budget : 89.12 + Network Project : 37.86 + NMITLI Projects : 4.74)
2013-14	115.17 (CSIR Budget : 68.70 + Network Project : 41.26 + NMITLI Projects : 5.21)
2014-15	111.47 (CSIR Budget : 76.93 + Network Project : 32.89 + NMITLI Projects : 1.65)

Laboratory reserve: Receipts

Year	₹ in Lakhs
2012–13	719
2013–14	712
2014–15	600



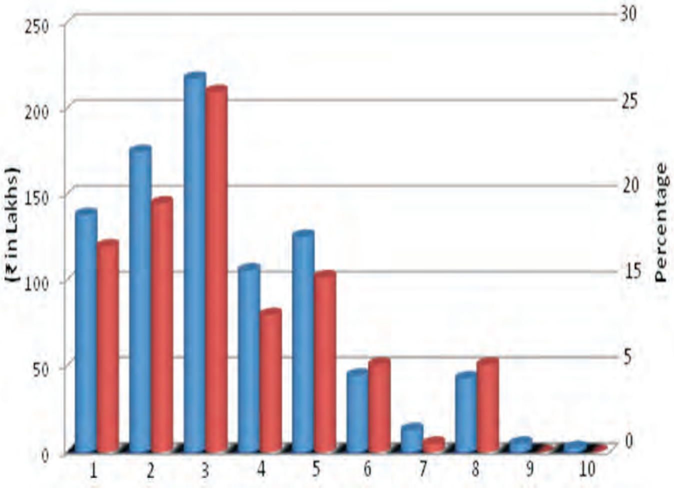
Laboratory reserve: Expenditure

Year	₹ in Lakhs
2012-13	483
2013-14	1128
2014-15	835

Financial Performance Indicators

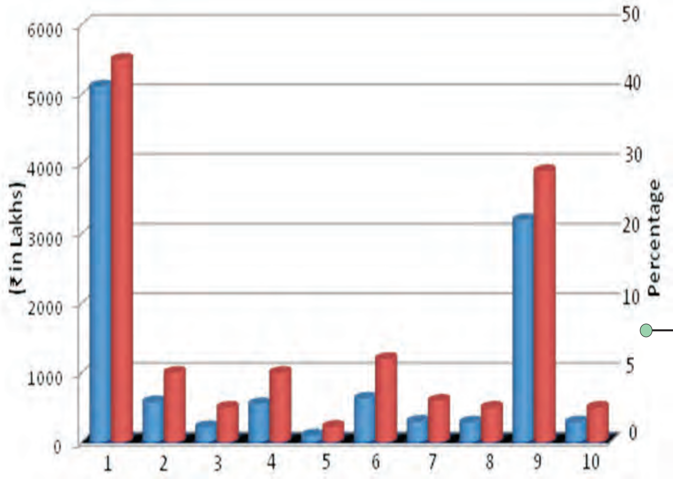
Expenditure: Laboratory reserve

Sr. No.	Expenditure head	Amount	%
1	Salary linked allowances	138.292	17%
2	Appliances and equipment + Comp. equipment	155.24	19%
3	Contingencies	217.708	26%
4	Maintenance (Lab. + Staff quarter)	100.169	12%
5	Chemicals & Consumables	125.579	15%
6	Work and services	44.666	5%
7	Furniture	8.269	1%
8	Construction of Staff Quarters	41.412	5%
9	Library	1.613	<1%
10	HRD	2.444	<1%



Expenditure: CSIR & Network Projects

Sr. No.	Expenditure head	Amount	%
1	Pay & Allowances	5017.444	45%
2	Contingency	580.000	5%
3	Maintenance (Lab+Staff Qtr)	221.000	2%
4	Chemicals	550.000	5%
5	Works & services	100.000	1%
6	App.& Equip+Comp. Equip.	630.000	6%
7	Library	300.00	3%
8	Constr. Staff Qtr.	290.000	2%
9	Netwotk projects	3196.516	29%
10	NMITLI projects	290.259	2%



Outputs and Outcomes

Category of Benefits	Benefit	Indicators	2012-13	2013-14	2014-15
Public and social goods	Generation of and dissemination of generic knowledge	Number of papers published (Calendar year)	431	455	546
		Number of invention disclosure (Calendar year)	116	176	150
		Number of patents filed in India (Calendar year)	86	118	112
		No of foreign patents filed ** (Calendar year)	96	66	78
		Number of PCT applications filed (Calendar year)	36	55	77
		No of US applications filed	26	24	50
		Number of PhDs produced (Calendar year)	52	73	68
	Highly trained man-power	Number of NET/GATE qualified students joined (including DBT JRF)	90	118	88
	Science awareness, popularization etc.	Number of popular S&T articles published (in all languages)	NA	3	4
		Number of national and regional workshops, seminars organized	9	4	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)	22	62	49
	Representation in global affairs	Official(s) in global/ trans-national organizations like the UN, WHO etc – IUPAC (Cumulative years of office held) (Data given in no. of years)	6	6	6

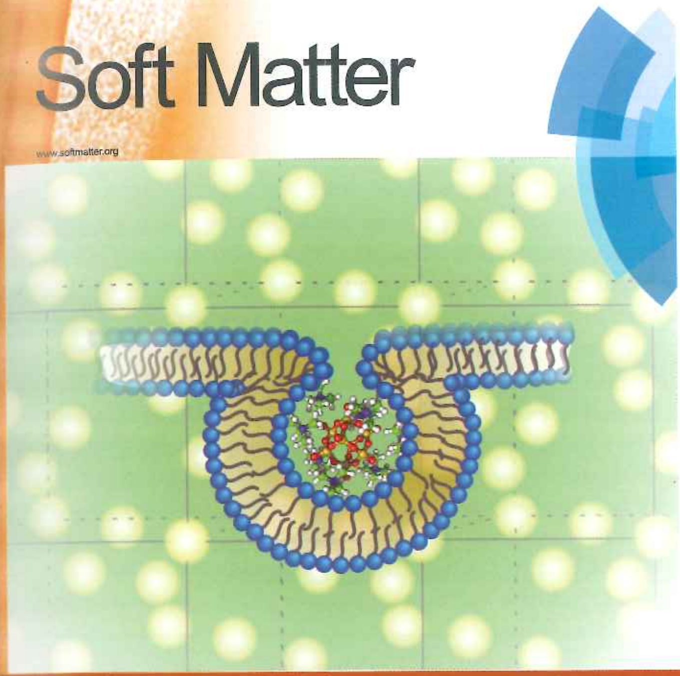
Outputs and Outcomes

Category of Benefits	Benefit	Indicators	2012-13	2013-14	2014-15
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)	10.18	7.42	18.09
	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)	4.81	0.22	5.39
Strategic goods and options	Other tactical and strategic developments	Total earnings from patent related transaction (₹ in crore)	–	–	–
		No. of patents in new Licensing /assignment/ option arrangements	–	1	1
		No. of unique Licensing /assignment/ option cases	–	1	–
		No. of Indian patents granted (Calendar year)	19	10	7
		No of foreign patents granted** (Calendar year)	22	68	49
	Contributions to projects involving valuable opportunities in the form of technology options	Money inflow from NMITLI projects and other similar strategic projects (₹ in Crore)	4.74	5.21	1.65
		Money inflow from Technology Mission & GIA projects (other than NMITLI) projects (₹ in Crore)	11.73	14.09	15.71
Intellectual assets and reputation	Quality, reputation and standing of scientific man-power	No. of Indian patents granted (Calendar year)	19	10	7
		No. of foreign patents granted** (Calendar year)	22	68	49
		Number of scientists who are members of editorial boards of international peer-reviewed journals, covered by SCI	NA	NA	NA
		Number of PhDs granted where lab scientists were research guides	52	73	68
		Number of staff who are members of National academies (Cumulative)	32	32	32
		Number of Bhatnagar awardees (Cumulative)	15	15	15
		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)	10.18	7.42	18.09

* – 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



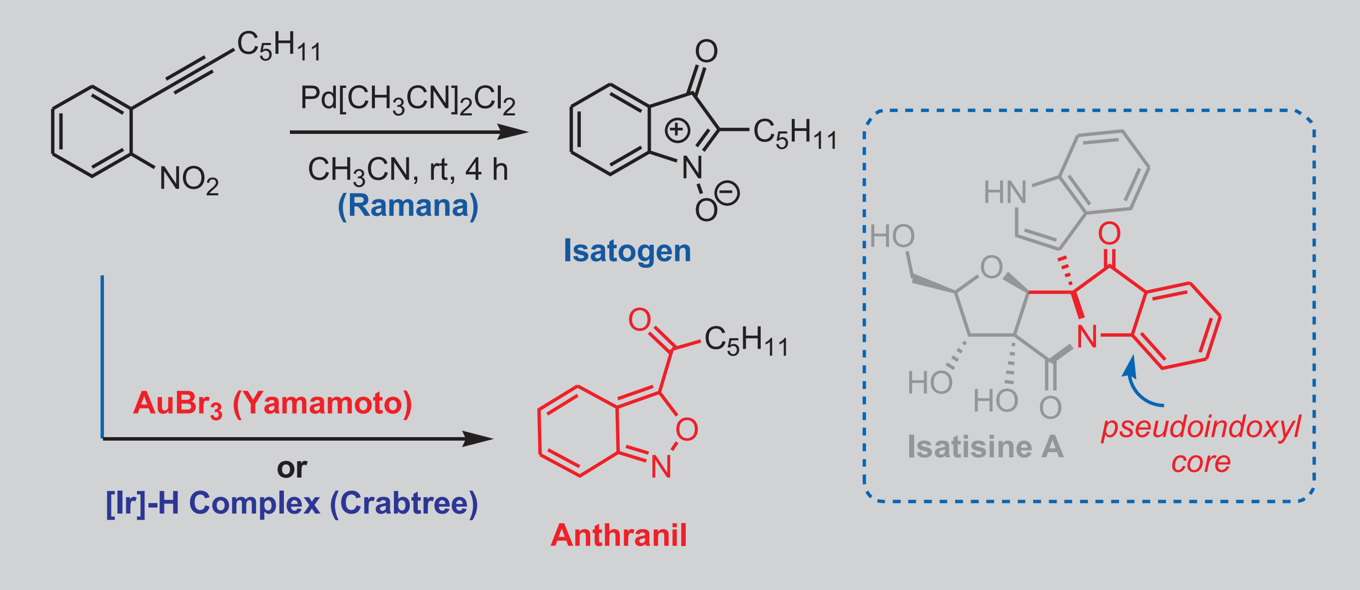
Research and Development Reports

Catalytic internal nito-alkyne redox reactions

C.V. Ramana
vr.chepuri@ncl.res.in

Internal nitroalkyne redox reactions were the centre of interest to deal with the total synthesis of Isatisine A wherein the group hypothesized the synthesis of pseudoindoxyl core employing an isatogen as the key intermediate. Isatogens (3–oxo–3H–indole–1–oxide) are unnatural and are able to undergo nucleophilic addition either at C2 or at carbonyl.

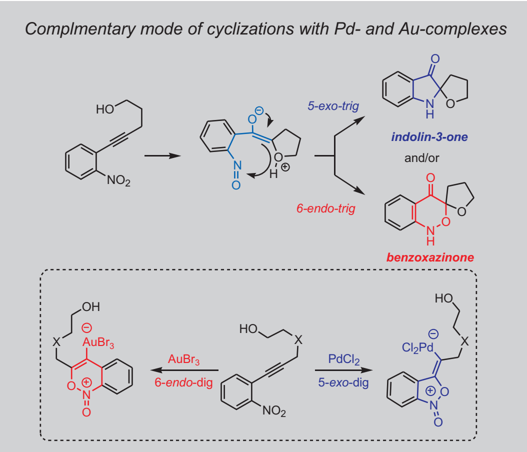
The Bayer's 1881 inaugural report on the cycloisomerization of o–nitrophenylpropiolates documented the first synthesis of isatogens. Several approaches were investigated to solve the problem of the initially employed harsh reaction conditions to facilitate the nitro–alkyne cycloisomerization. The base–mediated cycloisomerization of *o*–alkynylnitrobenzene derivatives (trivially known as *o*–nitrotolans) under thermal or photochemical conditions was employed conventionally for isatogen synthesis. It was reported recently that the nitro–alkyne cycloisomerization can also be effected under mild conditions in the presence of gold(III) bromide or an iridium hydride complex. The outcome was dictated by the nature of the alkyne substituent o–(arylalkynyl)–nitrobenzenes, for instance, were seen to give mixtures of isatogens and anthranils in the presence of catalytic amounts of gold bromide. The attention was on the synthesis of isatogens, however, the functional units at the C(2)–positions of reported isatogens were limited mainly to aryl groups, with even reports dealing with C(2)–alkyl groups being scarce. The development of a versatile catalyst that promotes the nitro– alkyne cycloisomerization to isatogens was warranted because the available catalytic transition metal protocols have limitations for 2–alkyl substituents. Considering the experience with the Pd–mediated cyclotrimerizations that was proceeded with the initial chloropalladation, it was hypothesized about the possibility of palladium(II)–mediated nitro–alkyne cycloiso–merization process that should provide exclusively isatogens.



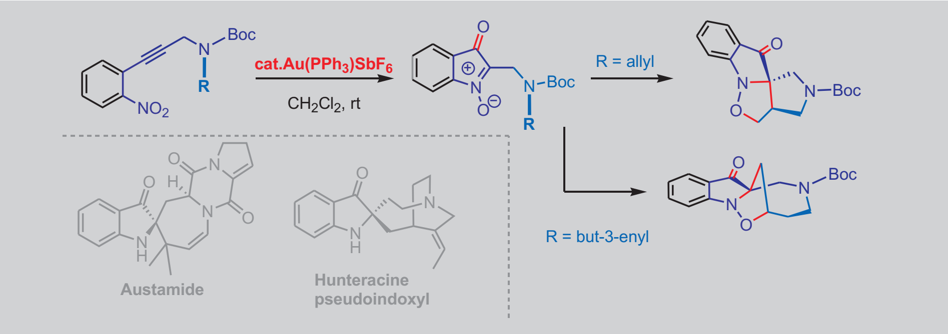
A general, efficient synthesis of isatogens was realized and documented successfully. It was the first general method for the synthesis of this class of compounds and also the first report that presented the synthesis of isatogens with diverse substituents at the 2–position (*Eur. J. Org. Chem.* **2010**, 5955).

The possibility of an intermediate nitroso stabilized Pd–carbene complex which is regiomeric to the one that forms either with Au– or Ir–complexes was proposed with the help of DFT calculations. An unprecedented nitroalkynolcyclosiomerization was designed and executed purely on the mechanistic hypothesis to address this issue. The intramolecular addition of nitro and alcohol units across the alkyne leading the spiro–indolin–3–one and spiro–benzoxazin–4–one derivatives was revealed by employing palladium and gold catalysts. Whilst A large variety of natural products comprised with spiro–indolin–3–one unit, the latter 2,3–benzaoxzinone unit is rare and present in important antitumor, antibiotic natural products.

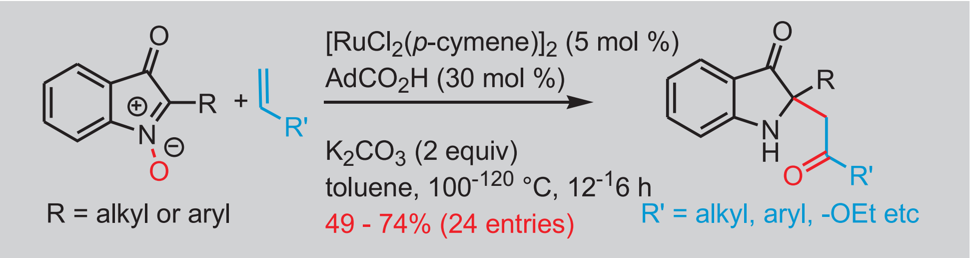
Funded upon the information that obtained from this nitroalkynolcycloisomerizatios, it was argued that Pd–complexes a 5–exo mode of cyclization is facile whereas with Au–complexes it was the 6–endo mode of cyclization that resulted in the complementary product formation (*Org. Biomol. Chem.* **2011**, *9*, 7327).



The total synthesis of Austamide was reported by Corey and Baran groups. The 2,2–spiropseudoindoxyl that forms the central tricyclic core of Austamide is another important and a rare structural motif and general methods for its synthesis are scarce. Keeping in mind the previous information on how the electronic factors influence the regioselectivity of the alkynol cycloisomerization, a hypothesis was made that the presence of an electron–withdrawing group such as nitrogen on a pendant chain should promote the 5–exo mode of cyclization inter alia isatogen formation. When the pendant group carries a suitably positioned olefin unit, the subsequent intramolecular [3 + 2]–cycloaddition should lead to the tricyclic spiro–pseudoindoxyl skeleton. The hypothesis was executed successfully to provide a simple approach for the construction of the complex spiro–indoxyl core present in a variety of pseudoindoxyl natural products. Some preliminary, yet important, observations on how to control the regioselectivity of internal nitroalkyne redox by employing the appropriate substituents at appropriate positions were revealed in this process.The Au–catalyzed nitroalkyne cycloisomerization leading to isatogens was combined with the intramolecular [3 + 2]–cycloaddition in a cascade fashion to arrive at the complex tetracyclic [6.5.n.5] frameworks in moderate to excellent yields (*Org. Lett.* **2014**, *16*, 4766).



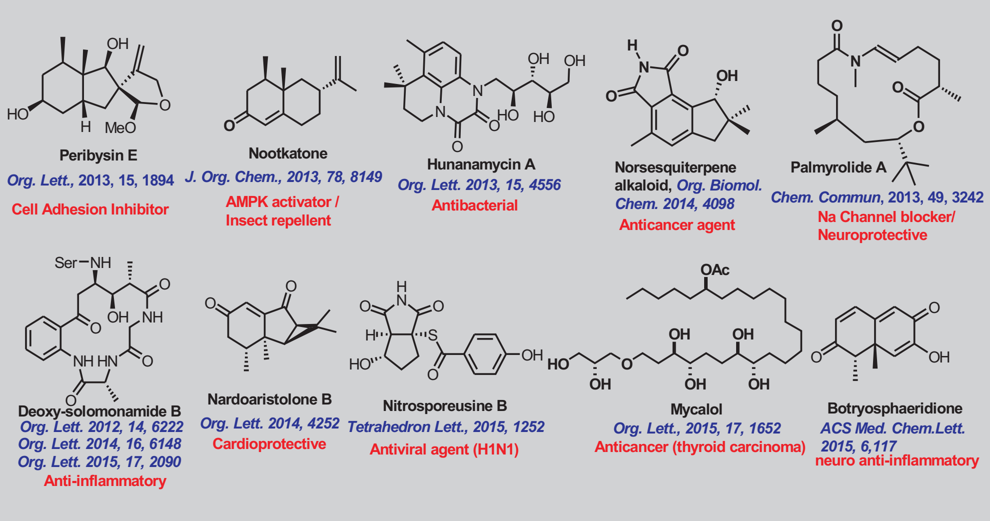
A novel metal–catalyzed one–pot [3 + 2]–cycloaddition of isatogens was developed with olefins followed by the Ru–catalyzed redox–neutral N–O bond cleavage of intermediate isoxazolidine executed as a simple method for the synthesis of 2,2–disubstituted pseudoindoxyls having proven potential as intermediates in the total synthesis of natural products and applications in inorganic materials chemistry (*Org. Lett.* **2015**, *17*, 2870).



Total synthesis of biologically active natural products using scalable routes

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

The total synthesis of natural products and their analogues with simplification of structure towards potential therapeutics is one of the exciting areas of contemporary interest in drug discovery. The group is involved in the total synthesis of several biologically active natural products. The target natural products are selected based on their biological activities. After the successful total synthesis of target natural products such as Peribysin E and Hunanamycin A, the group has prepared a focused library of their analogues. The structure-activity relationship studies (SARs) resulted in potent compounds and they are currently being profiled in biological assays.



Peribysin E
Org. Lett., 2013, 15, 1894
Cell Adhesion Inhibitor

Nootkatone
J. Org. Chem., 2013, 78, 8149
AMPK activator / Insect repellent

Hunanamycin A
Org. Lett. 2013, 15, 4556
Antibacterial

Norsesquiterpene alkaloid, *Org. Biomol. Chem.* 2014, 4098
Anticancer agent

Palmyrolide A
Chem. Commun, 2013, 49, 3242
Na Channel blocker/ Neuroprotective

Deoxy-solomonamide B
Org. Lett. 2012, 14, 6222
Org. Lett. 2014, 16, 6148
Org. Lett. 2015, 17, 2090
Anti-inflammatory

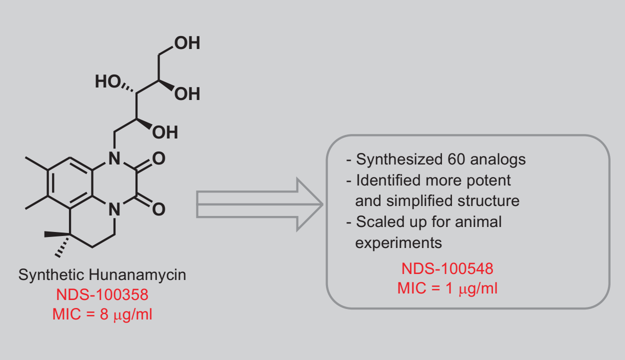
Nardoaristolone B
Org. Lett. 2014, 4252
Cardioprotective

Nitrosporeusine B
Tetrahedron Lett., 2015, 1252
Antiviral agent (H1N1)

Mycalol
Org. Lett., 2015, 17, 1652
Anticancer (thyroid carcinoma)

Botryosphaeridione
ACS Med. Chem.Lett. 2015, 6,117
neuro anti-inflammatory

Hunanamycin A was isolated from a marine-derived *Bacillus hunanensis* by MacMillan et al. in 2013. The compound showed anti-bacterial activity of 8 µg/mL against *Salmonella enterica* that was responsible for the foodborne illness. It was estimated that Salmonella ranks number one, accounting for 35% of total foodborne illnesses in the United States. The first total synthesis of Hunanamycin A was completed and systematic SAR studies were done; it resulted in more potent compounds compared to the natural product with more simplified structure. Further profiling of selected compounds is underway in this project.

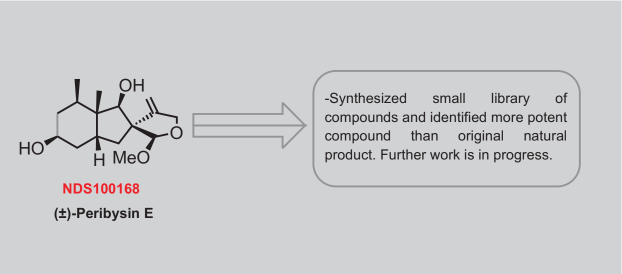


Synthetic Hunanamycin
NDS-100358
MIC = 8 µg/ml

- Synthesized 60 analogs
- Identified more potent and simplified structure
- Scaled up for animal experiments

NDS-100548
MIC = 1 µg/ml

Peribysins E was isolated by Yamada's group from a strain of Periconia byssoides OUPS-N133 originally separated from the sea hare, *Aplysia kurodai* showed potent cell adhesion inhibitory activity with IC_{50} value of 11.5 µM. The total synthesis of (±)-Peribysin E was accomplished using a short route. Eight new analogues of the natural compound were accomplished by means of "diverted total synthesis" in less than 10 steps and two compounds were showing better activity than Perbysin E. The development of a protecting group free shortest route to access these functionally embellished hydrindanes is a highlight of this work.



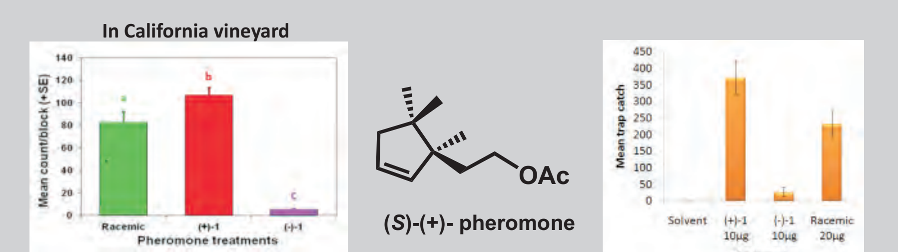
NDS100168
(±)-Peribysin E

-Synthesized small library of compounds and identified more potent compound than original natural product. Further work is in progress.

Access to enantiopure pheromones towards crop protection

The mealybug outbreaks can cause heavy losses to farmers. Controlling mealybugs using conventional methods like insecticides, biological routes are only partially effective, and may require interventions at certain points in the life-cycle of the mealybug or need repeated interventions to keep the problem under control over time. Pheromone is a secreted chemical factor that triggers a social response in members of the same species. Pheromones are known to be highly sensitive and some of them were identified and commercialized for use in pest management. Females of mealybug species produce powerful sex pheromones to attract males. The sex pheromone of the longtailed mealybug was identified after collecting odors produced by thousands of live unmated females over many weeks. The racemic synthetic pheromone provided to be biologically active for several months.

The group has synthesized both the enantiomers of the lontailed mealybug pheromone. The biological activities of these enantiomers were tested in California fields. The results showed that one of the enantiomer, (S)-pheromone was attractive to male mealybugs and the other enantiomer was inactive. The same material was also tested in New Zealand vineyards and similar results were obtained. Encouraged by this result, the group has developed a new route to synthesize enantiopure pheromones starting from readily available chiral synthons. This new route relies on reading available and cheap enantiopure starting materials and can be used for commercializing the product against the mealybug threat. Currenty, the group is exploring the activity of the pheromone in Indian fields. Since, these pheromones attract only mealybugs, and do not harm other beneficial organisms they are safer from an ecological point of view.

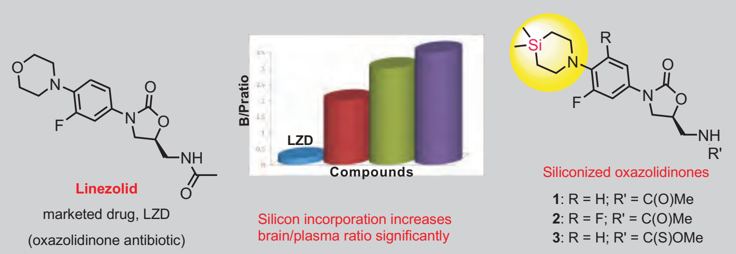


WO/2014/115172
J. Org. Chem. 2013, 78, 6281

J. Org. Chem. 2015, 80, 7785

Medicinal chemistry using silicon switch approach: Identification of brain penetrant linezolid analogues and potent anti-TB agents

Linezolid is an antibiotic used for the treatment of serious infections caused by Gram-positive bacteria that are resistant to other antibiotics. The central nervous system which coordinates the activities of all parts of the body has an additional protection called the blood-brain barrier (BBB). The BBB is highly selective and controls the entry of compounds into the brain. In a normal individual, the BBB efficiently protects the brain from pathogens that can easily cause infections in other parts of the body. While brain infections are not common, they can be difficult to treat in affected individuals due to the inability of drugs to cross the BBB. Recent reports on the potential use of linezolid in treating brain infections prompted the group to design novel compounds around this scaffold.



1: R = H; R' = C(O)Me
2: R = F; R' = C(O)Me
3: R = H; R' = C(S)OMe

WO 2013/054275 A1; US 20140296133 A1; *ACS Med. Chem. Lett.* 2015, 6, 1105

Two series of compounds showing potent activity against *mycobacterium tuberculosis* were also isdentified. Medications were known to treat TB; but they take long time with development of antibiotic resistance posing a serious threat. Along these lines, the pre-clinical candidate BM212 reported to be active against Mtb (MIC of 0.7-1.5 µg/mL) caught our attention. Several analogues were made with the incorporation of silicon and found that the incorporation of silicon increased the anti-TB potential of the series drastically. A series of silicon incorporated pyrazole derivatives which also showed potent activity was identified by the replacement of central pyrrole core of BM212.

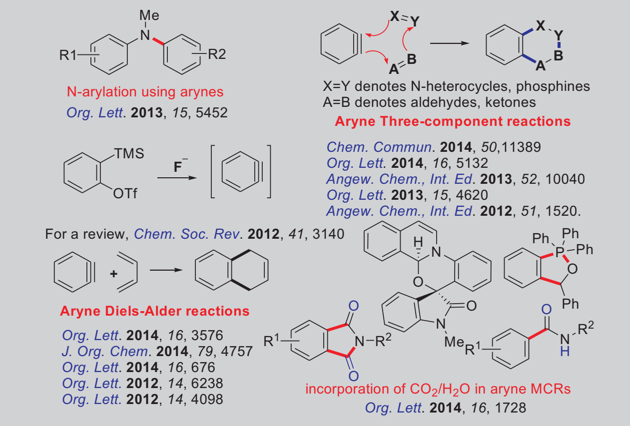
Transition-metal-free carbon-carbon and carbon-heteroatom bond-forming reactions using aryne chemistry and NHC-organocatalysis

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

The transition-metal-free carbon-carbon and carbon-heteroatom bond-forming reactions using aryne chemistry and N-heterocyclic carbene (NHC)-organocatalysis were investigated. New aryne multicomponent reactions (MCRs) involving arynes, initiated by N-heterocycles such as pyridine, and (iso)quinoline, and various phosphines were developed. The aryne chemistry was applied to various Diels-Alder reactions and insertion reactions. In addition, several NHC-organocatalyzed methods were demonstrated for the synthesis of various functionalized coumarins, highly enantioselective synthesis of various dihydropyranones, dihydropyridinones, functionalized pyrazoles and cyclopentenes.

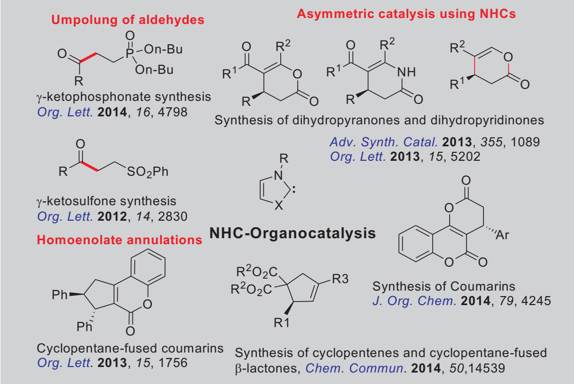
Aryne chemistry

A mild, efficient and scalable Diels-Alder reaction of arynes with challenging diene systems such as pentafulvenes, 1, 2-benzoquinones, styrenes, indenes/benzofurans, and tropones was recently developed. The synthetic utility of N-heterocycles such as pyridine, and (iso)quinoline in aryne multicomponent reactions (MCRs) was demonstrated for the synthesis of various heterocycles. In addition, aryne MCRs triggered by phosphines for the synthesis of functionalized benzooxaphospholes, and the use of CO_2 as a one-carbon synthon in aryne MCRs were developed recently. Furthermore, a transition-metal-free protocol for the N-arylation of tertiary amines was developed.



NHC-organocatalysis

A efficient and facile Stetter reaction using vinyl sulfones, and vinyl phosphonates as Michael acceptors were developed using NHC-catalysis. An efficient homoenolate annulation reaction with hydroxy chalcones for the synthesis of cyclopentane-fused coumarins was realized. The group is also working on asymmetric catalysis using NHCs. A facile method for the enantioselective synthesis of functionalized dihydropyranones and dihydro-pyridinones was developed by the reaction of modified enals with β-dicarbonyl compounds or enamines, enolizable aldehydes, and heterocyclic C-H acids. Furthermore, an enantioselective synthesis of functionalized cyclopentenes and β-lactone-fused cyclopentanes by the NHC-catalyzed reaction of 2-bromoenals with α-substituted β-diesters were reported.



Polymeric membranes for separation and fuel cell

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Polymeric membranes are used in various separation applications such as drinking water purification, waste-water treatment, chemodialysis, industrial scale gas/ liquid separations, etc. The membrane manufacturing efforts are too feeble and restricted mainly for the drinking water application in the Indian scenario. CSIR-NCL's membrane group devoted its efforts towards indigenous development of pilot-scale membranes and facility for various applications (water purification, N_2/O_2 enrichment of air, etc.). The group is involved in basic investigations of various polymeric membrane materials and their application development. The group is synthesizing various types of polybenzimidazoles (PBIs) and their structural variants for gas separation, PEMFC and chemodialysis. The MOF-polymer composite membranes for gas separation, development of PIL based CO_2 selective membranes, hollow fiber membranes for water purification and gas separation (O_2/N_2 enrichment, H_2 and CO_2 separation), acid separation using chemodialysis are the key challenging areas that are being addressed in the group.

Fuel cells are widely regarded as an efficient and clean energy alternative to limited fossil fuel resources, in which the polymeric membrane plays a niche role of transporting protons. The group has developed new proton exchange membranes (Fig. 1) for high temperature PEMFC, which are being utilized for developing stack for the generation of electricity. The performance of developed PBI based MEAs was benchmarked with the commercial MEAs and was found to be equivalent or superior (*J. Mater. Chem. A* **2014**, *2*, 14449; Patent: 0552/DEL/2014).

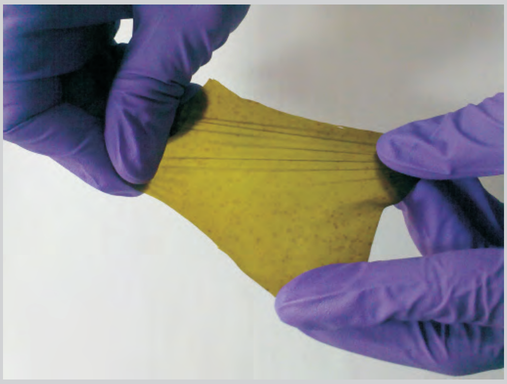

Fig. 1: Membranes developed at CSIR-NCL for PEMFC

The metal-organic framework (MOF) based composite membranes are gaining increasing attention for separation of gases and liquids. The composite membranes in both flat sheet and hollow fiber configuration were developed in CSIR-NCL. Their further modification is being done to address scale-up for gas separation application (Fig. 2) (*J. Mater. Chem. A* **2014**, *2*, 12962; *Nanoscale* **2015**, *7*, 7291; Patent(s): 3078/DEL/2014; 3324/DEL/2014).

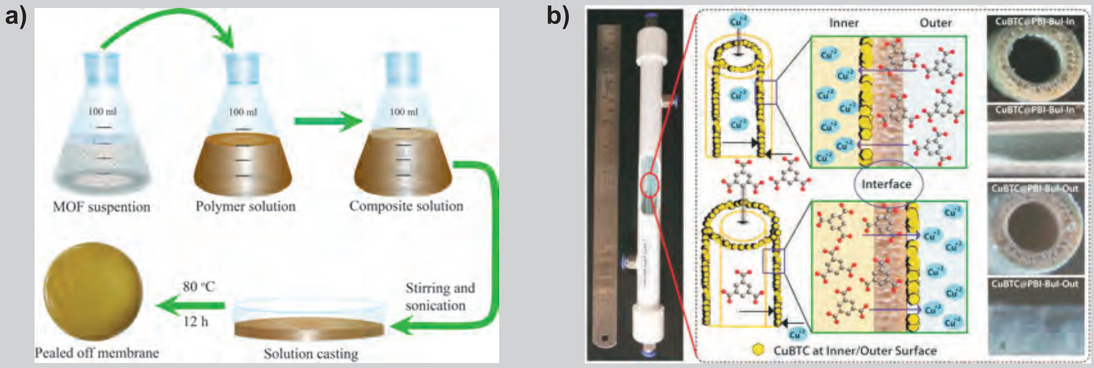

Fig. 2: a) Flat sheet; b) Hollow fiber based MOF-PBI composite membranes

The membrane based processes showed an advantage of physically removing pathogens from water. The hollow fiber ultrafiltration (UF) membrane was developed having pores small enough to retain viruses and bacteria. It can be operated at tap water pressure (0.4bar) and does not require electricity. In this regard, hollow fiber membrane based water purification unit (Fig. 3) development aiming at betterment of flux and selectivity, followed by up-scaling to semi-pilot scale led to technology transferto M/s. Technorbital Advanced Membrane Materials, Kanpur for commercial production.

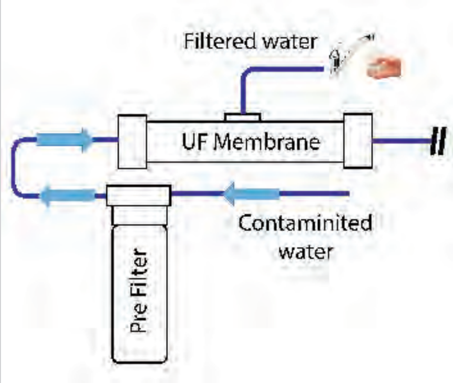

Fig. 3: Schematic of water purification unit

A new process based on chemically active membranes (in hollow fiber form), named as Chemodialysis, and is being up-scaled for acid separation (Fig. 4).

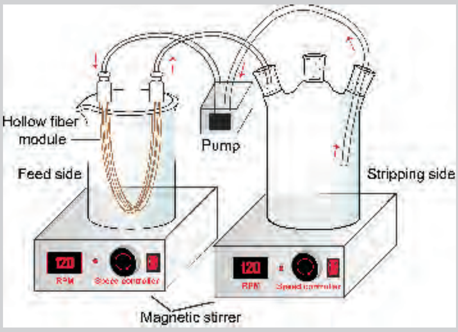

Fig. 4: Schematic of chemodialysis process

In present scenario, there is an urgent need at public / rural health centers for supply of oxygen enriched air that could be used for various medical conditions (asthma, chronic obstructive pulmonary disease (COPD), post-operative recovery, wound healing etc.). Hollow fiber membranes capable of enriching oxygen in air were developed and the technology is transferred to Genrich Membranes, Pune, for preparation of oxygen enrichment unit (Fig. 5). Developments are going on to further make the hollow fiber membranes for other gas separation applications.

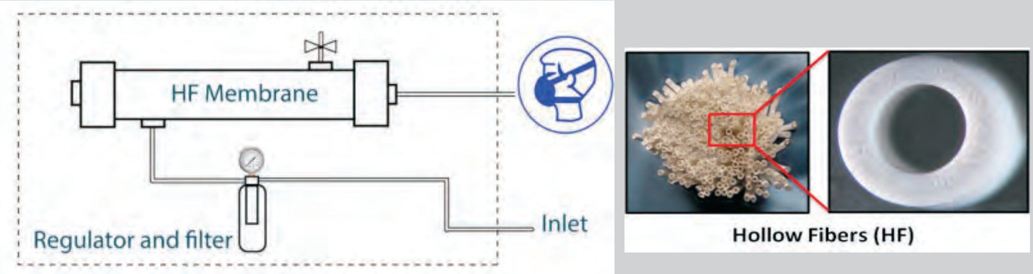

Fig. 5: Schematic of OEU

π Conjugated Oligomers and Polymers

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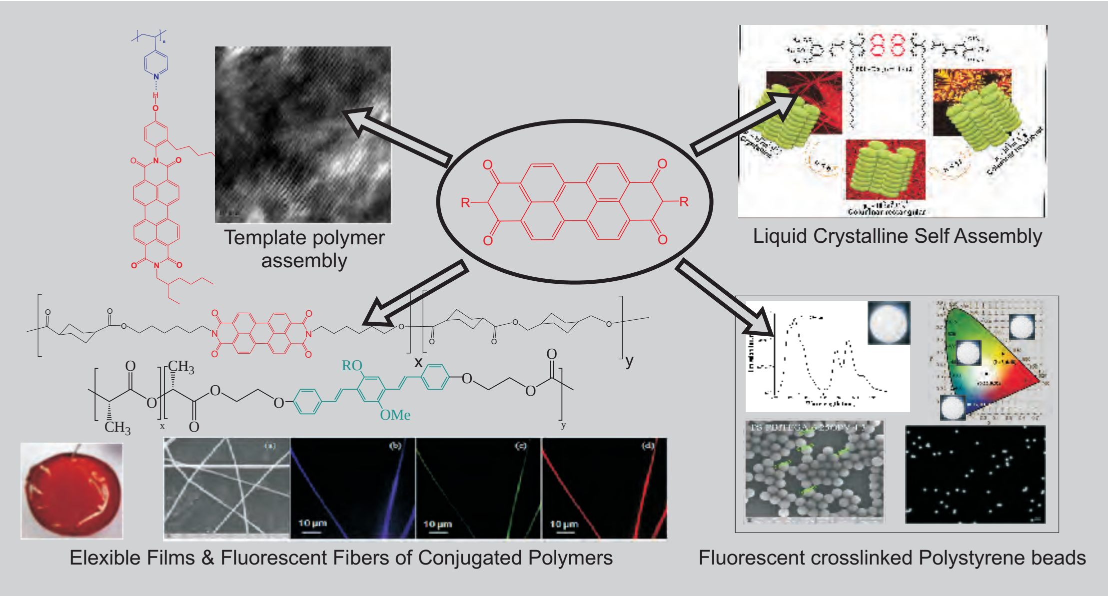
Unlike the vast majority of commodity polymers such as polyethylene, polypropylene, poly(ethylene terephthalate) or polystyrene which are insulators and are colorless, the conjugated polymers are semiconductors or conductors and can interact with light which makes them very interesting. These semiconducting polymer materials were characterized by high luminescence quantum yields, broad absorption bands and a HOMO-LUMO energy gap in the range of 1.5 eV to 3 eV, i.e., in the range of visible light and the near infrared, similar to inorganic semiconductors. The interesting photophysical characteristics make them applicable in devices like the organic light emitting diode (OLED), organic photovoltaics (OPV), organic field effect transistors (OFET) etc. The low solubility in common organic solvents due to their rigid aromatic nature is a big challenge for practical device applications. Another challenging aspect was the fact that the conjugated small molecules, which are highly crystalline with promising charge transport properties tend to lose these features upon covalent incorporation into the backbone of polymers. Retaining the crystallinity of the small molecule with the processability of a polymer is a highly desirable property in pi conjugated polymers for device applications.

In this regard the group has demonstrated that a self assembly approach could be adopted to meet the challenging task of combining the crystallinity of the small conjugated molecule with the processability and film forming nature of polymers resulting in several orders of improvement in the charge carrier mobilities (*Adv. Funct. Mater.* **2013**, *23*, 2033; *Polymer* **2015**, *65*, 115; *ACS Appl. Mater. Inter.* **2014**, *6*, 19434; *J. Mater. Chem. C* **2013**, *1*, 5925; **2014**, *2*, 6511).

Liquid crystalline ordering is another method to improve the charge carrier mobilities in these mesogenic conjugated chromophores (*J. Mater. Chem. C* **2014**, *2*, 9882).

When solid state light emission is desired, then covalent incorporation of small amounts of these conjugated fluorophores into high molecular weight polymers becomes a method of choice. Recently the group has showed that tailored molecular design principles coupled with appropriate polymerization strategies could be made use of to obtain chiral fluorescent fibers as well as white light emitting polystyrene (PS) microbeads (*ACS Appl. Mater. Inter.* **2013**, *5*, 12205, **2014**, *6*, 12457; *J. Mater. Chem. C.* **2014**, *2*, 2051; *J. Phys. Chem. B* **2013**, *17*, 13710, **2014**, *118*, 9467; *J. Polym. Sci. Polym. Chem.* **2012**, *51*, 509).

The PS beads with controlled particle size could be tuned for emission color depending on the amount and nature of fluorophore incorporated. These beads also showed promise as invisible inks that could be used for strategic application purposes.



Contemporary monomers and polymers

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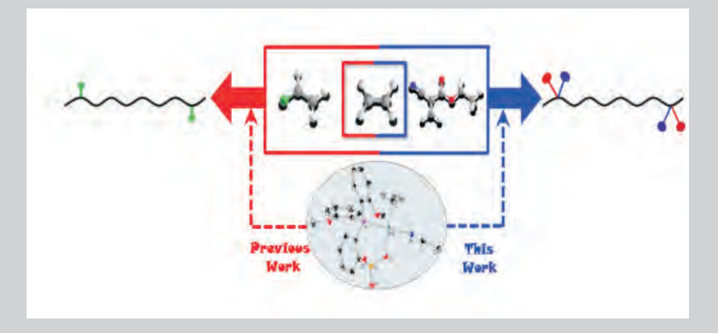
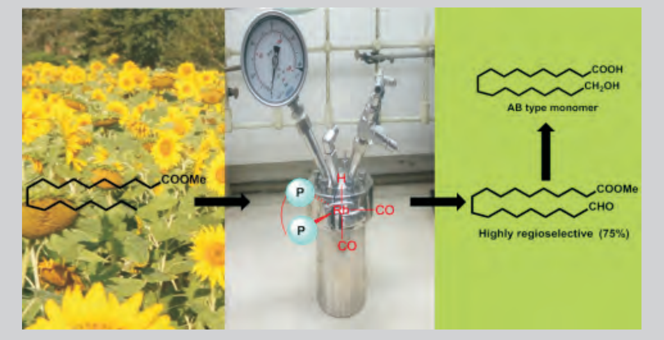
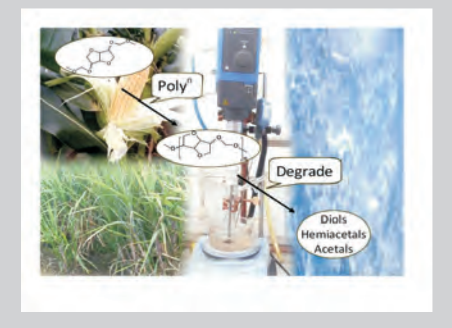
In the day-to-day life various materials come across (generally called polymers or plastics) starting from toothbrush to polyethylene bags (carry-bags) and clothes. Some of these materials were manufactured using metal catalyst. The group tried to understand the process of making these materials using various metal catalysts. A catalyst that can produce polyethylene which may stick to a surface was designed for the first time. It can be potentially used in printing inks, paints and adhesives as glue (*J. Polym. Sci. A Polym. Chem.* **2014**, *52*, 1; *ACS Macro Lett.* **2015**, *4*, 933; Patent: 2587DEL2014).



The above sticky polyethylene and majority of the carry bags and plastics used today are made from fossil fuel based building blocks and do not degrade. On the other hand, the global polymer demand continues to increase and fossil fuel reserves continue to dwindle. Therefore, scientists today have to make materials and plastics that can be grown every year like an agricultural crop and that can degrade in the environment without affecting the surroundings. The organometallic catalysts were improved to refine plant oils to synthesize various renewable building blocks (monomers). The resultant renewable material (polymers) will most likely mimic polyethylene (*ChemCatChem* **2015**, *7*, 3468).



The multifaceted approach was adopted for sustainable materials and a single step protocol was developed to convert sugars to useful building blocks and polymeric materials. Interestingly, these so called polyacetals derived from sugars degrade in slightly acidic media. Thus, the materials developed in the laboratory originate from plants (renewable resource) and degrade in the nature, meeting both the criteria i.e., renewable and degradable of futuristic materials (*Green Chem.* **2014**, *16*, 3810; Patent: WO2014181358 A2).



Controlling drug release from pharmaceutical formulations

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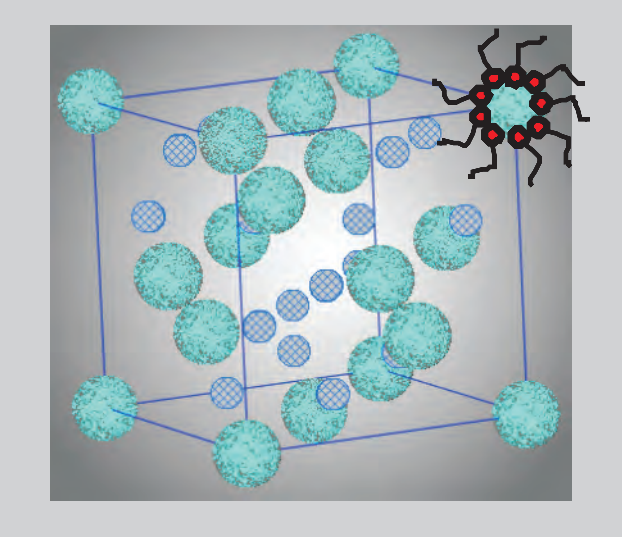
The research group observed a major challenge in pharmaceutical formulations to control the rate of drug release. In most nanoparticle based formulations, encapsulated drugs exhibit burst release, viz. they are rapidly released immediately after the medication is administered. This work addressed this issue by developing a formulation based on a food-grade lipid called monoolein. Monoolein is a commercial lipid used as an emulsifier in foods. It is highly hydrophobic and typically organizes into a structure that has a bicontinuous structure, viz. it has connected aqueous and hydrophobic channels that run through it.

A demonstration was performed for the first time by adding a class of water-soluble polymers to transform this structure into a discontinuous structure that encapsulates water droplets in a hydrophobic matrix. The release of water soluble drugs dissolved in these nanoscopic water droplets was retarded ten-fold relative to the normal bicontinuous structure. Apart from the implications of this work for drug release applications, it showed major implications for fundamental understanding of how to control lipid organization. The research work provided the first design rules for polymeric additives to transform lipid organization from a bicontinuous to a discontinuous phase. The demonstration was performed to prove that polar polymers that interact strongly with the lipid head group having a compact molecular architecture induced such structural transformation (*Soft Matter* **2015**, *11*, 5417, 5705; Patent: 3631/DEL/2014).



Computational studies in metal-free molecule activation

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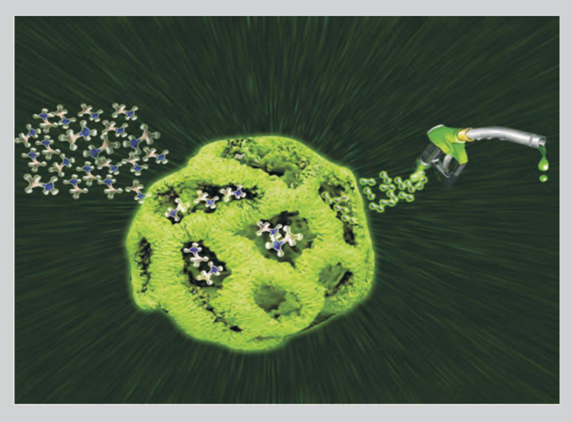
The small molecule activation is an important problem, with relevance in biological processes, as well as to important new areas of research such as hydrogen storage. Transition metal complex systems held a monopoly in this field. However, methods that employ systems that move away from transition metals hold special interest; because main-group systems have the advantage of being cheaper and greener than transition metal systems. The authors have investigated through computational studies employing density functional theory (DFT) small molecule activation by main group systems based on the concept of frustrated Lewis pairs (FLPs).

Specifically, the employment of 0D caged structures containing only carbon, nitrogen and hydrogen atoms as well as molecular caged structures were studied. Furthermore, computational studies with silylene and frustrated Lewis pair (FLP) systems yielded interesting results *vis-à-vis* making them more effective. The reactions like the catalytic dehydrogenation of ammonia borane (AB), dihydrogen activation, as well as the activation of other important small molecules such as carbon monoxide and carbon dioxide were investigated properly (*Chem. Commun.* **2011**, *47*, 11417, **2014**, *50*, 8522; *Phys. Chem. Chem. Phys.* **2013**, *15*, 20857; *Inorg. Chem.* **2013**, *52*, 4238; *Dalton T.* **2013**, *43*, 2194; *J. Org. Chem.* **2015**, *80*, 2081).



Novel nanoporous hollow structures

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Scientists have designed porous materials by borrowing ideas from nature. Interesting examples of natural porous structures include hollow bamboo, honey combs with hexagonal pores, diatomaceous earth and alveoli in the lungs. When the pore size is reduced down to the nanometer scale, novel porous materials with unique properties and applications are created.

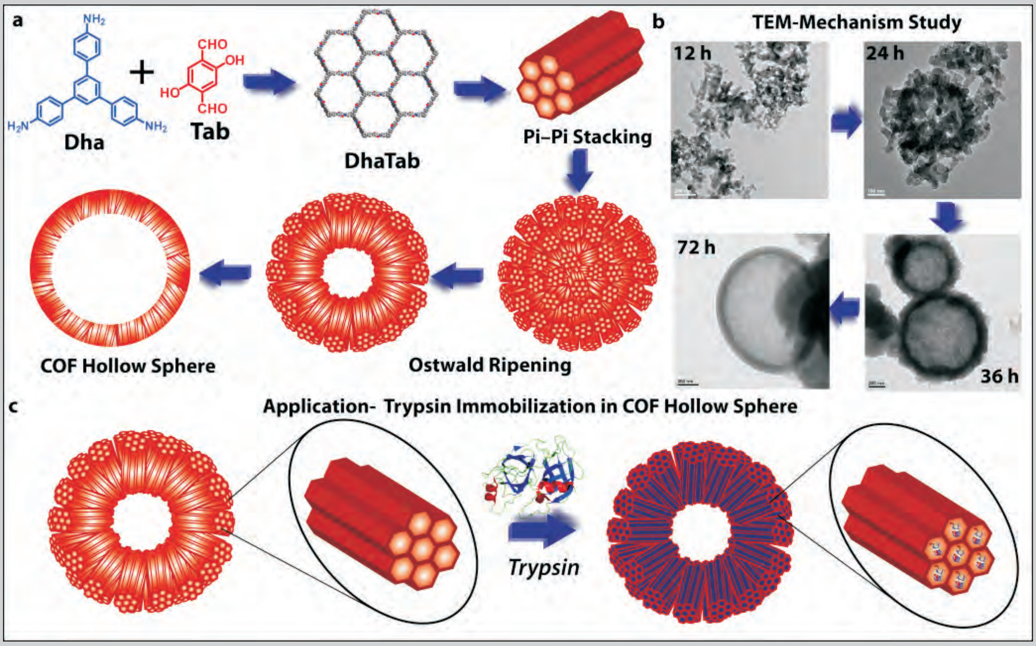
Nanoporous materials can be used for a variety of applications such as storage of molecules (e.g., gas molecules, drugs and biomolecules like enzymes), ion exchange, catalysis and sensing. The main examples of nanoporous materials are porous carbons, mesoporous silica, zeolites, metal organic frameworks and covalent organic frame (COF) works.

Notably, COFs are the newest member in this family and are unique because they are formed by rigid covalent bonds between organic building blocks. Consequently, they have low density and a large number of functional groups that can be tailored for various applications. Initial reports on COFs demonstrated their utility as effective gas storage media, catalytic supports, and semi-conductive and photoconductive devices (*Chem. Commun.* **2014**, *50*, 3169).

One of the drawbacks of COFs is their poor chemical stability in presence of water. This is important in applications such as gas storage since gases found in nature are often saturated with water vapour. The group for the first time demonstrated that introduction of intramolecular H-bonding improves the chemical stability of imine based COFs making them stable in boiling water, buffer and even in 9 N HCl (*J. Am. Chem. Soc.* **2012**, *134*, 19524, *Angew. Chem. Int. Ed.* **2013**, *52*, 13052).

While COF crystallites are known to adopt beautiful morphologies like belts, fibres, sheets, cubes, rectangular prisms, spheres and platelets in nano-dimension, the process of self assembly of the COF crystallites was hitherto unknown. The group first time shed light on the mechanism of formation of crystalline and nanoporous COF hollow spheres of high surface area (*Nat. Commun.* **2015**, *6*, 6786).

Electron microscopy of these self templated COF hollow spheres during synthesis showed formation of rod-like structures, which first self assembled into dense spheres and then converted into hollow spheres as the reaction progressed. It was reported that the demonstration of the immobilization of trypsin inside the 3.7 nm mesopores of COF-DhaTab hollow sphere increased the recyclability and stability of the enzyme.



Tandem catalysis

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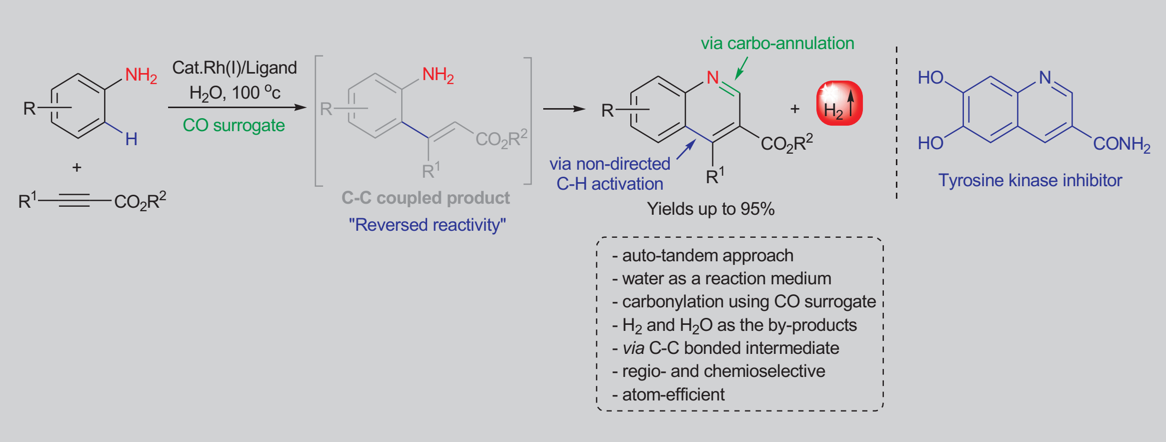
Effective catalysts are critical to develop efficient and clean chemical processes in the industry. Chemists are often inspired by nature in the pursuit of selective chemical transformations while designing new catalytic systems. One of the approaches mastered by nature involves the use of a tandem process (a multicatalytic approach consisting of two or more mechanistically distinct catalytic steps using a single–site catalyst) for rapid and straightforward access of structurally complex molecules. Tandem or cascade reactions are extremely valuable processes because of the potentially difficult work–up. The product associated with the isolation and purification of the intermediates in multistep sequences can be avoided and the generation of copious chemical waste is also minimized. Development of such tandem processes for chemical production is very challenging and sporadically mentioned due to the difficulty in the optimization of the separated processes independently.

The reversed reactivity of aniline with alkyne led to the formation of C–C coupled product as a potential intermediate in contrast to the archetypical C–N bonded products; it was disclosed for the first time. The product from this complementary approach (non–directed C–H activation strategy of unprotected anilines) was integrated with sequential carbonylation–annulation in an auto–tandem manner to form synthetically versatile quinolines with the concomitant generation of hydrogen gas. This auto–tandem reaction operates under mild, environmentally benign conditions using water as a solvent and CO surrogates as a carbonyl source with extremely good atom–efficiency (only H_2 and H_2O as by–products). The strategy facilitated the development of new synthetic protocols for the efficient and sustainable production of chemicals in an atom–economic way from simple, abundant starting materials (*Nat. Commun.* **2015**, *6*, 8591).



Process intensification: Continuous flow reactors

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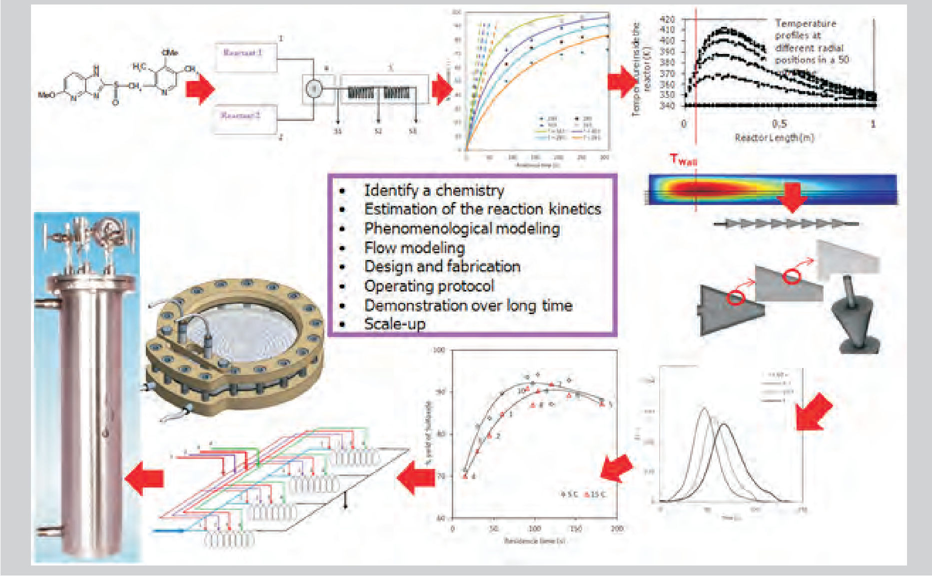
The group works on the development of continuous processes, designing of flow reactors, development of new concepts for flow reactors, and their applications for variety of reactions in an effort to change the way the fine and specialty chemicals are manufactured in India. The small volume continuous flow reactors offer very high heat transfer and mass transfer rates and rapid mixing, which helps to transform the conventional processes into an efficient and consistent synthesis protocol. Aromatic exothermic nitrations, sulfoxidation, amination, reduction, chlorination, bromination, diazotization etc. are among few of the reactions that were successfully transformed in continuous flow (*Org. Process Res. Dev.* **2015**, *19*, 1138; *J. Flow Chem.* **2014**, *4*, 210; *Green Process Synth.* **2014**, *3*, 279).

The products synthesized by the group included intermediates for API, agrochemicals, adhesives, dyes and pigments. The approach involved a multi-step protocol that included identification of the right chemistry, measurements of the reaction kinetics, development of a flow synthesis set-up, parametric studies aimed at maximizing the yield of the desired product, design of prototype, (1D, 2D and 3D) simulations of flow, heat transfer and reaction (either coupled or independent), fabrication and measurement of dispersion and its effect on performance, demonstration at laboratory and bench scale for long hours and then numbering-up to achieve the desired production capacity. The approach was extended for the flow synthesis of nanomaterials like Ag, Au, CuO nanoparticles and a method for their scale-up to produce as much as 100 g/day with a strict control on particle size and shape (*AIChE J.* **2015**, *61*, 4294; *Chem. Eng. J.* **2015**, *278*, 454; *Cryst. Growth Des.* **2014**, *14*, 4329; *Colloid. Surface A* **2014**, *443*, 149).

A few microreactor fabricators were developed so that the chemical manufacturing industries in India do not have to import these reactors in an effort to spread the method of continuous flow synthesis of *high-value-low-volume* chemicals in the manufacturing industry. The reactors developed as a part of this effort are explored in detail and the performance in terms of their hydrodynamics for flow of liquids, gas-liquid and liquid-liquid dispersion, liquid-solid suspension etc. were studied quantitatively to develop scale-up guidelines (*Ind. Eng. Chem. Res.* **2014**, *53*, 1916; Patent(s): 2957DEL2011, 3622/DEL/2013, 0292-NF-2013, 2012-NF-0133; Design(s): 247209; 247208).

One of the major challenges in using flow reactors for reactions involving solids is the blockage of channels. Such situations prevent the use of a promising technology for efficient manufacturing. New flow reactors that can be used for flow of suspension having about 20% solids to overcome the issue. Similarly another challenge is to achieve uniform flow distribution in a network of large number of channels where multiphase reactions take place. Various distributor designs for uniform flow distribution are being explored to ensure that a robust numbering-up approach can be developed.



- Identify a chemistry
- Estimation of the reaction kinetics
- Phenomenological modeling
- Flow modeling
- Design and fabrication
- Operating protocol
- Demonstration over long time
- Scale-up

Research Highlights

Identifyling diverse promoter architectures from genome-wide data

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Transcriptional regulation is critical for appropriate development and maintenance of cells. The core promoter—100bp near the transcription start site (TSS)—is believed to play a major role in this process by harboring sequence elements recognized by DNA–binding proteins. High–throughput technologies have helped produce genome–wide maps of TSSs in various cell–types, but the promoter architectures and elements involved in the process are still poorly understood. The biggest hurdle in the downstream analysis of promoters is the heterogeneity in TSS neighborhoods. Promoters can have diverse regulatory mechanisms. For example, one set of promoters may be characterized by elements X, Y, & Z, another by X & W, a third only by W, and a fourth by U & V. None of the traditional methods can identify such categories of promoters.

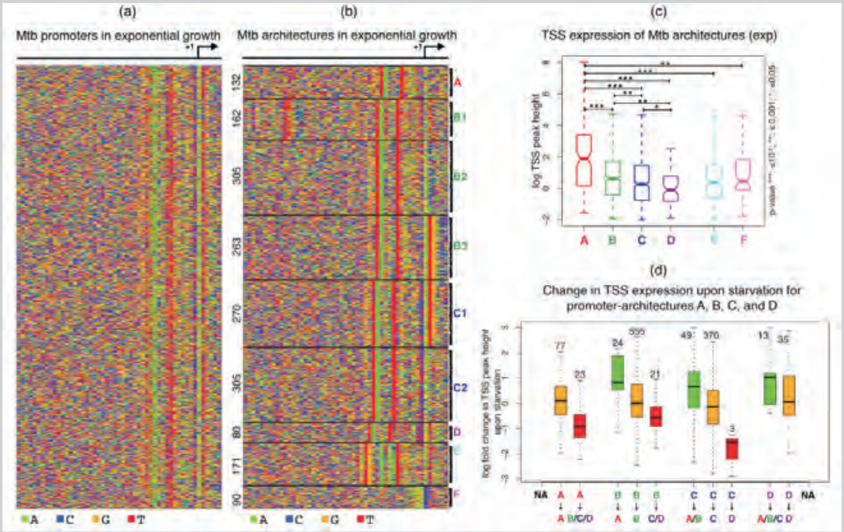
A new unsupervised learning method was recently developed that clusters promoters into similar architectures, while simultaneously identifying positions with respect to the TSS that are vital for characterizing each promoter (*Nucleic Acids Res.* **2014**, *42*, 12388).

The results are briefly mentioned, while the method was run on *M. tuberculosis* TSSs in exponential growth conditions (Fig. a) for other organisms and more details about the formulation of the model.

The primary distinguishing factor in the identified nine architectures (Fig. b) is the position of the –10 box from the TSS, which can appear at positions –11 (architecture A), –12 (architecture B, which is in fact identified as three separate architectures that were named B1, B2, and B3), –13 (architecture C, also separated into C1 and C2), or –14 (architecture D) relative to the TSS. Cortes et al. showed a modest correlation between the presence of the TANNNT motif and the expression level of the TSS. However, these results suggested that it is not the presence of the motif, but the spacing between the motif and the TSS that better explains the expression level of the TSS. The TSS expression is significantly higher in architecture A and monotonically decreases as the distance increases (Fig. c).

The TSS of 133 of these genes changed by one, two, or three bases under starvation condition such a way that they could be categorized as having transitioned into architecture with a different spacing. For genes where the TSS does not change, the TSS expression also does not change significantly (Fig. d).

In contrast, in cases where the architecture changes to one with a larger (smaller) spacing, the TSS expression goes down (up). Interestingly, this relationship between the spacing and TSS expression was found to be true only in *Mtb*, and not the other bacteria where data was available. No Promoter Left Behind (NPLB) is also available as a webserver hosted in NCL (nplb.ncl.res.in), which is a fast implementation of the method.



Advanced glycation end products in diabetes

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Advanced Glycation End products (AGEs) promoted protein cross-linking and formation of protease resistant aggregates, which were implicated in the pathogenesis of diabetes and its complications (*Mol. Cell Proteomics* **2013**, *12*, 228; *Proteom. Clin. Appl.* **2013**, *7*, 155).

Reducing AGE levels is considered as a useful therapeutic strategy in management of diabetes. A diagnostic fragment ion library for mass spectrometry-based quantification of glycated peptides of albumin was developed and the identification of glycation sensitive peptides was done that could be potential novel markers to assess the degree of glycation in diabetes (*Mol. Cell. Proteomics* **2015**, *14*, 2150).

Furthermore, it was unequivocally demonstrated that albumin protects low abundant plasma proteins from adverse effects of glycation and lower levels of albumin are associated with increased glycation of plasma proteins in general and HbA1c in particular, and vice versa (*J. Proteome Res.* **2012**, *11*,1391).

This association was also observed in about 900 clinical subjects in collaboration Chellaram Diabetes Institute, Pune. Thus maintaining higher or near normal levels of albumin in diabetes would help in reducing the plasma AGEs in vivo, while lower levels of albumin in diabetes could be a potential risk factor for glycation induced complications.

The work involved the repositioning of drugs for glycation inhibition. Several FDA approved drugs like Hydralazine, Rifampicin, Protriptyline and Isoprenaline were demonstrated to possess potent glycation inhibition activity. These molecules can be useful in the management of diabetes, as it is important to reduce AGEs along with glucose (*Sci. Rep.* **2013**, *3*, 2941).

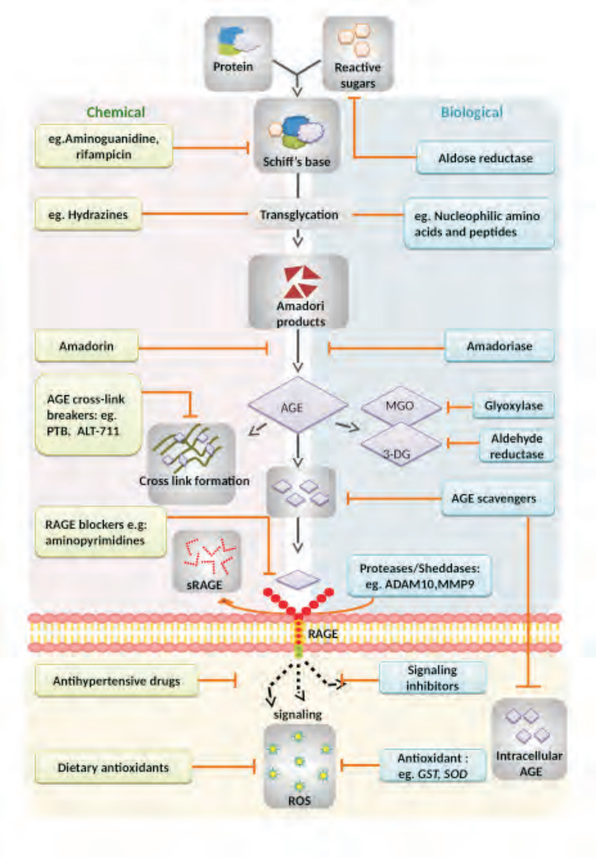

Fig: Chemical and biological intervention strategies for reducing AGEs

Dynamics of plant-insect interactions

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Available history manifests contemporary diversity that exists in plant-insect interactions. A radical thinking is necessary for developing strategies for crop protection since current agricultural practices can reduce species richness and evenness, and cause heavy damage to the ecosystem. Diverse natural products need to be studied and explored for their biological functions as insect pest control agents. In order to assure the success of an integrated pest management strategy, human activities needed to be harmonized to minimize the global climate changes (*Planta* **2015**, *242*, 761).

Unlike pathogen resistance, insect resistant crop varieties are rarely spotted in the primary or secondary gene pool. The scientific potential of such intriguing problem is pursued by the group by selecting *Helicoverpa armigera* as insect pest system. This insect uses multiple serine proteases to acquire nutrition and energy from ingested plant food for growth, development and reproduction.

On the other hand, plant produces protease inhibitors to disrupt digestive physiology of feeding insect. The contributions of the group are towards understanding protease inhibitor mediated plant defense against insect pests and their potential use in agriculture as pest management. The group studied the expression processing and tissue-specific distribution under steady state and induced conditions of *C. annuum* protease inhibitor (*CanPIs*) genes to explore the functional specialization of an array of it (*Planta* **2015**, *241*, 319).

The elicitation treatments regulated the accumulation of *CanPIs* corresponding to 4-, 3-, and 2-inhibitory repeat domains (IRDs). Based on the differentially elicited *CanPI* accumulation patterns, it is intriguing to speculate that generating sequence diversity in the form of multi-IRD PIs is a part of elaborative plant defense strategy to obtain a diverse pool of functional units to confine insect attack. Selected *CanPI* genes were cloned in *Pichia pastoris* to obtain recombinant proteins for further characterization. For example, *H. armigera* larvae fed on recombinant PIs individually incorporated into artificial diet showed mortality; in addition, significant reduction in weight gains in *H. armigera* larvae and pupae (*Phytochemistry* **2014**, *101*, 16).

Thus, some of the identified PIs have a strong potential to use in insect pest management (*Colloid. Surface. B* **2015**, *130*, 84).

The biochemical properties of *H. armigera* digestive proteases were evaluated and coupled with gene expression analysis to understand insect's responses to protease inhibitors (*Insect. Biochem. Molec.* **2014**, *54*, 129).

Advanced Materials

Nanostructured materials

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Tunable and NIR absorbing nanomaterials: The tunable, high quality and NIR absorbing lead sulfide (PbS) quantum dots were synthesized from colloidal synthetic root. The heavily doped copper selenide ($Cu_{2-x}Se$) nanocrystals were also synthesized for their plasmonic behavior.

Materials for energy: The materials were designed with the aim of implementing them to build efficient and cost effective photovoltaic devices. The various nanomaterials in fabricating solar cells were successfully implemented.

Functional Materials: The materials were designed such that they can play various roles in functioning of photovoltaic devices. For example TiO_2 and ZnO were synthesized and used as n type layer, PbS quantum dot layer acts as main light absorbing layer and plasmonic $Cu_{2-x}Se$ serve as a light trapping aliment in the solar cells.

Development of plasmonically enhanced quantum dot solar cell: The PbS quantum dots of varying size were investigated to achieve the band gap tunability. Fig. 1(a) shows the absorption spectrum of different size lead sulfide quantum dots synthesized from colloidal technique. The band gap energy was tuned from 1.34 eV, 1.12 eV and 0.89 eV respectively by increasing the size of the quantum dots. Such control tuning of band gap was exploited further in the development of solution processed quantum dot solar cells. The plasmonic light taping strategy was implemented in order to avoid transmission loss and to achieve higher order light trapping in quantum dot solar cells. The heavily doped semiconducting nanocrystals of $Cu_{2-x}Se$ were implemented for the first time for the plasmonic light trapping in solar cells. The absorption spectrum of $Cu_{2-x}Se$ nanocrystals in organic solvent (Toluene) is shown in Fig. 1b. Plasmonic resonance peak for $Cu_{2-x}Se$ nanocrystals appeared within the wavelength range of 600 nm to 1600 nm. The broad plasmonic resonance complements the transmission loss of PbS quantum dot solar cell in the NIR range.

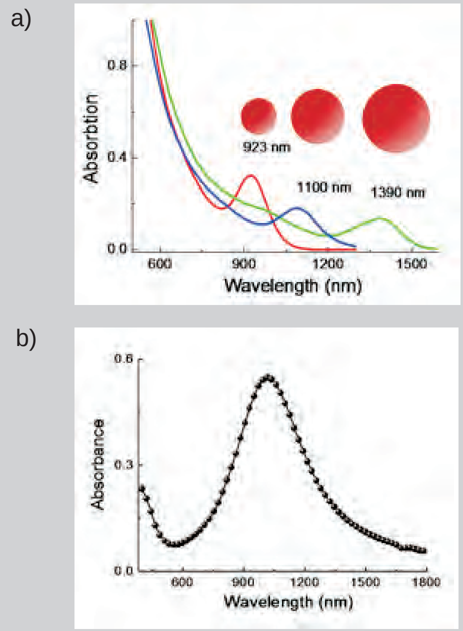

Fig. 1: (a) UV-VIS-NIR absorption spectrum of three different sizes PbS quantum dots. (b) Represents the absorption spectrum of Cu2-xSe nanocrystals in toluene

The efforts were extended to develop solar cells based on PbS quantum dots and $Cu_{2-x}Se$ nanocrystals. Fig. 2 (a) and (b) show the devise structures investigated. In Fig. 2 (a) pristine PbS quantum dot layer was used as light absorbing layer where as in case of figure 2 (b) $Cu_{2-x}Se$ nanocrystals were blended with the PbS quantum dot layer to obtain the plasmonic enhancement in solar cell performance. The strong plasmonic resonance of $Cu_{2-x}Se$ nanocrystals enhanced the light absorption within the same volume of the blend layer and there by contributed in performance enhancement of the solar cells. Fig. 2 (a) and (b) shows the solar cell performance of the devices without and with plasmonic active layer. As it was found in the preliminary study, the performance of the plasmonically modified solar cell was enhanced by 43%.

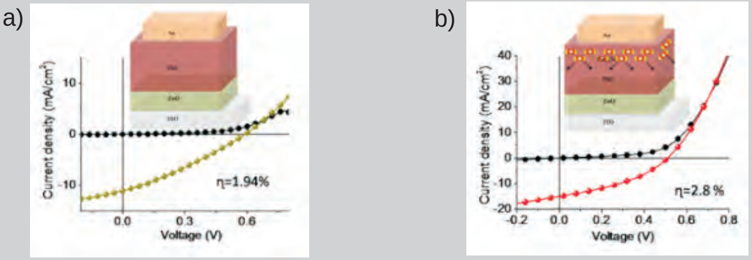

Fig. 2 (a), (b): The device structure and current voltage characteristics under dark and 1 sun condition for pristine and plasmonically modified devices respectively

Advanced Materials

Nanostructured materials

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The objective was to design catalytic materials with improved performance in terms of activity and stability which require nanoscale engineering of chemical components that constitue the final catalyst. It is possible to improve the overall activity either by engineering the support or by creating nano-architectures which specifically exposes active sites.

Core-Shell Au@Ti-SiO_2 catalyst for oxidation reactions: The overall performance of an Au- based catalyst was significantly improved by incorporating Ti (1-5 wt %) into a relatively inert SiO_2 matrix. Since the catalyst is in the form of core-shell morphology, the sintering issues associated with Au nanoparticles were also addressed by improving the stability and life time of the catalyst (*Chem. Cat. Chem.*, **2015**, *7*, 1222).

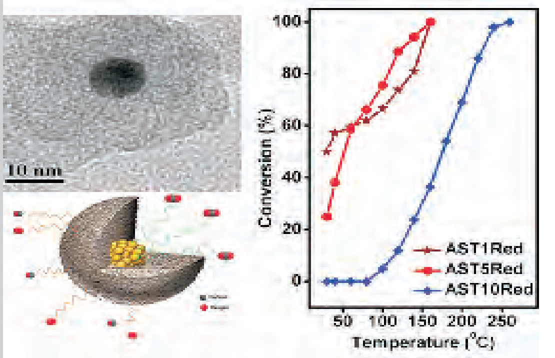

Fig. 1: CO oxidation profile for Au@Ti-SiO_2 core-shell catalyst from RT to 300°C

Structure sensitive CO oxidation on Ru nanochains: A seed mediated protocol reported for the synthesis of Au nanoparticles was adopted for the formation of Ru nanochains at mild temperatures (70°C) and in aqueous medium. Due to the abundant presence of defect sites the nanostructures showed much improved activity compared with its spherical counterparts (*Chem.Comm.* **2015,** *51,* 10178).

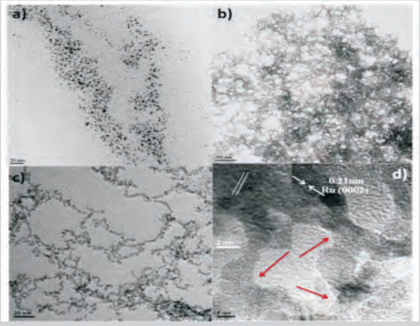

Fig. 1: The TEM image a) Ru seeds (~3nm) b) and c) low and high magnification images of Ru nanochains d) HRTEM images of the Ruthenium nanochains and grooves

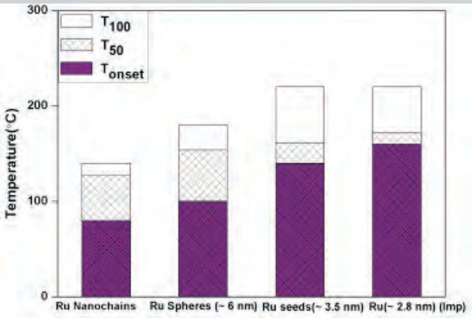

Fig 2: The CO oxidation activity profile for different Ru nanostructures supported on Ceria by sol immobilisation method

Advanced Materials

Nanostructured materials

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Eco-fabrication of extracellular metal sulfide nanoparticles from fungus *Fusarium oxysporum*: Technologically important metal sulfide nanoparticles of PbS, ZnS, MnS and NiS were biologically synthesized and complete characterization was done. The nanoparticles solution was found to be extremely stable with little evidence of aggregation even after months of storage. The long term stability of the nanoparticles was due to the proteins secreted by fungus in the nanoparticle solution which was bound to the surface of the nanoparticle and thus prevented aggregation. Moreover, all the nanoparticles were formed extracellularly (*Curr. Nanosci.* **2014**, *10*, 588).

Fungal bioleaching of fly-ash for production of extracellular silica nanoparticles: The demonstration was done for the first time to understand the ability of mesophilic fungus *Fusarium oxysporum* in the bioleaching of waste material such as Fly-ash for the extracellular production of highly crystalline and highly stable, protein capped, fluorescent and water soluble silica nanoparticles at ambient conditions. When the above fungus was exposed to Fly-ash, it selectively leached out silica nanoparticles of average 22 nm size dimensions and quasi-spherical morphology within 24 h of reaction. These silica nanoparticles were completely characterized (*PLOS ONE* **2014**, *9*, e107597).

Simple recovery of intracellular gold nanoparticles from peanut seedling roots: Intracellular formation of nanomaterials, due to the lack of a proper recovery protocol has always been dreaded. The recovery of intracellular gold nanoparticles was reported for the first time from dry and fresh roots of peanut by extracting separately with ethanol and distilled water, followed by sonication for 20 min. Water proved to be much better system as it provided well dispersed, stable gold nanoparticles and higher recovery. The recovered particles were further characterized by UV-Vis, TEM and ICP-AES (*J. Nanosci. Nanotechno.* **2015**, *15*, 1575).

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The group works extensively in the area of bottom up synthesis of nanoparticle dispersions. The recent highlights of the groups work in this area include the development of a simple and convenient method for the preparation of ultra-small palladium nanoparticles (Pd-NPs) and their utility for selective hydrogenation of terminal alkyne groups in organic molecules. The preparation of unconventional Aucore – Agshell nanoparticle dispersions was undergone using the amine molecules present on the surface of silver nanoparticles as reducing agents (*Colloid. Surface*. A **2015**, *478*, 30; *Nanoscale* **2015**, *7*, 872).

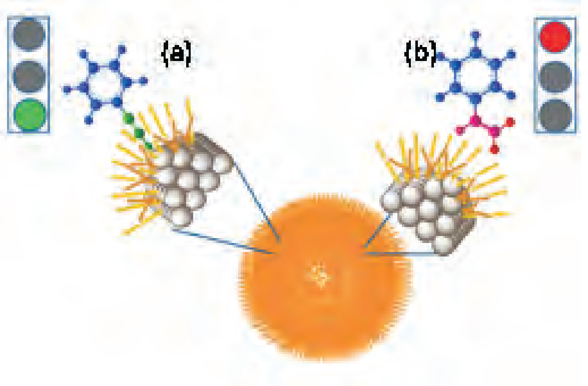

Fig. 1: (a) Favorable accessibility of nanoparticle surface to phenyl acetylene and (b) unfavorable accessibility of nanoparticle surface to styrene

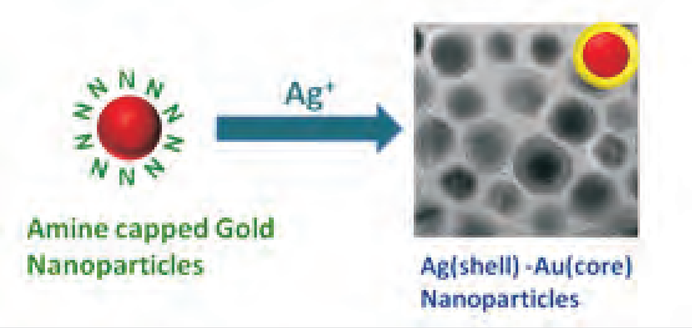

Fig. 2: Au_{core}-Ag_{shell} nanoparticle formation

Advanced Materials

Nanostructured materials

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Development of functional nanocomposite materials

The fabrication of designer functional nanostructures was reported by using large area, high throughput and simple nanofabrication techniques in order to improve their morphological homogeneity and functionality to enhance the performance of potential application. Approaches are based on improvement of functionality of existing known nanomaterials, and development of innovative composite material concepts for advanced applications (*Nanoscale* **2014**, *6*, 9148; **2015**, *7*, 11515; *Catal. Sci. Technol.* **2015**, *5*, 1251; *J. Nanopart. Res.* **2014**, *16*, 2372; *Sensor. Actuat. B-Chem.* **2014**, *191*, 837).

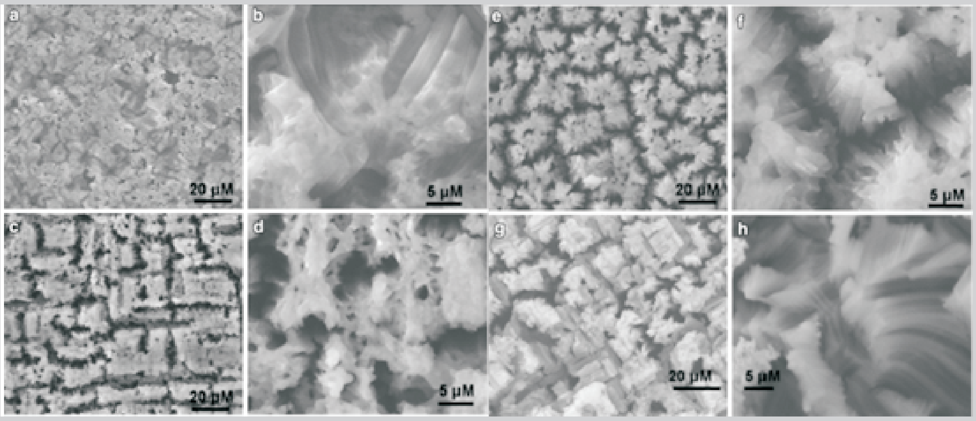

Fig. 1: SEM images of silicon nanostructures synthesized by evaporation-induced self-assembly of AuNPs

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The work was focused on the synthesis, characterization and application of copper based nanostructures. Tailoring of surface morphology of Cu based dendritic nano/ micro structures was achieved utilizing a very simple, rapid, scalable and versatile reaction strategy. Such nanostructures were extensively characterized with SEM, TEM, XRD, UV–Vis spectroscopy. These nanostructures found important applications in catalysis, chemical sensing, and for fabricating self–cleaning superhydrophobic surfaces. Successful demonstration of all of these applications was undergone using Cu dendritic nanostructures (Fig.1).

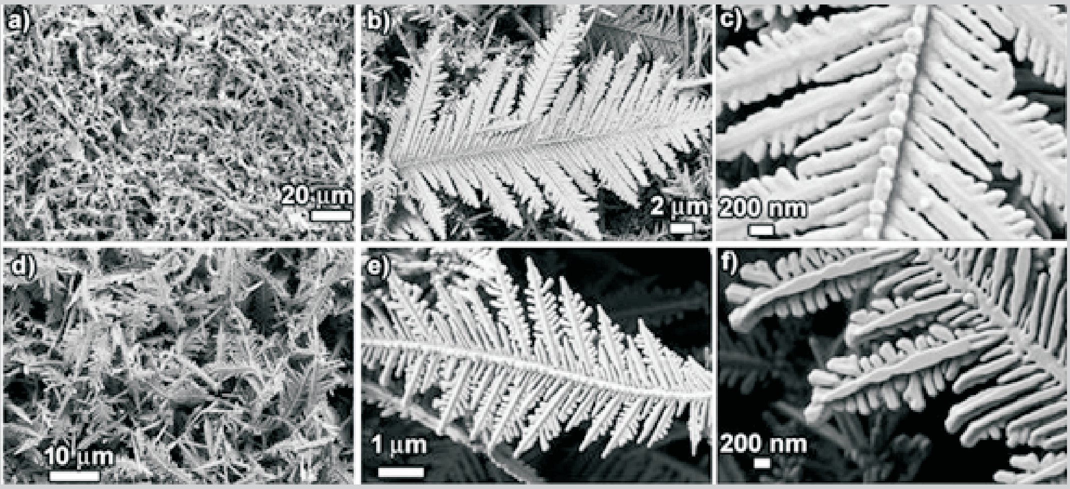

Fig. 1: Depicts surface morphology tailoring based on chosen reaction parameters during synthesis of Cu dendrites

Advanced Materials

Materials for energy

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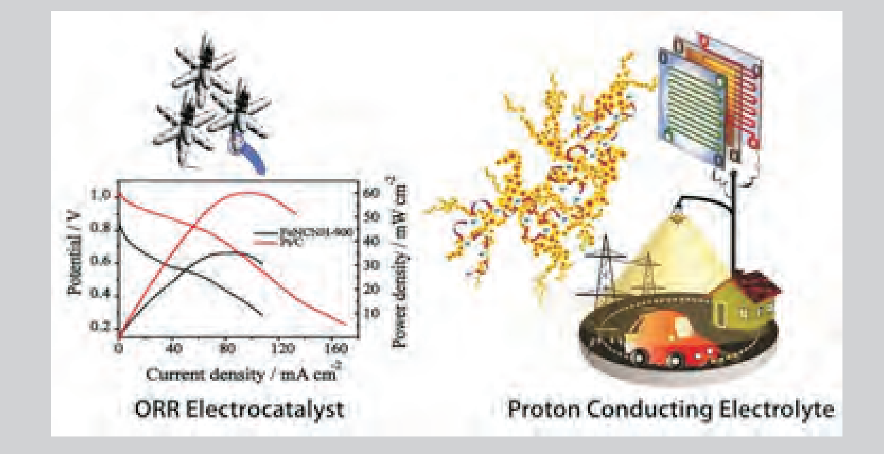
The focus was on the development of multifunctional materials towards fabrication of energy devices such as fuel cells, batteries and supercapacitors, as a plausible greener replacement for the depleting fossil fuels. A few electrodic materials for Oxygen Reduction Reaction (ORR), Hydrogen Evolution Reaction (HER) and Oxygen Evolution Reaction (OER) applications etc were developed successfully. A Fe–phytic acid based metallogel was tried for its anhydrous proton conducting ability under the fuel cell operation conditions. As prospective supercapacitor materials, hybrid systems based on conducting polymers like polyethylenedioxythiophene (PEDOT) and polyaniline (PANI) were also developed and effectively tested as active electrode materials for device fabrication. All these materials showed promising results in their respective areas.

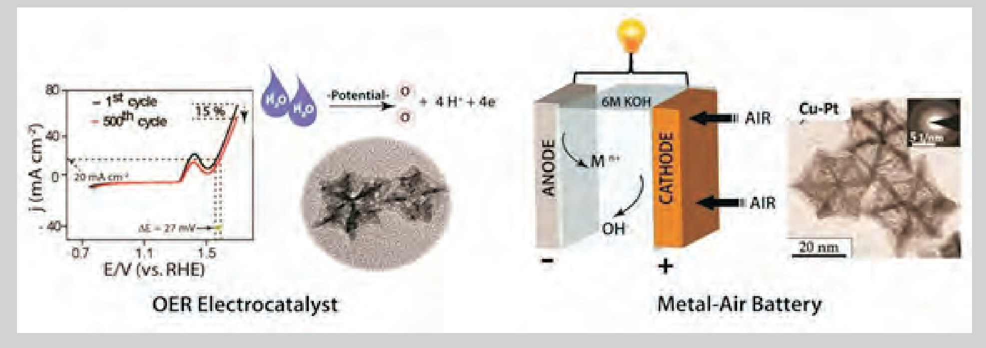
Utilization of Pt-free electrocatalysts and solid electrolytes for fuel cell operation: Pt-free electrocatalysts for oxygen reduction reaction were achieved by modulating the active reaction center density on Carbon Nanohorn (CNH) based catalyst wherein the CNH was annealed using higher loading of iron and nitrogen precursors. Thus synthesised FeGNT was ORR active in both acidic and alkaline mediums giving a maximum power density of 200 m W/cm^2 in PEFMC operating conditions. In another attempt, porous graphene was synthesized through a simple peroxide treatment. Simultaneous generation of nanoporous graphene (pGr) and photo luminescent graphene quantum dots (GQD) resulted after 72 h of oxidative treatment. The active sites of the porous graphene were further modulated through nitrogen doping onto the edges of the pores (NpGr-72). The NpGr-72 showed 60 mV overpotential compared to 20 wt% Pt/C with a maximum power density of 27 mW cm^{-2}, under anion exchange membrane fuel cell conditions.

One of the critical parameters dictating the overall efficiency of a PEMFC is the proton conducting ability of the separating membrane. An ability to conduct protons at high temperature (>100°C) in dry conditions apart from high mechanical stability forms the most vital criteria for any material to be used as a proton conducting membrane in fuel cells. In this direction, a Fe-phytic acid based metallogel was successfully tested for its anhydrous proton conducting ability under the fuel cell operation conditions. A Membrane Electrode Assembly (MEA) fabricated using the FNPA xerogel showed a maximum Open Circuit Voltage (OCV) of 1.02 V ± 0.02 at 120°C with high proton conductivity of 2.4×10^{-2} S cm^{-1}. At 0.60 V, a power density of 0.94 mW cm^{-2} was obtained, which thereby validated the proton conducting nature of the material (*Energy Environ. Sci.* **2014**, *7*, 1059; *Small* **2015**, *11*, 352; *Chem. Sci.* **2015**, *6*, 603).



Development of electrode materials for zinc-air battery: Zinc–air batteries belong to the class of powerful, inexpensive, metal-air batteries with high energy density, whose cathode demands an effective catalyst capable of reducing O_2 under alkaline conditions. With platinum being expensive, the lookout is on for a low Pt containing / Pt–free catalyst. In the group, intermetallic Cu–Pt nanocages (CuPt-NC) were synthesized and tested for the same. It showed ORR at 0.9 V *vs* RHE with 2.9- and 2.5-fold improved mass activity and specific activity, respectively in comparison to Pt/C. When used as a cathode in a primary zinc-air battery, CuPt-NC showed constant discharge stability with a specific capacity of 560 mAh gZn^{-1} and energy density of 728 Wh kgZn^{-1} at 20 mA cm^{-2}.

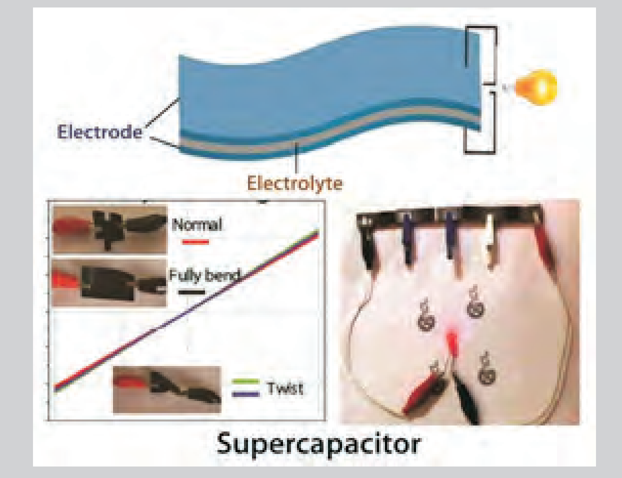
Materials for energy



OER Electrocatalyst

Metal-Air Battery

Development of supercapacitive materials with better electrode-electrolyte interface: High surface area materials are known to form a better electrode-electrolyte interface thereby improving the overall charge storage properties. High surface area polyaniline (PANI) was synthesized by in situ polymerizing aniline onto the graphene surface in presence of phytic acid. A homogeneous covering of 3D-PANI on the graphene surface was thus achieved and the resulting nano-composite G-PANI-PA showed an enhanced specific capacitance of 652 F/g with excellent durability than the unsupported PANI. The group also focused on developing solid-state supercapacitors with close matching charge storage characteristics with its liquid-state counterpart even under extreme temperature and humidity conditions. In one such attempt, highly conductive polyethylenedioxythiophene (PEDOT) paper was prepared by simple roll coating technique with conductivity and sheet resistance amounting to 375 S cm^{-1} and 3 ohm cm^{-1}, respectively. A highly flexible solid–state supercapacitor was demonstrated with very high durability (90 % retention over 2500 cycles). Additionally, an inter–digital 3.6 V flexible supercapacitor was fabricated using a single large PEDOT paper (*ACS Appl. Mater. Inter.* **2015**, *7*, 7661; *Energy Environ. Sci.* **2015**, *8*, 1339).



Supercapacitor

Singlet triplet gaps in polyacenes

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Renewable and alternate energy technologies: Singlet–triplet gaps in polyacenes are important in the process of singlet fission. These gaps were calculated with the perturbative spin flip equation of motion coupled cluster methods. A delicate balance was observed between static and dynamic correlation which are crucial to the accurate estimation of these gaps. The extrapolated gaps showed no singlet–triplet cross–over. The nature of the singlet ground state was understood which becomes more di–and poly–radical in nature as the size of the polyacene increases. The study was followed up by studies into understanding singlet fission processes that are important for solar cell technologies. Use of a method developed in the group will make it feasible to study large systems (*Phys. Chem. Chem. Phys.* **2015**, *17*, 9849).

Advanced Materials

Materials for energy

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Nanostructured electrode materials for solar energy conversion and charge storage

Carbon nanomaterials for supercapacitor: A cheaper and green approach was developed for the synthesis of CNOs and demonstrated a supercapacitor based on these CNOs which provided a higher specific capacitance than conventional graphitic/ mesoporous/ activated carbons. A composite of these CNOs was synthesized with metal oxides like MnO_2 and RuO_2 that showed high enhancement in specific capacitance of this supercapacitor with high rate capability and long cycle life. Carbon nanohorns and nanodiamond particles were also evaluated as an electrode material for supercapacitor (*J. Mater. Chem. A* **2014**, *2*, 2152; *Carbon* **2014**, *68*, 175).

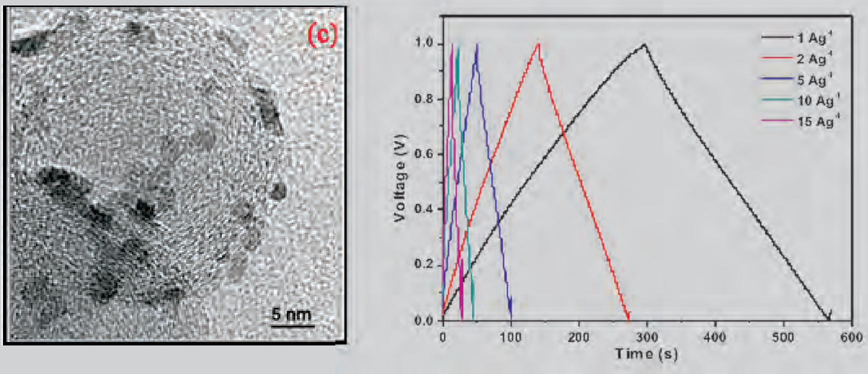

Fig. 1: Multilayer fullerene-metal oxide nanoparticlecomposite supercapacitor electrode

Nanostructured materials as photoelectrodes: Silicon nanowires as efficient photoelectrodes: Quantum dot-decorated wide band gap semiconductors, such as TiO_2, ZnO, SnO_2, etc., which have electron mobilities of less than 200 $cm^2\ V^{-1}\ S^{-1}$ were studied as the photoelectrodes for photovoltaics and photoelectrochemical water splitting. CdSe quantum dot decorated-silicon nanowires (SiNWs) and SiNW-TiO_2 core shell nanostructures were reported with sandwitch carbon layer as photoelectrodes for photoelectrochemical water splitting. Gold nanoparticle decorated SiNW-TiO_2 core-shell structures were also synthesized for enhanced photoactivity (*J. Mater. Chem. A* **2014**, *2*, 13352; *Sci. Rep-UK* **2014**, *4*, 4897; *Phys. Chem. Chem. Phys.* **2014**, *16*, 17786).

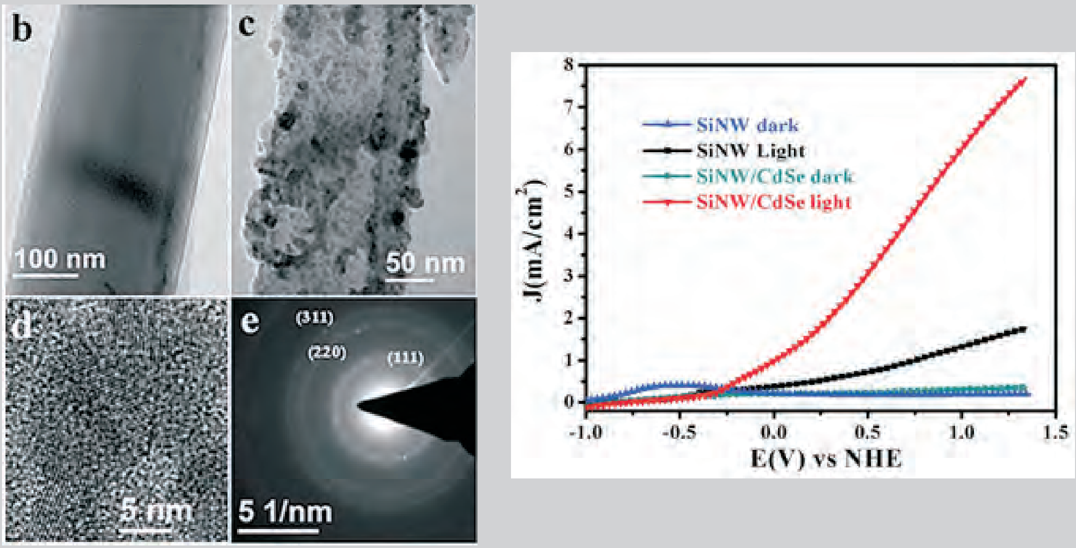

Fig. 2: HRTEM images of the SiNWs and CdSe-deposited SiNWs with SAED pattern.Current–voltage characteristics of the SiNWs (dark & light) and of the CdSe quantum dot-decorated SiNWs (dark & light)

Materials for energy

Plasmon-enhanced photocurrent generation from click-chemically modified graphene: Graphene oxide (GO) and partially reduced graphene oxide (rGO) have numerous electro-active sites due to oxygen functionalities on the basal plane and the edges. It allows non-covalent, covalent based chemistry on its surface so as to recover the electrical strength and practical utilization of graphene in the devices. Self Assembled Monolayers (SAMs) which are ultrathin molecular films can be used to modify surface and interface electronic properties of Graphene. The influence of AuNPs assembled on different SAMs on the rGO surface and subsequent plasmonic enhancement in the photocurrent generated from chemically modified rGO/AuNPs hybrid was explored (*Chem.–Eur. J.* **2014**, *20*, 7402).

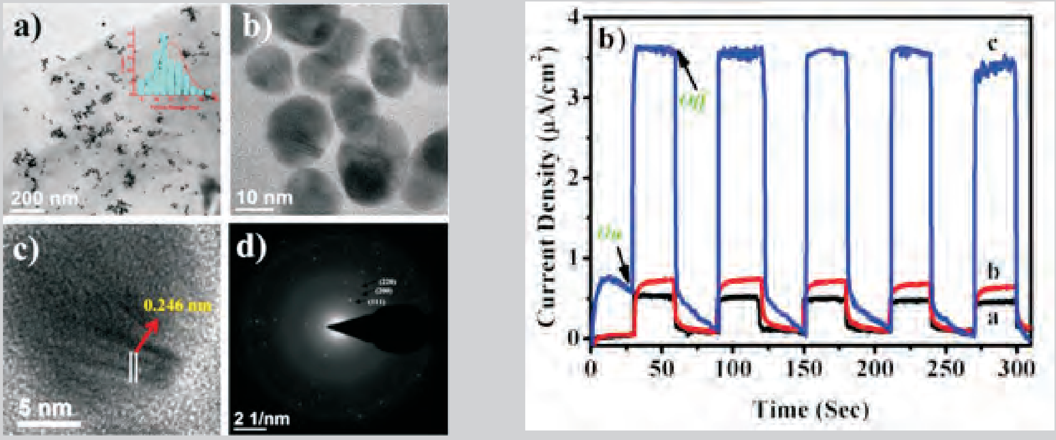

Fig. 3: TEM images and photocurrent responses of a) FTO/rGO, b) FTO/rGO (APTMS)/Au and c) FTO/rGO (Click)/Au electrodes

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The research interests included harnessing both coordinative interactions as well as various non-bonding interactions for realizing desired functions of a molecule or molecular assembly.

Molecular recognition and imaging reagent for intra-cellular application: A new phenanthroimidazole-rhodamine conjugate constituted a unique example of the role of a secondary bond to achieve a distinct TBET process induced by the Hg(II)-η^2-arene π-interaction in pure aqueous medium with a large pseudo-Stokes shift of 200 nm. This molecule was used as an imaging reagent for detection of the cellular uptake of Hg^{2+} as low as 0.2 ppb in Hct 116 colon cancer cells (*Chem. Commun.* **2015**, *51*, 3649).

Molecular aggregates with predictive optical responses: A purpose-built gelator molecule showed an ESIPT coupled AIEE process for generating multiple luminescent color, including white colour with varying aggregation as a function of the water content in THF-water mixture. *J*-aggregated state of this molecule formed a luminescent gel in THF and this luminescent property was retained even in solid state (*Chem. Commun.* **2015**, *51*, 2130).

Designing sensitizer molecule for DSSC application: Low-cost and adaptability are two important factors that have made DSSC a popular for developing a promising photovoltaic cell for conversion of sunlight to electricity. Developing a better insight in interfacial electron transfer dynamics was crucial for achieving an efficient system. Ultrafast charge-transfer dynamics for CdSe quantum dots (QD) with new Re(I) derivatives as sensitizer were studied to unveil the crucial role of charge recombination process. Role of the anchoring functionality of the sensitizer dye to the QD surface was also described (*J. Phys. Chem. C* **2015**, *119*, DOI: 10.1021/jp5122068).

Sensors for important biomarkers: A new cell membrane permeable reagent with insignificant toxicity towards Hct 116 cancer cells was utilized as an imaging reagent for detection of endogenous Cys as well for quantitative estimation of Hcy and GSH in human blood plasma sample (*Chem. Commun*. **2014**, *50*, 9899; Patent(s): 1697/DEL/2014; PCT/IN2015/000250).

Advanced Materials

Materials for energy

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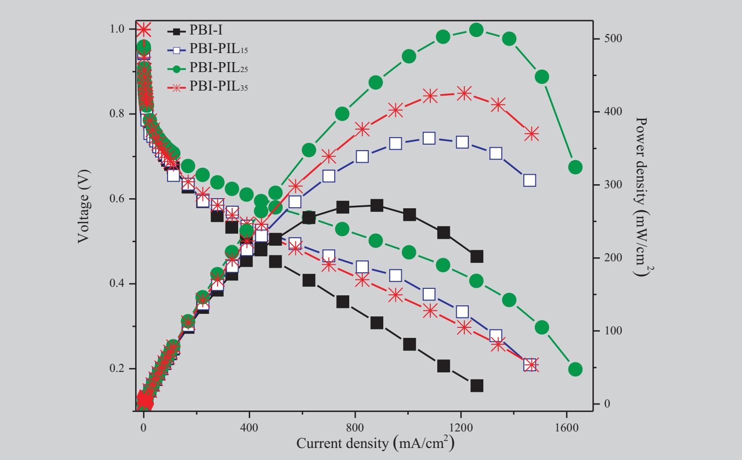
Polymeric ionic liquid- Polybenzimidazole blends for PEMFCs: Nafion, well established as the membrane material for PEMFC, has major drawbacks such as the need for water for proton transport, limiting operational temperature to <80^{o}C (resulting in lower electro–kinetics and poor CO tolerance of 10 ppm), poor mechanical property under water absorbed conditions and fuel crossover impose limitations on its wide practical applicability. The draw backs of Nafion membranes were addressed by operating PEMFC at 160^{o}C using PBI membranes. Although these membranes are capable of operating at high temperature, its performance is lower than the Nafion membrane. The blended membranes of polymeric ionic liquid (PIL) and PBI as a membrane material for HT–PEMFC were developed for the first time to mitigate this issue. The membranes have almost doubled the performance than that of pristine PBI–based membrane (*J. Mater. Chem. A* **2014**, *2*, 14449; Patent: 0552/DEL/2014).



Performance of PBI-PIL blend membranes

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Squaraine based dyes for dye sensitized solar cells: In dye sensitized solar cell(DSSC), dyes with Donor-π-Acceptor configuration plays an important role in harvesting the solar energy from visible to NIR regions. Apart from the design p-spacer for the extended light absorption, suitably introducing alkyl groups either in the donor or conjugated spacer units avoid the dye aggregation, and unwanted charge recombination processes. Recently most of the dyes synthesized by invoking out-of-plane branching units in the p-conjugated spacer showed better efficiency in compared to the dyes containing in-plane alkyl groups. Squaraine (SQ), a NIR active dye that possessed Donor-Acceptor-Donor configuration provided an opportunity to introduce the branched alkyl chains in the donor unit. As the SQ dyes aggregated in solution and solid state, controlling the aggregation was realized by suitably functionalizing the dyes with out-of plane branching unit. An efficiency of 7.93 % was achieved with I^-/I_3^- electrolyte and this efficiency was highest reported so far for this family of dyes. A Series of squaraine dyes were synthesized to study the importance of out–of–plane alkyl groups in the squaraine dyes in different positions.

Orthogonally functionalized dyes for DSSC: Most of the organic dyes explored in metal free organic dyes based DSSC were planar; aggregation of dyes on the semiconducting TiO_2 surface is a common problem that hampers the efficiency of the devices. In order to avoid such aggregation properties, either introducing alkyl groups to the dyes, or optically transparent additives with anchoring groups are utilized. It was envisaged that introducing a spiro spacer, that possess the orthogonally functionalized planes which help in avoiding aggregation of dyes on the TiO_2 surface. In this design, a dye had two anchoring groups that facilitated the stronger binding with TiO_2. Both symmetrical and unsymmetrical orthogonally functionalized dyes were synthesized by utilizing Pd calalyzed C-H activation following with condensation reactions. The unsymmetrical dye was synthesized by selecting two different dyes that covered from 400-700 nm (towards panchromatic light absorption) of the solar spectrum.

Advanced Materials

Functional materials

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The objective was to synthesize atomically thin nanosheets of various inorganic layered materials including graphene. Various chemical and dry process routes for applications were used including field effect transistor, photodetector, gas sensor, supercapacitor, and catalyst for hydrogen generation and field emission based electron source for vacuum nanoelectronics device application.

Atomically thin nanomaterials for novel device systems: Various 2D inorganic nanomaterials were synthesized using chemical methods such as hydrothermal, chemical vapor deposition, wet chemical, microwave, electrochemical etc. and dry process routes such as micromechanical exfoliation, pulsed laser deposition, sputter etc. followed by their characterization using various techniques.

2D Material based Nanoelectronic devices: The 2D nanosheets were utilized for various applications including photodetector, gas sensor, supercapacitor, catalyst for hydrogen generation and field effect transistor which shows the good performance at room temperature. Especially the layered SnS_2 nanosheet showed the photosensitive field emission behavior under visible light. The F-N plot, in the dark, is nonlinear in nature representing the semiconducting behavior. It became more linear in nature under illumination. This property was exhibited in the presence of various color filters during illumination. The emission current enhancement is only due to the photoconductivity and has no contribution by thermionic emission. The enhanced field emission current along with the photoswitching property was explained on the basis of the band structure. The study makes SnS_2 nanosheets a promising cold cathode material, finding applications in field emission based optoelectronic devices (*Appl. Phys. Lett.* **2015**, *106*, 23111; *Nanoscale* **2015**, *7*, 13293; *RSC Adv.* **2015**, *5*, 5372, 21700, *6*, 41887; *CrystEngComm* **2015**, *17*, 3936; *Eur. J. Inorg. Chem.* **2015**, *9*, 1598; *11*, 1973; *ACS Appl. Mater. Inter.* **2015**, *7*, 5857; *Nanomater. Nanotechno.* **2015**, *5*, 1; *J. Vac. Sci. Technol. B*, *33*, 03C106).

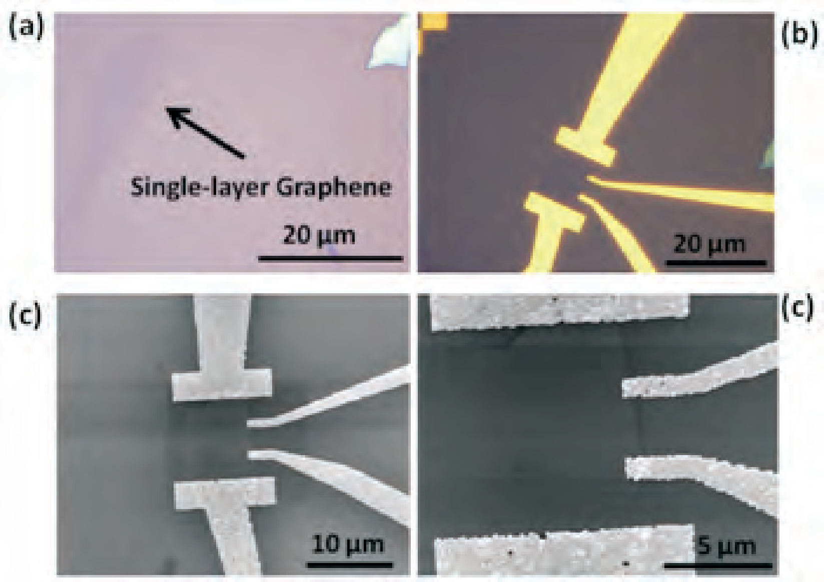

Fig 1: Typical optical images of single-layer graphene sheet (a) before patterning the electrode and (b) after patterning the electrode. Typical SEM images of the single-layer graphene field-effect transistor (c, d)

The charge-transfer doping caused by an interaction with strong electron acceptor molecules affected the transfer curve of the field-effect transistor device of a single-layer graphene, which makes graphene to a more *p*-type. The shift in the Dirac points towards positive gate voltage as a function of increasing concentration indicated the magnitude of doping increases with increasing in concentration. The performance of our single-layer graphene transistors was improved by reducing the defects and damage creation during preparation and transfer processes to meet the requirements of various device applications including thin film solar cells, flexible touch screen panels and nano-electronic papers (*Adv. Device Mater*. **2015**, *1*, 52).

Advanced Materials

Functional materials

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The chemistry of exfoliation mechanism of bulk powder into nanosheets by rapid freezing of hydrated powder in water and rapid heating of the powder resulted in separating out the nanosheets of various inorganic layered materials.

The synthesis of transition metal dichalcogenide nanosheets were carried out using rapid quenching method. The thirty cycles of rapid freezing (30s in liquid nitrogen bath) and heating (20 min in oil bath at 60ºC) were carried out. The post reaction product gave yield > 60 wt%. It indicated that this method can be utilized for large production of 2D nanosheets. As synthesized products were then characterized using TEM which depicts the nanosheet like morphology. Raman spectroscopy data confirmed the high quality of the nanosheet sample. The exfoliated samples showed good electrochemical performance. Among all TMDC samples, WSe_2 nanosheet sample showed better performance due to the uniform morphology, large surface area and less defects (*Eur. J. Inorg. Chem.* **2015**, *11*, 1973, 19, 3102; *J. Phys.-Condens. Mat.* **2015**, *27*, 285401; *J. Nanomed. Res.* **2015**, *2*, 15; *JSM Nanotechnol. Nanomed.* **2015**, *3*, 1033).

Self-assembled functional organic soft materials for advanced applications

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Self-assembly of functional π-conjugated systems is one of the advanced topics of research. Drastic developments are witnessed in the last decade to convert information at the molecular level to the nano-macroscopic levels. The research interest included room temperature solvent-free π-liquids that expected to deliver wonders in printable electronics.

Seeded on-surface supramolecular growth for large area conductive donor-acceptor assembly: The charge transport features of organic semiconductor assemblies are of paramount importance still large area extended supramolecular structures of donor-acceptor combinations are hardly accessible. Seeded on-surface supramolecular growth of tetrathiafulvalene and tetracyano-p-quinodimethane using active termini of solution formed sheaves were introduced to form large area conductive donor-acceptor assembly. The on-surface assembly via both internally formed and externally added sheaf-like seeds open new ways in supramolecular chemistry and device applications (*Chem. Commun.* **2015**, *51*, 10439).

Paradigms shift when solvent-less fluids come into play: Solvent-less organic fluids are a new class of functional soft materials. The available fluid matrix makes it equally competitive with the solvent assisted systems. The ways in which organic fluids challenge the established and accepted paradigms was highlighted here. Solvent-less fluids challenge the paradigms by realizing it in the neat, solvent-less and ambient condition. A few representative examples were discussed to point out the challenges

Hydrogel derived soft materials for biomimetic and energy related functions: Supramolecular assembly of molecules leading to gelation of large amount of solvents is always a fascinating topic of research. Hydrogels were exploited to generate soft materials with mechanical anisotropy, tunable rigidity, self-healing etc. and with photocatalytic H_2 production.

Advanced Materials

Functional materials

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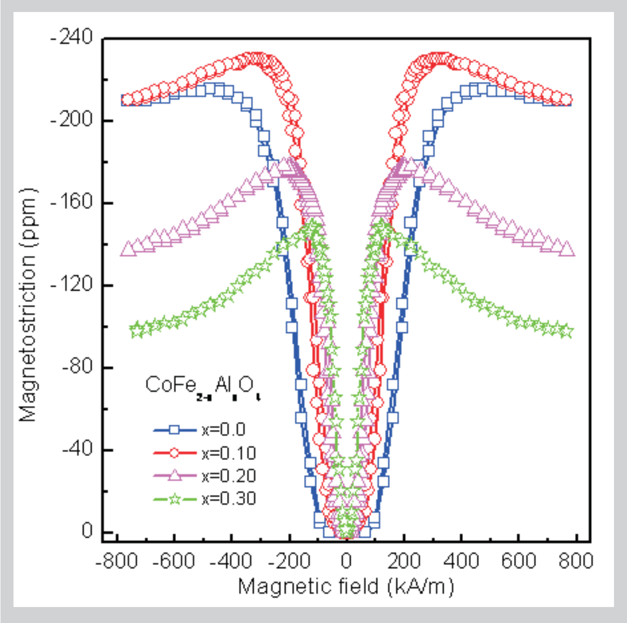
Ceramic magnetostrictive materials with high strain sensitivity: Magnetostrictive smart materials are very important class of materials due to its wide applications. Cubic spinel type cobalt ferrite ($CoFe_2$O4) is known to exhibit large magnetostriction at room temperature but with very low strain sensitivity. Aluminium substituted cobalt ferrite compositions derived from nanosized powders synthesized by a citrate-gel method showed larger magnetostriction and higher strain sensitivity at low magnetic fields compared to that for the unsubstituted cobalt ferrite. A very high strain sensitivity of 4.5 x 10^{-9} m/A was obtained for a magnetically annealed sample which is larger than that reported for any substituted cobalt ferrite samples. The combination of high magnetostriction coefficient and strain sensitivity is suitable for device applications (*J. Mater. Sci.* **2015**, *50*, 6510).



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Bioactive polymersomes self-assembled from amphiphilic PPO-GlycoPolypeptides: Synthesis, characterization, and dual–dye encapsulation: Glycopoly–peptide–based polymersomes have promising applications as vehicles for targeted drug delivery because they are capable of encapsulating different pharmaceuticals of diverse polarity as well as interacting with specific cell surfaces due to their hollow structural morphology and bioactive surfaces. The glycopolypeptide-b-poly(propylene oxide) was synthesized and characterized. The formation of glycopolypeptide-based polymer-somes was demonstrated from the self-assembly of glycopolypeptide-b-poly (propylene oxide) in which the presence of an ordered helical glycopolypeptide segment was required for their self-assembly into spherical nano-scale (~50 nm) polymersomes (*Langmuir* **2015**, *31*, 3402).

Advanced Materials

Functional materials

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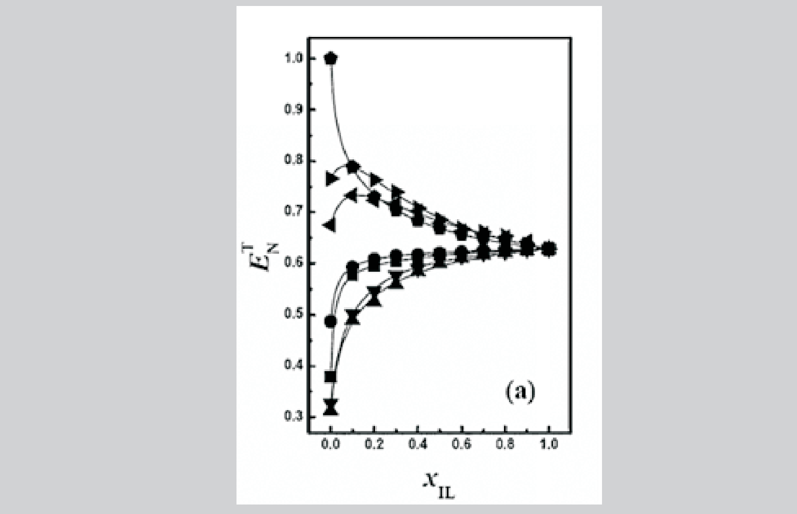
Physical chemistry of organic reactions in unusual media

The objective was to investigate the structure–property relationship in ionic liquid systems involving micro–emulsions. The qualitative and quantitative study of the interfacial reactions was done. Physical chemistry of organic reactions in supersaturated solvent solvents was reported. The hydrophobicity and enthalpies in non–reactive and biologically active molecules, liquid–liquid equilibrium and reaction mechanism was also investigated.

Synergistic effects and correlating polarity parameters in binary mixtures of ionic liquids: Ionic liquid binary mixtures were studied to understand the effects of hydrogen–bond acceptor basicity (β) of solvents on the "synergistic effects" found in ionic liquid–alcohol mixtures, the interrelation between the polarity parameters in binary mixtures and the application of a model for the description of normalised electronic transition energy for all the binary mixtures. A detailed analysis of polarity parameters in both hydrophilic and hydrophobic ionic liquids was carried out. A three–parameter model developed by Roses et al. was found applicable to all the binary mixtures. The synergistic effects were generated as a result of high β values of alcohols compared with those of the ionic liquids. A strong correlation was observed in the β values and hydrophobicities of pure ionic liquids, suggesting that β values can play a role in describing synergism (*ChemPhysChem* **2015**, *16*, 1026).



Aqueous hydrophobic ionic liquid confined media: Insights into microviscosity and microporsity: Investigations of physicochemical properties of water confined in dibutylimidazolium bis(trifluoromethanesulfonylimide) ($[C_4C_4im][NTf_2]$) reverse micelles through the NMR relaxation measurements provided an understanding of microviscosity and pH in the confined condition. Experimental results on phase behavior, diffusion, structural characteristics and pH in aqueous ionic liquid-confined media were represented. Microviscosity of the aqueous confined media was calculated from the measured T_1 relaxation time values by applying the Debye–Stokes equation and correlated with the bulk viscosity of the samples. It was observed that both the microviscosity and bulk viscosity showed inverse relationship. The fraction of bound and free water molecules were calculated from the measured T_1 values. NMR spin–spin relaxation time (T_2) of water molecules in its homogeneous microemulsion systems were measured with the varying pH of the aqueous core. A change in the T_2 relaxation time of the water proton was observed proposing an exchange of proton between the H_2O and –OH group of the TX-100 molecules. Finally, methyl orange (MO) was used as UV–vis spectrophotometric molecular probe and the measured $_{max}$ values of the probe were used for the detection of micropolarity of the homogeneous aqueous confined media and was found to be increase with the increase in the size of the confined media (*J. Phys. Chem. B* **2015**, *119*, 1641).

The organic reactions in ionic-liquids and at interfacial media: A quantitative study of the kinetics and mechanism of the Baylis–Hillman reaction in the presence of ionic liquids as solvent media was reported. A simple Baylis–Hillman reaction was occurred by two different exclusive mechanisms in ionic liquids. The delicate balance of these mechanisms was maintained by the ionic environment employed. The main features of the possible mechanism are described here along with interesting kinetic consequences. The measurement of rate constants and activation energy parameters demonstrated that as the medium becomes basic, the order of the reaction changes from 1 to 2. An unexpected change in the mechanism of the reaction was observed with a change in the nature of the ionic liquid. The Linear solvation energy relationship was used as an investigating tool to delineate the respective contributions of the cation and anion of the ionic liquid. The observation strongly dictated the dependency of the mechanism of the Baylis–Hillman reaction on the nature of the anion of the ionic liquids undertaken for this study.

The investigation of 1,3-dipolar cycloaddition reaction under heterogeneous conditions was carried out in another study in order to inspect the hydrophobic contribution towards rate enhancement at the interface on addition of prohydrophobic salts. The influence of different substituents on the reactivity of 1,3-dipole was explored. Kinetic studies divulged a conspicuous role of prohydrophobic salts under these conditions. No rate enhancement was observed at higher salt concentration. Role of “active'' interfacial area was found to be crucial for the desired enhancement in heterogeneous reaction conditions, which has implications in determining the optimum salt concentration and conditions required for such reactions (*RSC Adv.* **2015**, *5*, 2994).

Physical chemistry of organic reactions in supersaturated solvent solvents: New super-saturated solvent which acts as a potential solvent to promote organic reactions like Diels-Alder reactions was introduced in this work. Systematic kinetic and thermodynamic studies of the Diels–Alder reactions in new super-saturated solvent established the potential of such solvent as a new reaction media. New super-saturated solvent was a medium of interest due to the presence of excess of carbohydrates and their –OH groups which increase the possiblity of formation of hydrogen bonding during course of the reaction. The physico-organic investigations revealed the potential of new super-saturated solvent as an efficient environment–benign reaction medium as compared to other solvents (*J. Phys. Org. Chem*. **2015**, *28*, 665).

Elucidation of ionic interactions in the protic ionic liquid solutions by isothermal titration calorimeters: Thermal behaviour in terms of excess partial molar enthalpies, H^E_{IL} of aprotic ionic liquids in the presence of low relative permittivity solvent i.e. chloroform was investigated. The H^E_{IL} values as measured by isothermal titration calorimeter (ITC) at 298.15K were used as a diagnostic tool to investigate the interactions in these solutions. The study suggested the presence of ion-pairs of the ionic liquids in the ionic liquid-chloroform solutions and the interactions prevailing between these ion-pairs and the chloroform molecules. The interactions were expressed in terms of virial coefficients and their dependence on the cationic substitution of alkyl chains and nature of both cations and anions were discussed. The relative apparent molar enthalpies, ϕ_L of the solutions were analysed using a modified Pitzer equation.

Dissociation of equimolar mixtures of aqueous carboxylic acids in ionic liquids: Role of specific interactions: The Hammett acidity (H_0) of equimolar mixtures of aqueous formic acid, acetic acid and propionic acid was measured in 1-methylimidazolium-, 1-methylpyrrolidinium-, and 1-methylpiperidinium-based protic ionic liquids (PILs) and 1-butyl-3-methylimidazolium-based aprotic ionic liquid (AIL) with formate ($HCOO^-$) anion. Higher H_0 values were observed for the equimolar mixtures of aqueous carboxylic acids in protic ionic liquids compared with those of the aprotic ionic liquid because of the involvement of the stronger specific interactions between the conjugate acid of ionic liquid and conjugate base of carboxylic acids as suggested by the hard–soft acid base (HSAB) theory. The different H_0 values for the equimolar mixtures of aqueous carboxylic acids in protic and aprotic ionic liquids were noted to depend on the activation energy of proton transfer ($E_{a,H+}$). The higher activation energy of proton transfer was obtained in AIL, indicating lower ability to form specific interactions with solute than that of PILs. Thermodynamic parameters determined by the “indicator overlapping method” further confirmed the involvement of the secondary interactions in the dissociation of carboxylic acids. On the basis of the thermodynamic parameter values, the potential of different ionic liquids in the dissociation of carboxylic acids was observed to depend on the hydrogen bond donor acidity (α) and hydrogen bond acceptor basicity (β), characteristics of specific interactions (*J. Phys. Chem. B* **2015**, *119*, 5537).

Advanced Materials

Functional materials

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Terahertz spectra in molecules and organic molecular crystals

The main focus of the group was to understand relation between structure and properties of materials by employing ab initio DFT based techniques. The ultimate goal was to predict and design materials with desired properties.

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

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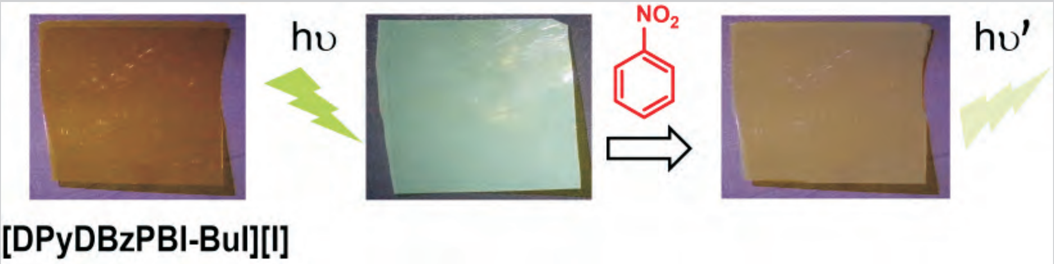
Fluorescent polymeric ionic liquid films for nitroaromatic explosives detection: Detection of nitroaromatics (NACs) is considered as one of the vital factors of security in modern society and is widely needed at locations, such as airports, ports and borders to combatterrorism. Research was done to develop an applicability of film forming polymeric ionic liquids (PILs) which possess pyrene and anthracenefluorophores for the detection of NACs. The functionalized PILs were synthesized via post modification of thermo–chemically and mechanically stable polybenzimidazole. The formed PILs showed ability to detect NACs through quenching of fluorescence intensity (*J.Mater. Chem. A* **2014**, *2*, 13983; Patent: 0552/DEL/2014).



Fluorescentpolymeric ionic liquids (PILs) films for NACs detection

Advanced Materials

Polymers

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Dynamics and thermodynamics of model molecular glass formers with different interaction potential

Two model liquids with different interaction potentials were studied. It exhibited similar structure but significantly different dynamics at low temperatures. The differences in the dynamics of these systems were understood in terms of their thermodynamic differences by evaluating the configurational entropy.

The contribution from two body and higher order correlations to the total configuration entropy was separated out for the first time. It enabled the access to its individual contributions to the dynamics. The calculations showed that the general notion was correct. The analysis of the individual contributions led to counter intuitive observations. The common belief was that if thermodynamics drives the dynamics then it should be the higher order correlations which will lead to the difference. However, it was found that although the structures appeared very similar to the difference in the dynamics which was driven by the pair correlation entropy obtained from the structure. A small structural change played a significant role in changing the dynamics. The higher order correlations which usually expected to slow down the dynamics actually facilitated it. The temperature, at which the pair configurational entropy vanished, was found to be similar to a temperature where mode coupling theory (MCT) predicted a divergence of the relaxation time. MCT is a mean field theory which ideally has no connection to entropy. So the coincidence of the two temperatures is completely unexpected and it was crucial to evaluate the real connection between MCT and theory (*Phys. Rev. Lett.* **2014**, *113*, 225701).

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Structure, dynamics and flow behavior of charged microgels with uniform polymer density profile: Ionic microgels of Poly (N-isopropyl acrylamide– acrylic acid) were synthesized successfully using a new and controlled synthesis procedure. It produced microgels with uniform polymer density profile rather than the generally reported core shell structure. The aim of this work was to test and verify the hypothesis on the double yielding flow behavior of neutral microgels of P (N-isopropyl acrylamide) observed in the previous investigation. The microgel particles prepared with this new procedure were highly monodispersed and formed colloidal crystals at moderate to high concentrations and glasses at very high concentrations (Fig. 1). The glass transition behavior of these microgel suspensions was studied as a function of concentration and temperature at a constant pH.

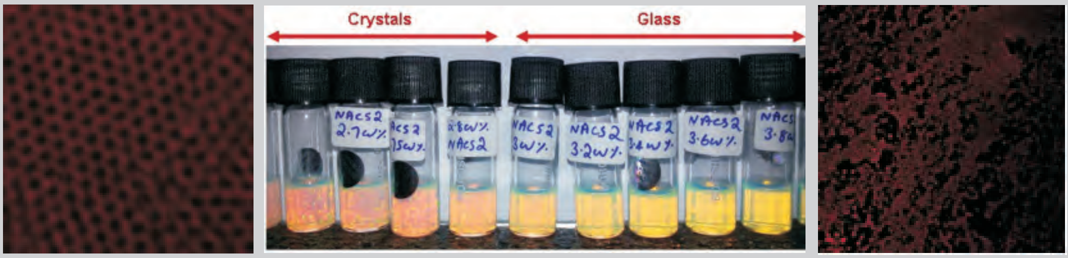

Fig 1: Visual and confocal microscopy images of ionic microgels

The particles that go from soft to hard in nature were prepared by varying the crosslinker content during the synthesis procedure. 3D-dynamic light scattering, confocal microscopy and rheology techniques were used to study the crystalline and glassy transitions in this material. The preliminary investigations were in support of the earlier observation that the double yielding in these materials was due to the core shell nature of the microgels prepared with conventional synthesis procedures. The glass and crystalline transitions were very much different from the neutral systems due to the ionic nature as well as due to the uniform polymer density profile. The double yielding nature was also seen to change with these parameters. These particles were used as models for soft dipolar liquids to investigate its concentration and temperature dependent structures, dynamics and phase diagrams under external alternating electric fields with uni-, bi-and tri-axial polarization.

Advanced Materials

Polymers

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Applications of NMR spectroscopy

The research was aimed to address various structural problems in the area of chemical science and material science for structure–property correlation applying methodologies based on solid state and solution state NMR spectroscopy.

Materials Chemistry: Information obtained from detailed NMR investigations on novel thermo–associating polymers such as PEPO (poly(ethylene oxide–co–propylene oxide) grafted carboxymethyl guar(CMG), carboxymethyl tamarind (CMT), poly *N*–isopropylacrylamide–*g*–NN dimethylacrylamide, poly *NN* dimethylacrylamide–*g*–*N*–isopropylacrylamide etc. provided the molecular level insight to its properties. ^{13}C CP-MAS NMR was employed to study transformation of cellulose to oxidized cellulose and the 6 carboxycellulose formed during the oxidation (*Carbohyd. Polym*. **2014**, *113*, 615; **2015**, *117*, 331; *Polymer* **2015**, *60*, 164).

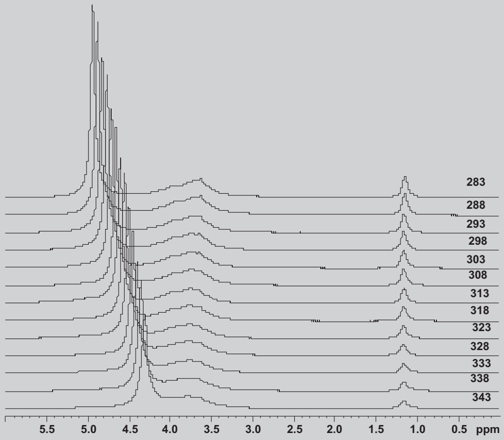

Fig. 1: Stack plots of ^{1}H proton spectra of CMG-g-PEPO in D$_2$O at temperatures 10–75°C

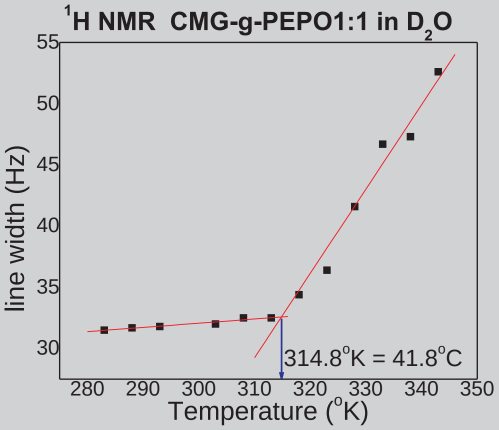

Fig. 2: Plot of proton line width of CH$_3$ peak at different temperatures

Engineering of organic molecules for terahertz tagging applications

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Tetrahertz spectroscopy was used to study a variety of physical phenomena ranging from atomic transitions to dynamics of biological molecules and hence involved a wide range of disciplines including physics, chemistry, engineering, astronomy, biology, and medicine. The present invention relates to heterocyclic and aromatic compounds containing amide and urea groups and binary molecular complexes based thereon with varying molecular mass and hydrogen bond strengths demonstrating several resonances below 10 THz which are customizable for various applications (Patent: WO 2015104722 A1 20150716).

Advanced Materials

Composite materials

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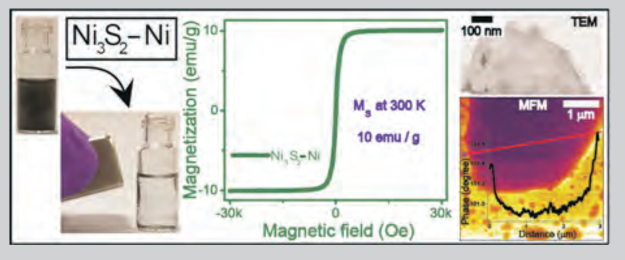
The group recently demonstrated that metal thiolates that exist as lamellar assemblies in the neat state, were disassembled into individual molecular sheets simply by dilution in apolar organic solvents. It formed ultrathin metallic/metal sulfide composite layers on substrates upon heat treatment. An easy and convenient preparation of nanometer-thick sheets of Ni_3S_2 and Ni_3S_2–Ni from solution processed molecularly thin sheets of Ni-thiolates was reported. It was observed that both the Ni_3S_2 and Ni_3S_2–Ni possessed the sheet-like morphologies and displayed room temperature ferromagnetic characteristics (*Cryst. Growth. Des.* **2015**, *15*, 2584).



Biomaterials

Tautomerization in cytosine

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The tautomerization barrier in cytosine and the effect of ionization and solvation on it was studied. Since tautomerization of cytosine in DNA is related to DNA damage, the evaluation of the effect of ionization and solvation on DNA damage was tried. It was noticed that the tautomerization barriers were significantly reduced by ionization and solvation. Understanding the processes in DNA was crucial to understand the DNA damage as well as DNA photoprotection (*J. Phys. Chem. A* **2014**, *118*, 5323).

Functionalized magnetic nanoparticles for hydrophobic drug delivery

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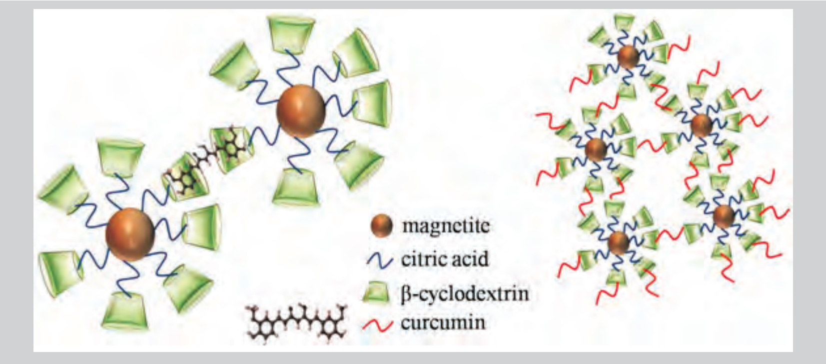
Targeting and release of hydrophobic drugs is an area of intense research using nanomaterials with an emphasis on their multi-functionality. Nanoparticles with super paramagnetic iron oxide (magnetite) core and drug coating were simultaneously used for imaging, targeting and drug delivery. Water-dispersible magnetite nanoparticles functionalized with citric acid modified β-cyclodextrin were prepared. The hydrophobic anti-cancer drug curcumin was loaded inside the cavity of cyclodextrin. The water-dispersible, citrate modified β-cyclodextrin functionalized magnetite nanofluid was found to be an efficient carrier for water insoluble curcumin. It was used for magnetic drug targeting or drug delivery as well as for contrast enhancement in MRI due to the super paramagnetic magnetite core (*RSC Adv.* **2015**, *5*, 22117).



Advanced Materials

Materials for environmental and healthcare applications

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Novel polyfluorene based conjugated polymers for bio-sensing and chiral separation: A water soluble polyfluorene was successfully developed by appending D-glucuronic acid at the 9, 9' position. D-glucuronic acid is a water soluble carbohydrate that performs the key function of removal of several insoluble toxic substances like bilirubin through glucuronidation and subsequent urinal excretion as glucuronides in the human metabolism. The appendage of D-glucuronic acid made the polyfluorene water soluble enabling the sensing of bilirubin in human blood serum in the clinically relevant levels (< 25 mol/L to > 50mol/L) with high selectivity (*Macromolecules* **2015**, *48*, 3449; Patent: WO 2015/015517 A1).

Appendage of the chiral L-Glutamic acid at the 9, 9' position of fluorene resulted in chiral polyfluorene that enabled efficient heterogeneious enatioselective separation and chiral sensing of a wide variety of substrates from their aqueous racemic mixture in an easy 'filter-and-separate' method. The helical fibrous polymer with pores on the walls selectively adsorbed L isomers within its pores from their racemic mixture leaving the D enantiomer in the water. The highest enantiomeric excess of 95 % was observed for 2-amino-1-propanol and more than 86 % for phenylalanine (*Chem. Commun*. **2015**, *51*, 8931).

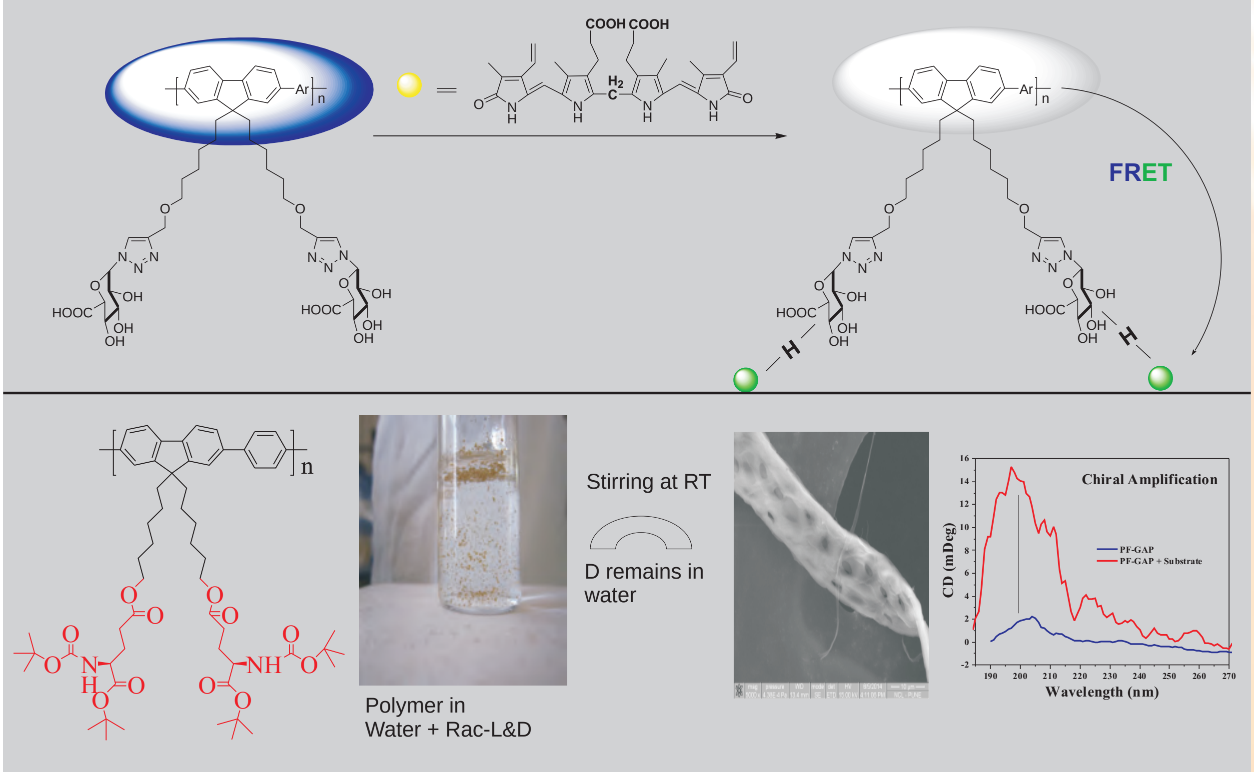

Fig. 1: FRET based sensing of bilirubin in human blood serum (Top); Heterogeneious enatioselective separation and chiral sensing (Bottom)

Advanced Materials

Materials for environmental and healthcare applications

New materials from biomolecules

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The objective was to design the materials using various biomolecules for value added applications. The idea of using functional bio-molecules was to minimize harmful petroleum derived products and to balance the ecosystem from deterioration.

Egg albumen as gel electrolyte: Egg albumen is highly functional protein with remarkable gelling /crosslinking ability. It was functionally modified to enhance the conductivity and was applied in the form of a gel electrolyte in dye sensitized solar cell (DSSC) architecture to enhance its durability. A hybrid gel comprising of poly(acrylic acid), PAA, polyaniline, PANI and modified egg albumen (FEA) was synthesized. The cell efficiency, stability and durability of the corresponding DSSC device were studied. Egg albumen was chemically modified with ethylenediaminetetraacetic dianhydride which showed an improved crosslinking, micro structural and conductivity properties of the gel. DSSC with the egg albumen-based electrolyte demonstrated a conversion energy efficiency of 4.6% and modified egg albumen (FEA) yielded remarkable 5.75% conversion efficiency. Fig. 1A shows preparation of modified egg albumen based gel electrolyte, its surface morphology and IV plot of the gel electrolyte (*ACS Sustain. Chem. Eng.* **2014,** *2*, 2707).

Antibacterial curcumin oligomers as nanofibers: The monomers of curcumin acrylate were synthesized by reacting curcumin and acryloyl chloride in order to exploit the properties of curcumin. The curcumin monomers were polymerized by free radical polymerization to attain oligomers of curcumin acrylates. The oligomers were fabricated into non-woven nanofibers by blending them with poly (l-lactide). The oligomers showed antibacterial properties (27mg/mL). The material showed potential applications in textile industry and health care products as well. Fig. 1B shows synthesis of oligomers of curcumin, fabrication of nanofibers and antibacterial property (*New J. Chem.* **2015**, *39*, 4464).

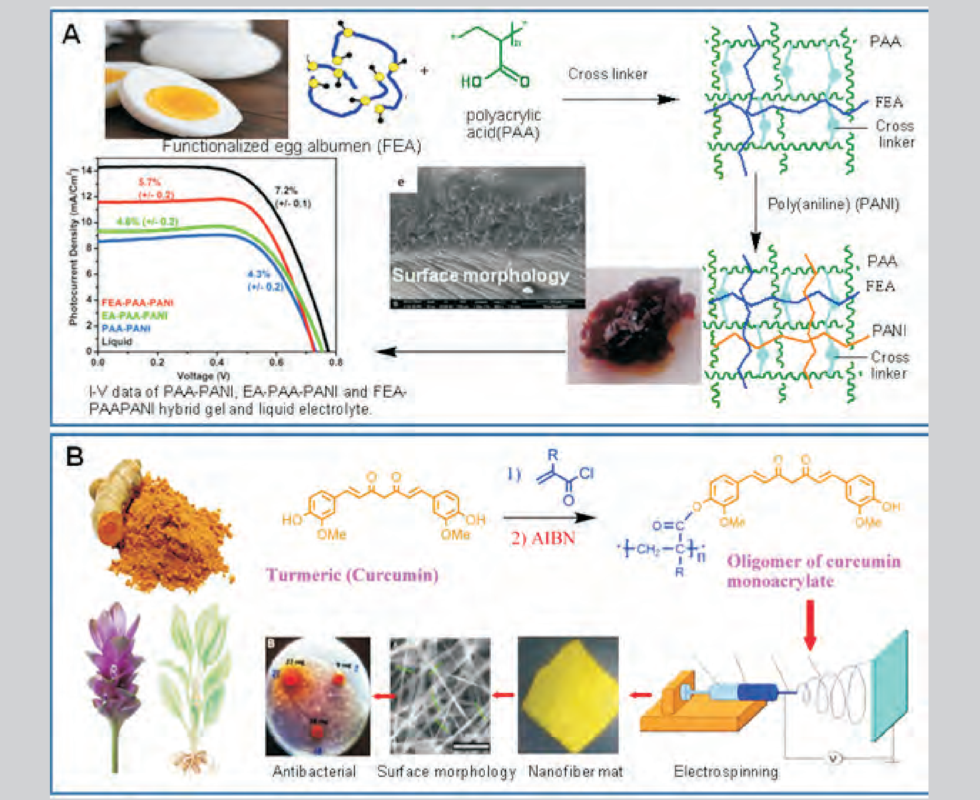

Fig. 1: A) Preparation of modified egg albumen based gel electrolyte B) Synthesis of oligomers of curcumin

Advanced Materials

Materials for environmental and healthcare applications

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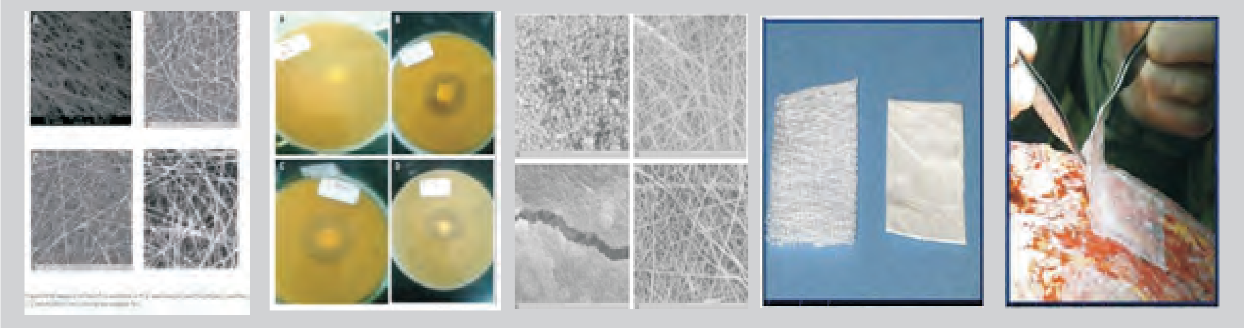
A vast number of biodegradable polymers were synthesized recently and degraded in presence of microorganisms and enzymes. Environmental pollution by a synthetic polymer proved to be a dangerous threat in the developing countries. Attempts were made to solve such problems by introducing biodegradability into the polymers in everyday use through slight modifications of their structures or total replacement using biodegradable polymer. India is a major sugar cane producing country. The sugar is produced from sugar cane and the remaining molasses are used for lactic acid which is a precursor monomer for preparation of Poly (lactic Acid). It can mimic all the properties of petroleum based polymers. Poly(lactic acid) was prepared using various synthetic strategies (*Polym. Bull.* **2015**, *72*, 405).

Poly (lactic Acid) is widely used in biomedical applications in various forms such as sutures, stents etc. Stannous octoate is a conventional catalyst used worldwide. However, it is toxic and cannot be removed from polymer matrix completely. Therefore, biocompatible zinc based catalyst was developed which helped to prepare Poly(lactic acid) with high molecular weight (Patent: Wo2013 108271A1).

Bacterial infection is a frequent complication associated with various types of wounds (normal, diabetic and burn). In an effort to address this problem, Ciprofloxacin was conjugated with polylactides (CP–PLA) through secondary amine group of piperazine ring using polylactide (PLA) and 7–(4–(2–chloroacetyl) piperazin–1–yl)–1–cyclopropyl–6–fluoro–1, 4–dihydro–4–oxoquinoline–3–carboxylic acid. Non–woven nanofiber matrices were fabricated using electrospinning. The release kinetics and bacterial studies showed that these mats can be used for 24hr for wound healing (*Int. J. Nanomed*. **2014**, *9*, 1463).



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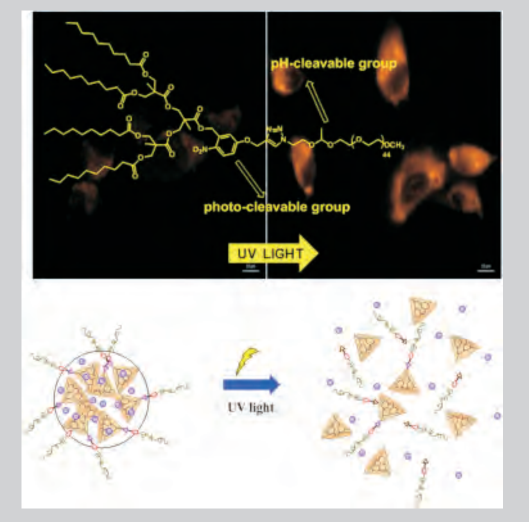
Polymer micelles as controlled release vehicles of anti-cancer drug: A biocompatible amphiphilic linear–dendritic block copolymer was developed that formed micellar aggregates in water similar to surfactant micelles. The polymer showed two groups –one sensitive to light and the other sensitive to pH. The polymer breaks down in response to UV light (365 nm) or acidic pH and the micelles disintegrate. It was demonstrated that the polymer micelles were capable of transporting the anti–cancer drug (Doxorubicin) into cancer cells (MDA–MB–231) and releasing it upon irradiation with UV light in a controlled manner. Studies with hydrophobic dye as a model drug showed that both light and pH were applied as stimuli, simultaneously to accelerate the disruption of micelles and release the dye (*Polym. Chem.* **2015**, DOI: 10.1039/c5py00792e; Patent: IN 2013DE01872 A).



Agriculture, Food and Nutrition

Crop protection

Genomic-proteomic studies of stress and defense related proteins of chickpea

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Analysis of UDP-glycosyltransferases genes abundant in chickpea genome: Glycosyltransferase (EC 2.4.x.y) glycosylates are the important plant products for proper functioning and survival in adverse conditions. 96 Uridine 5'–diphospho–glycosyltransferase (*UGT*) genes were identified in chickpea and compared with close orthologs in four other dicot plants. Their abundance must be related to glycosylation of a diverse array of acceptor substrates. RNA–seq data and expressed sequence tag libraries in NCBI database indicated differential expression in various chickpea tissues. Functional assignment was achieved for 74 of the identified UGTs (*PLoS ONE* **2014**, 9, e109715 doi:10.1371/journal.pone.0109715).

Structure-function studies of proteases and protease inhibitors in *Cicer arietinum*: Proteases and protease inhibitors (PIs) are involved in biological processes of biotic and abiotic stress responseincluding suppression of pathogen invasion. Proteases belonging to four families and cysteine and serine protease inhibitors were identified in chickpea. Their genes were characterized for chromosomal location, domain classification, gene architecture, gene duplication and expression. The profiles revealed differential expression pattern in multiple tissues. Three–dimensional structures were modelled and binding affinities with cognate molecules were also evaluated. Molecular dynamics studies revealed the strong interactions with target molecules (*Comput. Biol. Med.* **2015**, *56*, 67).

The four blades are numbered as I, II, III and IV. The bound calcium, chloride, sodium and iodide ions are shown in blue, cyan, light pink and magenta spheres, respectively, and arranged in a queue in the central channel. Orange sphere represents the chloride ion, near blade II which is at the dimerization interface.

The His180 and Lys181 are from blade IV while the carboxy–late groups are contributed by Asn15 and 16 from blade I. The solvent accessibility in the decreasing order for these residues is N15, K181, H180 and N16. The bound ions in the central channel are also shown.

Crystal structure of a chickpea albumin possessing hemopexin fold and hemagglutination activity: The plant albumin (PA2) from *Cicer arietinum* possessed the hemagglutination activity. This was the first structure of a plant albumin having hemaglutination activity. The polypeptide chain organized in four β–sheets (I–IV) was radially arranged like a four–bladed propeller (Fig. 1). The pseudo 4–fold symmetry axis passing through the centre formed a funnel shaped channel (Fig. 2) that provided the binding sites for ions. The four–bladed β–propeller structure provided unique multivalent binding sites for lectin function and also bound the hemin, plant hormones and hydrophobic groups (*Planta* **2015**, *241*, 1061).

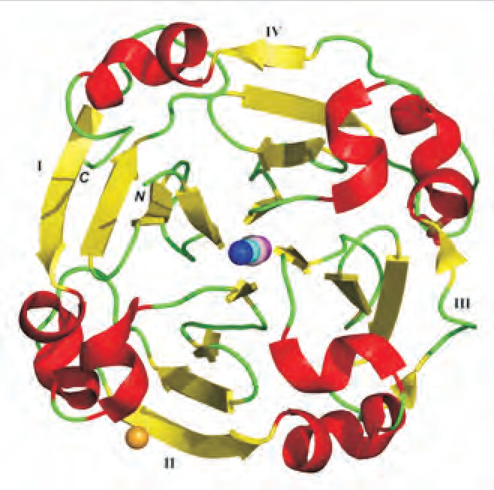

Fig. 1: The four-bladed β-propeller fold of PA2 viewed along the pseudo four-fold axis

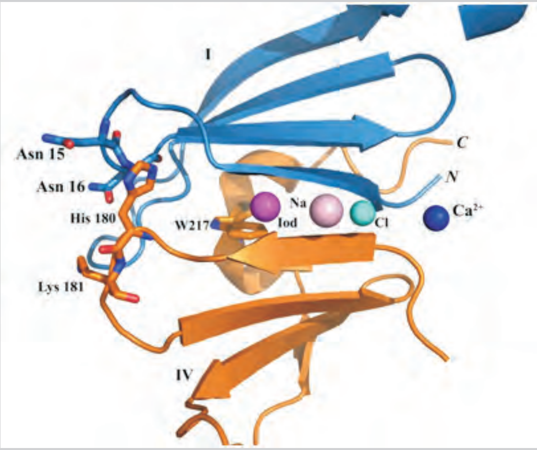

Fig. 2: Putative residues involved in sugar recognition by PA2 inferred using chemical modification studies

Agriculture, Food and Nutrition

Crop protection

Crop protection, bio-prospecting and identification of lead molecules

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Control of insect pests and pathogens: This work was carried out with the collaboration of Dr. A. P. Giri from the Biochemical Sciences Division. *Metarhiziumanisopliae* conidial germination was affected by chemical insecticides against mealy bug (20–30%) and fungicides (40–60%) against pathogens. The *Myrotheciumverrucaria* hydrolytic enzymes retained 66–70% activity after 5 h exposure to chemicals. The applications of biocontrol agents singly and sequentially in grape field were effective against mealy bugs. The enzyme mixture with additives controlled the downy (71% control) and powdery (80% control) mildews similar to the farmers practice.

Development of new antifungal agents and fungicides from Pseudomonas sp.: This work was carried out with the collaboration of Dr. C. V. Ramana from the Organic Chemistry Division.

An antifungal metabolite produced by a *Pseudomonas* was purified and identified as Phenazine 1–carboxamide (PC). Human pathogenic yeasts and filamentous fungi were inhibited by PC (MIC$_{90}$ 32–64 µg ml^{-1}). After exposure to PC (20 µg ml^{-1}), 75–80% yeast cells of *B. poitrasii* and *C. albicans* NCIM 3471 showed high intracellular reactive oxygen species (ROS) production. ROS further led to hyperpolarization of mitochondrial membrane, subsequently induction of apoptosis and finally death in *B. poitrasii* (*J. Appl. Microbiol.* **2014**, *118*, 39).

Antifungal diterpene from *Polyalthialongifolia var. pendula*: 16α-hydroxycleroda-3,13(14)Z-dien-15,16-olide, a diterpene from *Polyalthialongifolia* was found to exhibit antifungal activities having MIC$_{90}$ values of 50.3, 100.6 and 201.2 µM against *Candida albicans* NCIM 3557, Cryptococcus neoformans NCIM 3542 (human pathogens) and *Neurosporacrassa* NCIM 870 (saprophyte), respect-ively. The mode of action of *C. albicansis* was due to compromised cell membrane permeability, and also probably due to disruption of cell wall structures (*Eur. J. Med. Chem.* **2015**, *94*, 1).

Antifungal 1,2,4-triazole thiol substituted strobilurin derivatives: Total seventeen 1,2,4-triazole thiols and 1,2,3-triazole substituted strobilurin derivatives were synthesized. 1,2,4-Triazole thiol substituted strobilurin derivatives inhibited the growth of plant pathogens such as *Fusarium oxysporum, Magnaporthegrisea, Drechsleraory-zaeand* human pathogens *Aspergillus-fumigatus* and different strains of *Cryptococcus neoformans*, with MIC in the range of 16-256 µg/ml. Antifungal action of the compounds was due to inhibition of mitochondrial respiration (*Ind. J. Chem. B* **2015**, *54B*, 908).

1,4-dioxa-8-azaspiro [4,5] decanes fungicides: Various substituted 1,4-dioxa-8-azaspiro [4,5] decanes were synthesized and their usefulness as fungicides was demonstrated (Patent: US 8841296 B1).

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***In vivo* role of bile salt hydrolyse (BSH) like enzymes in bacteria and archea:** BSH–like enzyme includes pharmaceutically important enzymes that cleave the acyl side chains of penicillins, thus paving the way for production of newer semi–synthetic antibiotics. The research was focused on the studies of biochemical and structural characteristics of recently discovered penicillin acylases. The group has attempted to organize the available insights into the possible *in vivo* role of penicillin acylases and related enzymes, and emphasize the need to refocus research efforts in this direction (*Crit. Rev. Biotechnol.* **2014**, doi:10.3109/07388551.2014.960359).

Agriculture, Food and Nutrition

Crop protection

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Identifying QTL clusters governing dough rheology traits in wheat: Genetic dissection of dough rheology traits (DRT) in hexaploid wheat was conducted using nine mixograph characters evaluated in three agro-climatic zones of wheat. Composite interval mapping using a linkage map of 202 SSR markers identified 144 DRT QTLs of which, 96 were detected in single–and the rest in two to five year-locations. Majority of the DRT QTLs showed location-specificity and suggested selection of QTLs targeted for individual agro-climatic zones for breeding wheat for dough quality (*J. Cereal. Sci.* **2015**, *64*, 82).

Molecular analysis of GA3 response in grapes: Cluster compactness is an important character determining grape quality (Fig. 1). GA3 application at different stages of cluster development produces bold and uniform-sized berries. High-throughput transcriptomics and metabolomics approaches were employed to understand the molecular mechanisms of GA3 application on berry development. The suitability of 10 candidate reference genes were assessed for real time-PCR analysis and three most stably expressed genes were also determined. The expression of GA3 signaling gene, VvSpy, was analyzed to validate the stable reference genes (*Biol. Plantarum.* **2015**, *59*, 436).

Fig. 1: Result of the gibberellic acid spray at rachis stage

Mango is considered as the King of Fruits because of its flavor and nutritional importance. It is a source of energy, growth factors, carbohydrates, dietary fibers and antioxidants. Furaneol and mesifuran are the important flavor components of mango due to their sweet, fruity and caramel like aroma; and their appearance during Alphonso ripening. The gene encoding *O*-methyltransferase, which is involved in the biosynthesis of the aroma volatile mesifuran, was isolated and characterized from Alphonso mango. This will enable production of the mango flavor component mesifuran which offers caramel like aroma (Patent: 0098-NF-2015: 1737-DEL-2015).

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Characterization of molecules exerting antibiosis to *Helicoverpa armigera*: The efficacy and specificity of three inhibitory repeat domain (IRD) variants from *Capsicum annuum* PIs viz., IRD-7, -9 and -12 against H. armigera proteases was assesed. IRD-9 exhibited strongest effects on larval growth, survival rate and other nutritional parameters. The screen identified caffeic acid (CA), a natural phenolas a potent inhibitor of *H. armigera* gut proteases. The structure–activity relationship of CA highlighted that all the functional groups were crucial for inhibition of protease activity. The findings suggested that IRDs and CA explored further for development of effective strategies for crop protection (*Phytochemistry* **2014,** *101,* 16; *J. Agric. Food Chem.* **2014,** *62*, 10847).

Role of microRNAs in regulation of *Helicoverpa armigera* digestive protease: Deep sequencing of 12 small RNA libraries was performed from H. armigera larvae fed on artificial diet or recombinant *Capsicum annuumprotease* inhibitors (rCanPI-7). Homology analysis revealed that most of the identified miRNAs were insect-specific. Several candidate miRNAs (conserved and novel) were differentially expressed in rCanPI-7 fed larvae. These miRNAs were found to have target sites in protease genes. The negative correlation in the relative abundance of miRNAs and their target mRNAs were evident from gene expression data. The investigation revealed potential roles of miRNAs in *H. armigera* protease gene regulation (Insect *Biochem. Molec.* **2014,** *54*,129).

Potential delivery system for identified molecules for agricultural application: An attempt was made by the group to formulate the identified molecules for its potential application as spray. These formulations were being tested for the control release of active molecules and effect on plant growth and physiology. It was intended to confirm specificity in protease regulation for microRNAs (*Colloid. Surface. B* **2015,** *130*, 84).

Agriculture, Food and Nutrition

Crop protection

Molecular analysis of plant-pathogen interactions

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Molecular analysis of plant-pathogen interactions: The group is working on two major diseases such as the spot blotch of wheat (caused by *Bipolaris sorokiniana*) and wilt of chickpea (caused by *Fusarium oxysporumf.sp. ciceri*). Ten *B. sorokiniana* isolates were characterized at molecular, biochemical and morphological levels and three isolates were sequenced. SAGE and RNA–seq analysis of chickpea–Fusarium interactions revealed several disease resistance genes. Non–targeted metabolomics revealed many antifungal metabolites like aurantionobstine, β–glucosides and querecitin to induce in resistant plants after pathogen attack (Fig. 1) (*Phytochemistry* **2015**, *116*,120).

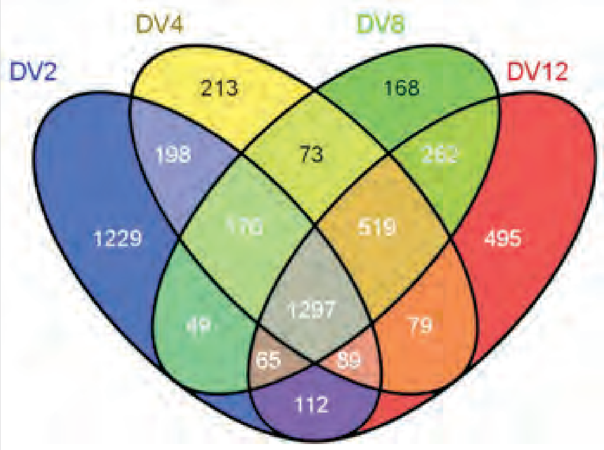

Fig. 1: Four-way Venn diagram showing the number of accumulated metabolites in resistant chickpea variety upon Foc inoculation

Molecular analysis of salinity tolerance in grapes: Soil salinity is a major problem in grape cultivation, which reduces the life of grapevines and seriously affects production. The group has used the high–throughput transcriptomics and proteomics approaches to understand the molecular mechanisms of salinity tolerance in grapes. The suitability of 10 candidate reference genes was assessed for real time–PCR analysis and determined three most stably expressed genes. The expression of a GA3 signaling gene, *VvSpy*, was analyzed to validate the stable reference genes (*Biol. Plantarum* **2015**, *59*, 436).

Structural and functional transitions of selected insect and fungal proteins

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Subtilase from *Beauveria* sp.: Conformational and functional investigation of unusual stability: The stability of Bprot towards denaturants (GdnHCl), organic solvents (methanol) and other proteases indicated the unusual stability of the enzyme which can be attributed to the rigidity of the structure, i.e. protein being difficult to unfold. Firstly, due to the structural rigidity, access of GdnHCl to the hydrogen–bonded protein interior could be prohibited. Secondly, altered favorable hydrophobic interactions and hydrogen bonding may impart the resistance towards organic solvents. Third, adoption of compact structure under harsh conditions like acidity and proteolytic environment protected Bprot from denaturation. All the above factors led to the conclusion that Bprot has a rigid structure (*Eur. Biophys. J.* **2014**, *43*, 393; *Glycobiology* **2015**, *25*, 357).

Agriculture, Food and Nutrition

Plant diversity and bio-prospecting

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Genetic diversity analysis in *Symplocos racemosa* from Western Ghats: The effects of anthropogenic activities on genetic diversity and population structure of a medicinally important tree species, *Symplocos racemosa*Roxb. from Western Ghats (WG) were analyzed. The variation in intergenic sequences of chloroplast and mitochondrial genomes was analyzed from seven sites from protected, semi–protected, and disturbed areas of WG. Total diversity was high although within–sites diversity was lower. The protected sites were highly diverse, while the disturbed areas possessed less genetic diversity indicating the effect of anthropogenic activities (*Int. J. Biodiversity* **2014**, Article ID 296891).

Genetic diversity analysis in *Symplocos laurina* from two biodiversity hotspots: *Symplocos laurina* is an important medicinal tree species. The group has analyzed 208 accessions of *S. laurina* from 13 populations belonging to three ecoregions in India including Western Ghats, Eastern Ghats and Northeast India to comment on the genetic diversity and population structure of the species. Of the 100 inter simple sequence repeat primers screened; eight polymorphic ISSR primers produced 1,014 bands from 208 accessions. Within–population variance was higher than among–population variance that indicated high intra–population genetic diversity (*Plant. Syst. Evol.* **2014**, *300*, 2239).

Plant secondary metabolites and pathway analysis

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Inducible metabolites from *Ocimum kilimandscharicum*: The overall biochemical and metabolic changes in *Ocimum kilimandscharicum* were examined to gain deeper insight into inducible defense metabolites that occurred in response insect feeding. Metabolic analysis revealed that the primary and secondary metabolism of local and systemic tissues in *O. kilimandscharicum* was severely affected.

Levels of specific secondary metabolites like camphor, limonene and caryophyllene significantly increased in leaves upon insect attack. Larvae fed on artificial diet supplemented with camphor, limonene and caryophyllene showed growth retardation, increased mortality rates and pupal deformities. Selected metabolites from *O. kilimandscharicum* possessed significant insecticidal activity (*PLoS ONE* **2014,** e104377).

Energy and Environment

Conventional energy coupled with CO_2 capture, storage and utilization

Hydrate based gas separation process for CO_2 capture

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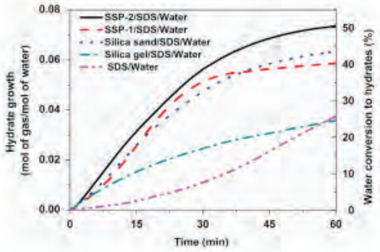
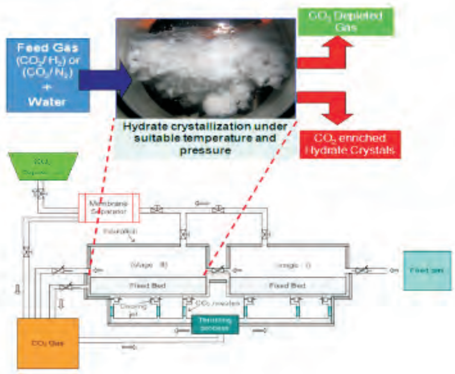
Hydrate based gas separation (HBGS) process requires selective partition of CO_2 between the solid hydrate phase and residual gas phase. It is imperative that faster hydrate formation rate maximum water to hydrate conversion is achieved. Highly conductive metallic packings were used to study hydrate formation kinetics in a fixed bed arrangement for faster hydrate growth. In presence of suitable kinetic promoters, significantly higher gas uptake rate of 115 mol.min.$^{-1}$m^{-3}and water to hydrate conversion of 70% was achieved in an hour of hydrate formation. Amount of CO_2 gas captured per mass/volume of packing material was significantly higher for metallic packing compared to silica sand and silica gel, which is an important parameter for scale-up of the process.



Conceptual protocol for potential application: Based on the lab scale experimentation a conceptual process flow diagram of the proposed HBGS process in a continuous mode for separation of carbon dioxide from fuel gas mixture was developed. The HBGS process comprised two thermodynamic phase changes; a hydrate formation stage to convert most of the liquid water into solid hydrate phase through selective enclathration of CO_2 from fuel gas (mixture of CO_2 and H_2), followed by a hydrate decomposition stage which converted the solid hydrate phase back into liquid water and CO_2 rich gas. The proposed process operated like a conventional tray dryer. There were two advantages of this arrangement, firstly a metallic bed ensured efficient heat transfer for hydrate formation and decomposition stages; passing a coolant (to maintain temperature of the reaction) at the bottom of the tray was easy to implement during scale-up. Additionally a tray dryer like arrangement ensured no bed clogging due to solid hydrate formation and thus lower pressure drop. Large surface area necessary for better water to gas contact (for tackling higher flow rate of fuel gas mixture) was created by just increasing the numbers of trays (*Ind. Eng. Chem. Res.* **2014**, *53*, 9849; *Chem. Eng. Sci.* **2015**, *122*, 78).



Energy and Environment

Conventional energy coupled with CO_2 capture, storage and utilization

Carbon dioxide sequestration in geological formations in sea bed

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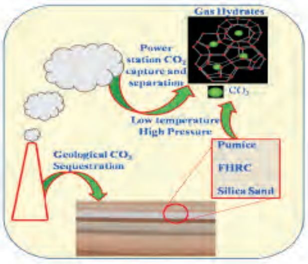
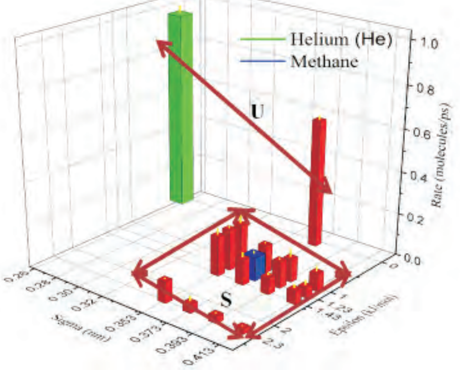
A comparison study on CO_2 hydrate formation kinetics using siliceous volcanic materials such as pumice and FHRC (a model material), which are available in plenty in the Indian subcontinent, is valuable to assess the feasibility of sequestering CO_2 in the form of hydrates. In this work pumice and FHRC were used as packing materials in a fixed bed setup to study hydrate formation kinetics. Carbon dioxide hydrate formation kinetics was studied at 3.0 MPa pressure and 274 K temperature.



CO_2 sequestration by methane replacement in marine gas hydrate reserves: Suitable MD simulations were done to explore systematically how the properties of guest molecules in fully occupied SI type hydrate cages affect the rate of hydrate decomposition. Lennard Jones (LJ) potential was used to calculate the non-bonded interactions between the particles (atom/molecules). As the size of the particle while using LJ potential is defined by sigma and the hydrophobicity/ hydrophilicity which is governed by epsilon parameter, the stability of the SI hydrate cages were checked with varying epsilon and sigma values. Rate of decomposition calculated for these hydrate suggested that guest molecules of slightly larger in size and more hydrophilic than methane were more stable than methane hydrate. The research work clearly showed the replacement of methane hydrate with CO_2 molecule that led to a more stable system making the molecular replacement approach quite feasible. H_2S is another guest molecule candidate which replaced CH_4 from natural gas hydrates (*ACS Sustain. Chem. Eng.* **2015**, *3*, 1205; *Phys. Chem. Chem. Phys.* **2015**, *17*, 9509).



Renewable and alternative energy technologies

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The efforts were made to tap alternative energy sources by employing photocatalysis and green chemistry.

Sunlight driven water splitting with $In_{1-x}Ga_xN@ZnO$ to generate hydrogen: Importance of In1-xGaxN lies in its ability to absorb the entire wavelength range of near IR, visible and UV light available in the direct sunlight. Its synthesis is difficult due to different ionic sizes and volatility of In and Ga. The tiny nanoparticles of In1-xGaxN in ZnO were embedded to minimize the structural stress and make it more stable, since it belongs to the same class of Wurtzite structure. $In_{1-x}Ga_xN@ZnO$ was successfully synthesized and demonstrated for water splitting to H_2 and O_2 in simulated sunlight. It is also shown to convert sunlight into electricity at no applied potential (Fig. 1). It indicated its high potential for solar energy harvesting applications (*Dalton T.* **2014**, *43*, 12546; Patent(s): WO2014195974-A1; WO2014195974-A4).

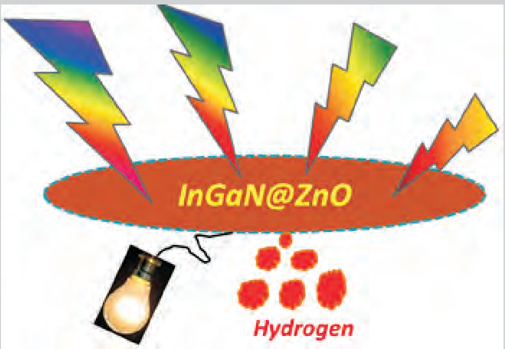

Fig. 1: The applicability of $In_{1-x}Ga_xN@ZnO$ for harvesting sunlight

Energy and Environment

Renewable and alternative energy technologies

Lithium battery

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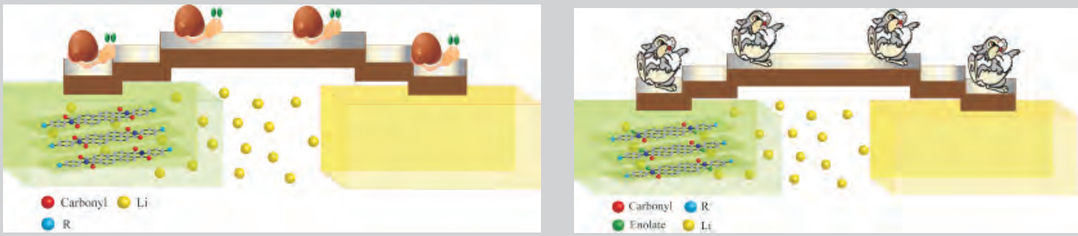
Quick recharging battery: The objective was to develop batteries that charge rapidly. The batteries based on organic materials are an added advantage. The organic materials render the possibility of fabricating light weight, thin and flexible batteries. These are not able to deliver the power consumed during the charging. A perylenediimide based (PDI) molecule as an electrode in lithium battery was synthesized to accomplish the objective of efficient organic electrode based lithium battery. The performance of this molecule was found to be poor. A small amount of reducing agent as dopant was added in order to increase the efficiency of the molecule. The doped battery's performance was excellent. The battery exhibited specific power of 8548 W/kg and specific energy of 213 Wh/kg with a coulombic efficiency of 100%. The battery was able to charge and discharge rapidly (*Chem. Mater*. **2015**, *27*, 2121).



The undoped battery slowly charge (left) and the doped battery charges rapidly (right)

Clean coal technology

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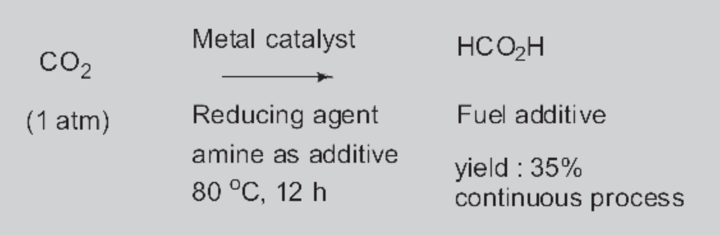
The objective was to establish a viable chemical process for the production of industrially useful products using carbon dioxide as a renewable feedstock. Hence, new catalytic systems for catalytic reduction of CO_2 to formic acid were developed.

Reduction of CO_2 to HCO_2H using various metal hydrides and borohydrides were carried out. Addition of $^{i}Pr_2NH$ as an additive in catalytic amount led to formation of formic acid. $^{i}Pr_2NH$ activated the $Co(BH_4)_2$ through its co-ordination to Boron and enhanced its reduction potential to deliver H^- easily (Scheme 1).



Scheme 1: Reduction of CO_2 to formic acid

Energy and Environment

Emission and effluent control including water and soil management

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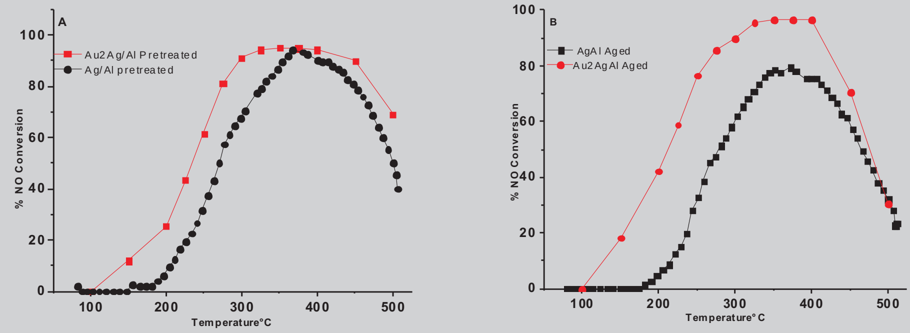
Non-nobel metal based diesel oxidation catalyst: The noble metal-based catalysts particularly Pt and Pd supported on alumina were used for the oxidation of CO, HCs (100 to 450°C) to clean up the diesel engine exhaust while meeting the stringent environmental regulations. Oxidation of NO to NO_2 is also important for oxidation of soot using formed NO_2 on oxidation catalyst. The major drawback of the noble metal based catalyst is its very high cost, sulfur poisoning and sintering of noble metals at high temperature. Development of non-noble metal based diesel oxidation catalyst (DOC) was done using ceria as a support. The oxidation activity of NCL catalysts showed promising results when compared with in-house prepared 1%Pt/Al_2O_3 as reference catalyst. NCL1 catalyst showed 100% conversion of CO and propene at 120 and 180°C respectively with a very low light off temperature (25 and 78°C respectively) compared to 1% Pt/Al_2O_3. The catalyst showed better tolerance for sulfur (10 ppm SO_2) and H_2O (9%) (Patent: 0009-NF-2014).

Catalyst for removal of NOx from automobile exhaust engines: Modification of the bench-mark catalyst composition (2%Ag/Al_2O_3) by doping gold (1 wt%) widened the temperature window for HC-SCR of NOx with 100% selectivity for N_2 over the entire temperature window. The aim of the study was to improve the low temperature activity as well as widen the temperature window (250-500°C) for SCR activity of the benchmark catalyst. 1Au–2Ag/Al_2O_3 catalyst showed maximum NO conversion of 94% at 325°C compared to 74% at 350°C on 2% Ag/Al_2O_3. Aging of the bimetallic catalyst in the reaction feed at 500°C for 12 h was considerably improved low temperature activity with ~42% NO conversion at 200°C. Presence of Au contributed for the improved high temperature activity as well as 100% selectivity for nitrogen in entire temperature range of study. Improved SCR activity was attributed to formation of well dispersed metallic Au and $Ag_n^{\delta+}$ clusters during pre-treatment and aging (*Appl. Catal. B-Environ*. **2015**, *162,* 11; *174*, 145).



Comparison of the SCR activity of Au2AgAl with AgAl (A) after pretreatment at 250°C in H_2 (B) after aging in the reaction feed at 500°C for 8h.

Dissolution POP idols: The Ganesh idols are being made from Plaster of Paris (POP) after immersion in water become harder and do not disintegrate causing environmental pollution. Due to sentimental issues associated with Ganesh idols, the idols cannot be disposed of by crushing. A project was jointly taken up by NCL with Pune Municipal Corporation, Cummins India Foundation and Mojj Engineering Systems Ltd. to disintegrate the Ganesh idols in an eco-friendly way. The POP idols were converted to ammonium sulphate which is very good fertiliser and calcium carbonate which could be used as additive in cement industry for making different cement articles as well as making chalks. The prototype designed and fabricated for eco-friendly immersion of four idols showed very encouraging results.

POP idols during the disintegration

Energy and Environment

Emission and effluent control including water and soil management

Desulfurization of transportation fuels

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Cleaner environment is not just priority goal for developed countries, but is an essential and priority agenda for developing country like India which housed numerous petrochemical industries and face severe pollution due to Sox emissions. The objective was to address the issues pertaining to the pollution control and emphasize mainly on the deep desulfurization of transportation fuels –below 15 ppm sulphur.

Adsorption technology: Adsorption technology is an attractive alternative in achieving deep desulfurization for removal of refractory sulfur compounds from organics. The application is specifically useful in petroleum industry for transportation fuels and industries that uses organic feed where sulfur is a problem e.g. Camphor industry. Newer adsorbents/ modified adsorbents are being developed for increased sulfur removal capacity with ease of regeneration. Development of newer tailor–made adsorbents, modification methodologies for improved adsorption, process integration using cavitation for desulfurization etc. extensive work was carried out recently on synthetic fuels comprising Thiophene, Benzothiophene and Dibenzo–thiophene and also using real Diesel (*J. Environ. Chem. Eng.* **2014**, *2*, 1495).

Studies on the hydrogen production by water splitting using doped TiO_2-SiO_2

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The use of TiO_2–SiO_2 mesoporous composites for water splitting was explored to achieve the enhanced performance of TiO_2 in photocatalytic water splitting process. The feasibility of using ethyl silicate, a less expensive polymeric version of ethyl silicate in place of TEOS was attempted to make the preparation of mesoporous SiO_2 more cost-effective. The titania was loaded in different proportions on mesoporous silica by sol–gel method to achieve the optimum photocatalyst. The research was aimed to prepare the potential visible active photocatalyst by extending the absorption of the optimized sample by doping with transition metals like Co, Sn etc.

The Fig. 1 presents the amount of hydrogen generated in mmoles/h/g of TiO_2 over MTi20, MTi40, MTi60, 1.0Pt/MTi60, MTi80 and 1.0Pt/MTi100 samples. The rate of evolution of H_2 was found to increase from 0.04028 to 0.08805 mmol of H_2/h/g of TiO_2 with increase in TiO_2 from 20 to 60%, further increase in TiO_2 upto 80%, the rate was found to decrease to 0.02238 mmol of H_2/h//g of TiO_2. Among the tested catalysts 1.0Pt/MTi60 showed the best result (*J. Mater. Sci.* **2014,** *49,* 6383).

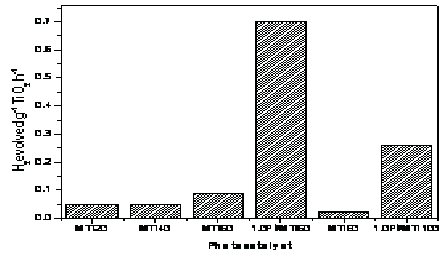

Fig. 1: Rate of hydrogen generation for water splitting over MTi20, MTi40, MTi60, 1.0Pt/MTi60, MTi80 and 1.0Pt/MTi100 samples under UV light

Energy and Environment

Water: treatment, disinfection, purification

Industrial wastewater tratment, recycle and reuse

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The objective was to address the issues pertaining to the pollution control and emphasize on water intensive industry in its wastewater treatment programs to such an extent that reclaimed water can be recycled and reused.

Industrial wastewater treatment: The group of scientists is working on Industrial wastewater treatment, water recycle and reuse. The activity mainly is focused on development of newer separation processes and how to combine or redefine finer aspects of existing methods– physico-chemical and biological methods. Specific aspects in developing wastewater treatment methodologies for effective separations were investigated using new/ novel adsorbents, ion exchange processes, coagulation/ cavigulation/ solvent extraction, membrane separations and cavitation, in isolation and in combination Emphasis was given to industrial applications and removal of pollutants in wastewater treatment to such an extent that reclaimed water was recycled and reused. A workshop entitled 'Indus Water' [Industrial waste water treatment, recycle and reuse [see http://induswater.ncl.res.in for more information] was conducted recently. The focus was on these and other aspects to realize environmentally benign and globally competitive processes and technologies through the research and industrial work (*Chemical Industry Digest* **2014**, *27*, 82).

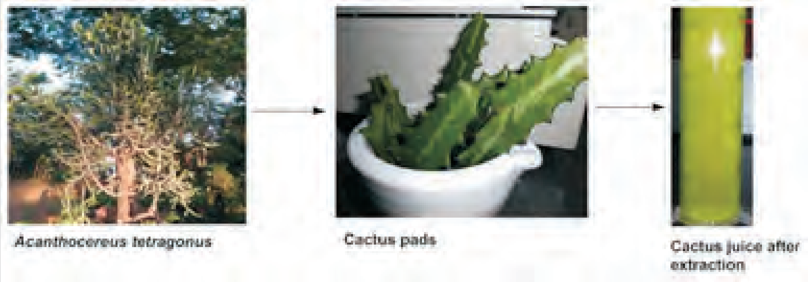
Cavitation technology: A technology was developed based on hydrodynamic cavitation for treatment of industrial waste. Cavitation technology is used for the treatment of any industrial effluent for removal of COD and colour. The technology was implemented alone or in combination with other processes such as biological treatment process, oxidation, adsorption, ion exchange or coagulation. The technology showed potential for effective removal of COD levels significantly at low cost of operation. When combined with anaerobic process, it enhances profitability through increased gas yield along with Digester stabilization.

Cavitation & Process Intensification Pilot Plant at CSIR-NCL, Pune (Capacity: 1 m3/h)

Coagulation technology: Coagulation technology was used for the treatment of any industrial effluent for removal of COD and color. The technology generally needed to be effectively implemented in combination with other processes such as biological treatment process, cavitation, oxidation, adsorption, ion exchange etc. to optimize distribution of pollutant removal load in different treatment stages. The technology showed potential for effective removal of COD levels significantly at low cost of operation. When used in the form of coagulant formulations, it dramatically enhanced the performance and reduced the cost of operation. A newer form of inorganic polymeric coagulant with high molecular weight and basicity, was developed in the laboratory is expected to offer substantial improvement as compared to existing coagulants. The development of biocoagulants and biocoagulant-formulations for improving coagulation process and cost benefits is also done (*J. Environ. Res. Dev.* **2015**, *9*, 813).

Water: treatment, disinfection, purification

Adsorption technology: Adsorption technology was used for the treatment of any industrial effluent for removal of COD and color, especially for removal of refractory pollutants. The technology was implemented alone or in combination with other processes such as biological treatment process, oxidation, cavitation, ion exchange or coagulation. The technology showed potential for effective removal of COD levels significantly at low cost of operation. The group is working on the development and application of novel adsorbents in wastewater treatment.



Industrial wastewater treatment: synthesis and application of biocoagulant

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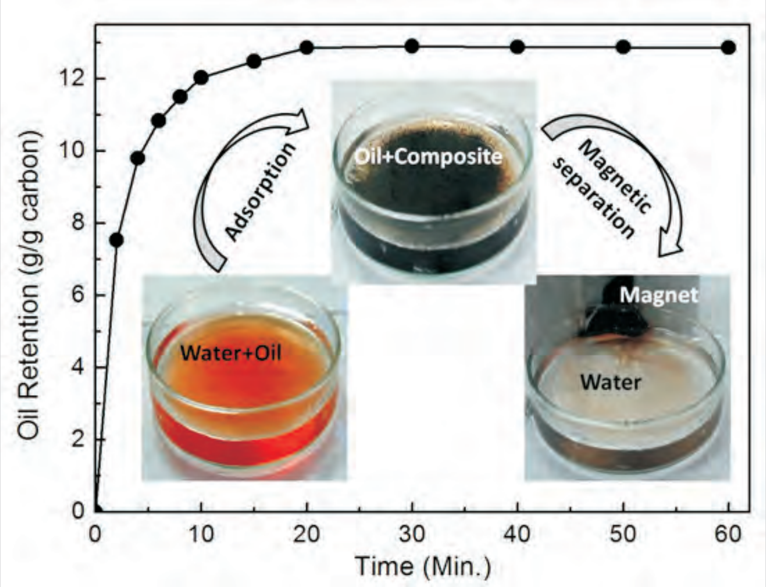
Coconut shell carbon based magnetic nanocomposite for cleaning oil spills: Coconut shell is one of the widely used materials for preparing activated carbon due to its easy availability and low cost. High surface area activated carbon derived from coconut shell is generally used for cleaning of oil spills in water bodies, which is considered as a serious environmental issue. A magnetic nanocomposite material of coconut shell based activated carbon and iron oxide nanoparticles was prepared in order to make the removal of oil spills more effective. The composite material was easily recovered using an external magnet after oil adsorption. The instantaneous oil adsorption by the composite material made it more efficient in preventing the spreading of oil on the surface of water. The magnetic nanocomposite can be recycled without much decrease in the retention capacity and therefore is a potential candidate for removal of oil spills by magnetic separation (*J. Environ. Chem. Eng.* **2015**, *3*, 2068).



Energy and Environment

Water: treatment, disinfection, purification

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Treatment of industrial wastewater by using advanced oxidation processes: Recently advanced oxidation processes (AOPs) showed great promises to provide alternatives for better protection of public health and the environment. A visible active photocatalyst for treatment of pharmaceuticals contaminated wastewater was developed. The effect of various parameters such as adsorption, pH of the solution, initial concentration, and effect of presence of anions and cations on photocatalytic degradation of pharmaceutical pollutant particularly paracetamol, Naproxen and ciprofloxacin HCl was studied in details. Developed BiOS photocatalyst was regenerated and reused. It implied that the chemical structure of BiOS showed photocatalytic activity intact. BiOS don't show disintegration into its individual components i.e bismuth or sulfur in treated water. A pilot scale slurry photoreactor was developed for the treatment of wastewater. It was found to be a viable proposition for photocatalytic degradation (PCD) using concentrated solar radiation.

Treatment of textile industrial wastewater by using advanced oxidation processes: The treatment of wastewater collected from textile industry (Manpasand Textile Processors Pvt. Ltd., Ichalkaranji, Kolhapur was attempted by using AOPs process. Initially experiments were carried out at scale of 500 ml/batch. Many experiments were performed in order to optimize the Photo-Fenton process. A viable solution was given to treatment of textile wastewater. The cost of treatment process was found less than 4 paise/L. Subsequently demonstration of textile wastewater at pilot scale 50000 L/batch was conducted at client site and got satisfactory results that showed complete color removal. COD value was reduced more than 60%. It can recycle the treated water along with fresh water for some of the dying operation which is an advantage of suggested process. The following photographs show actual trial taken at client site.

Appearance of textile wastewater before the treatment

Appearance of textile wastewater during the treatment

Demonstration of treatment of textile wastewater at Manpasand Textile Processors Pvt. Ltd. Ichalkaranji, Kolhapur

Sewage water treatment using AOPs: The treatment of actual sewage wastewater collected from STP Pune was attempted by AOPs process. The comparison of various AOPs for the treatment of sewage water was performed. The Photo-Fenton showed highest TOC reduction followed by Photo-Fenton persulfate and Aeroxide P-25 TiO_2 photocatalyst. Further detail studies on treatment of sewage water using photo Fenton process was carried out. Following figure shows the results of various batches conducted by using photo-Fenton process. The scale up of photo-Fenton process was done at scale of 10 L/batch and got promising results. Discussions are on with Pune Municipal corporation authority on the demonstration of suggested process at STP site (Patent filed: 14/584, 168).

Recovery of water from domestic waste water using membrane based systems: India produces around 22,900 MLD of domestic waste water apart from 13,500 MLD of industrial waste. Compared with the amount of waste water produced, there are only 234 sewage water treatments plants present in some of the major cities. In order to overcome the water crisis in the future there is a need for an efficient, cost effective and low maintenance waste water treatment plant which does not require skilled technical labour for its operation. The work was carried out on the possibility of effectively utilizing the natural microbial flora/ consortium, enriched with the rapidly growing algae, standard algal isolates along with MBR for the treatment of sewage as economical alternatives. The treatment of raw domestic sewage using micro algal photobioreactor (PBR) and combination of microalgae followed membrane bioreactor (MBR) process was studied. The isolation and screening of micro algae having potential to grow in sewage water was done. The performance of different microalgae and mixed culture were studied for the removal of nutrients using PBR in batch mode as well as fed batch mode of operation using MBR. Further studies on optimization of process parameters for the treatment of sewage water are under progress.

Healthcare

Natural products and methodology

Asymmetric total synthesis of biologically active compounds and development of synthetic methodologies

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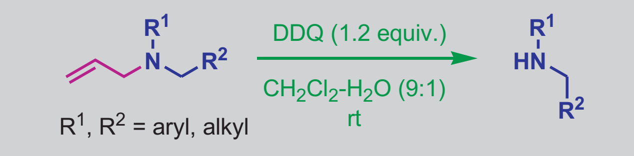
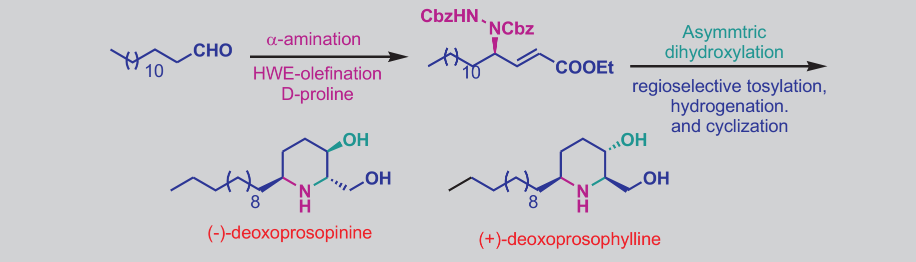
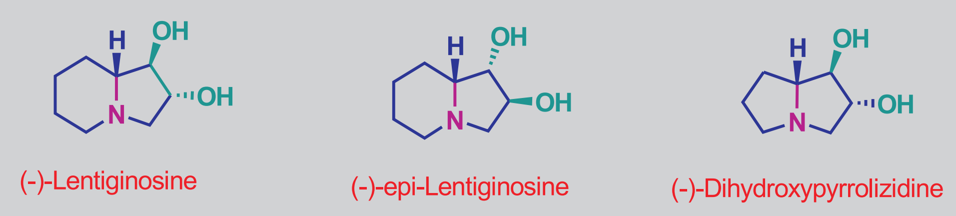
Chemoselective deprotection of N-allylic amines using DDQ: A highly chemo selective and simple method was developed for the deprotection of N–allylic amines using DDQ. The use of DDQ in dichloromethane–water provided a mild and efficient one–step deallylation of a wide variety of orthogonally protected tertiary amine derivatives (*Tetrahedron Lett*. **2014**, *55*, 7172).



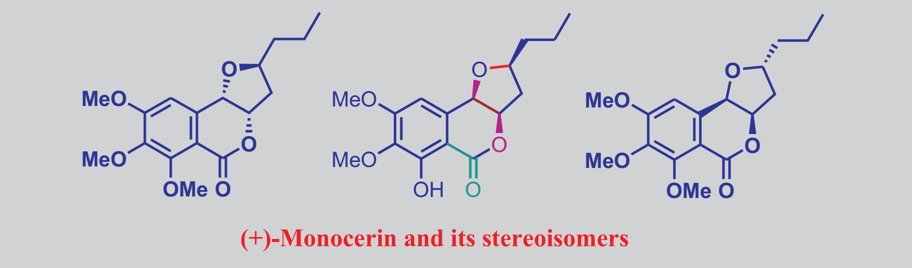
Stereoselective approach to 2,6-disubstituted piperidin-3-ol: synthesis of (-)-deoxoprosopinine and (+)-deoxoprosophylline: A simple and highly efficient approach was devised to an enantio enriched 2,6–disubstituted piperiin–3–ol skeleton from an aldehyde using organocatalysis and asymmetric dihydroxylation as the key steps. Its application to the synthesis of (–)–deoxoprosopinine and (+)–deoxoprosophylline was reported (*Eur. J. Org. Chem*. **2014**, 4897).



Stereoselective approach to indolizidine and pyrrolizidine alkaloids: Total synthesis of (–)–lentiginosine, (–)–epi–lentiginosine and (–)–dihydroxypyrrolizidine: A simple and highly efficient approach was devised to hydroxylated pyrrolizidine and indolizidine from an aldehyde using organocatalytic and asymmetric dihydroxylation reactions as key steps. Its application to the total synthesis of (–)–lentiginosine, (–)–epi–1,2–lentiginosine and (–)–dihydroxypyrrolizidine was demonstrated (*Org. Biomol. Chem*. **2014**, *12,* 4454).



Total synthesis of (+)-monocerin: A novel synthesis of (+)–monocerin was accomplished from 3–buten–1–ol employing hydrolytic kinetic resolution, Julia olefination, intramolecular tandem Sharpless asymmetric dihydroxylation-S_N2 cyclization and a novel copper mediated tandem cyanation–cyclization as the key steps (*Org. Biomol. Chem*. **2014,** *12*, 5973).



Healthcare

Natural products and methodology

Synthesis of allylic amines, tamiflu, (2R, 3R)-3-hydroxy pipecolic acid

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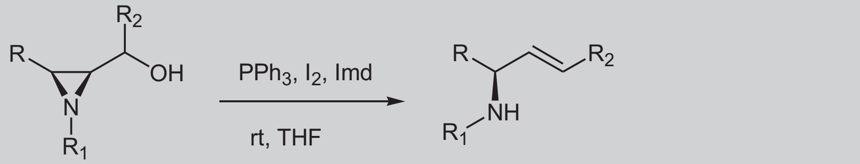
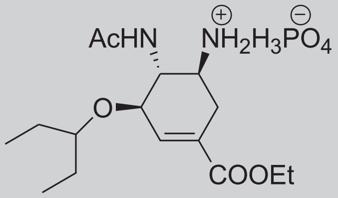
Efficient and mild method for the preparation of allylic amines: Chiral aziridine-2-alcohols represent attractive tool for the synthesis of chiral allyl amines. An efficient, practical method was developed using PPh_3/I_2/imidazole for the direct conversion of aziridine alcohols to chiral allyl amines giving well to excellent yields in a straightforward manner from chiral aziridine-2-alcohols under mild conditions (*Tetrahedron Lett.* **2014**, *55*, 5905).



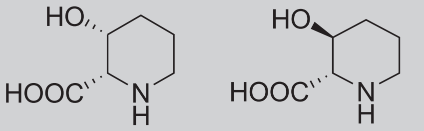
R=H, CH_3CH_2, 1,3-dioxalane; **R_1**=H, Benzyl, Allyl, Tosyl, Boc; **R_2**=H, Allyl, Phenyl

Synthesis of tamiflu: The formal synthesis of tamiflu was achieved from inexpensive, abundant and easily available L-cysteine as the renewable resource. An azide and aziridine free route was developed utilising a novel stereospecific amidoalkylation, Ramberg-Backlund reaction, azide free protocol in an efficient manner for synthesis of neuraminidase inhibitor drug tamiflu. The strategy involved stereoselective epoxidation, Sharpless-Reich protocol for the transformation of epoxide to access allylic alcohol and utilised the Ramberg-Backlund reaction for the first time for the synthesis of tamiflu as a key step to construct the cyclohexene intermediate which furnished desired vicinal trans diamine (*RSC Adv*. **2014**, *4*, 62281).



Oseltamivir phosphate
Tamiflu

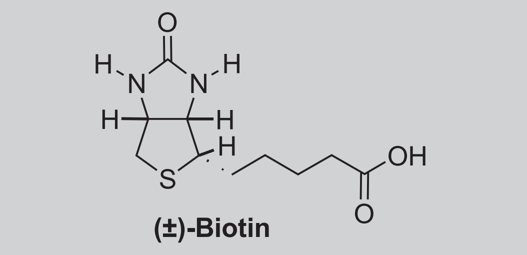
Formal syntheses of (2*R*, 3*R*)-3-hydroxy pipecolic acid and (2*R*, 3*S*)-3-hydroxy pipecolic acid from L-ascorbic acid: Formal synthesis of both cis and trans 3-hydroxy pipecolic acids were achieved from L-ascorbic acid. Present synthesis describes use of chiral pool approach in which epimerization, Staudinger reaction and cyclztion reactions were employed as the key steps. L-ascorbic acid was converted in to key synthon required for the synthesis of three hydroxy pipecolic acids. It was carried out by transforming the key synthon into alcohol which on oxidation and 2-carbon homologation provided unsaturated ester. The ester on hydrogenation gave an inseparable mixture of diastereomers. The reduction of ester to alcohol followed by its transformation into azide provided a key azide synthon as the diastereomeric mixture. This azide was cyclized under Staudinger reaction conditions and the diasteromers were separated to achieve formal synthesis of their respective 3-hydroxy pipecolic acid (*Tetrahedron Lett*. **2014**, *56*, 805).



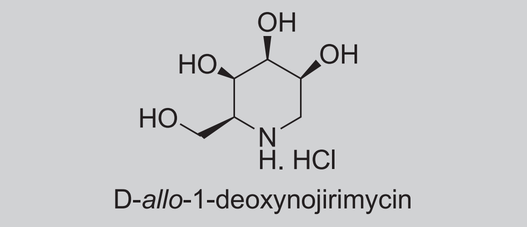
cis-3-hydroxy pipecolic acid
trans-3-hydroxy pipecolic acid

Natural products and methodology

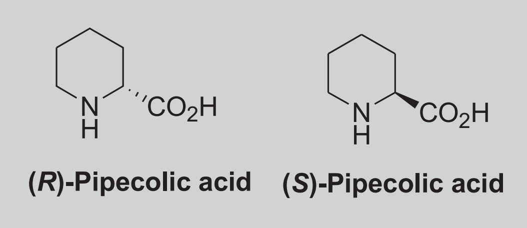
A facile and convenient synthesis of (±)-biotin: The interest in the synthesis of biologically important molecule led to explore a practical route for biotin. This strategy describes a facile and convenient synthesis for total synthesis of biotin which involved notable features like $MgCl_2/Et_3N$ mediated C-C coupling reaction, Mitsunobu inversion, ozonolysis, Staudinger reduction, novel urea formation and subsequent dibenzylation as the key organicreactions. Synthesis of biotin was accomplished in 13 purification steps with 13.7% overall yield. This method showed great value in terms of its simplicity in the construction of urea, tetrahydrothiophene ring and also elaboration of the pentanoic acid side chain of biotin skeleton. Investigation of the enzymatic and catalytic asymmetric reduction procedures to accomplish the asymmetric total synthesis of (+)–biotin is currently under way and the results will be reported in due course (*Synlett* **2014**, *25*, 2879).



Total synthesis of D-allo-1-deoxynojirimycin and L-*talo*-1-deoxynojirimycin: Synthesis of polyhydroxypiperidine framework for L–*talo*–1–deoxynojirimycin and D–*allo*–1–deoxynojirimycin was achieved from L–tartaric acid by employing flash dihydroxylation and reductive lactamisation as the key steps. The synthesis of D–*allo*–1–deoxynojirimycin and L–*talo*–1–DNJ was aimed by a chiral pool strategy using L–tartaric acid as the renewable starting material. The main synthetic challenge was the construction of piperidine moiety and installation of hydroxy groups in a stereoselective manner for the L–talo–1–DNJ and D–allo–1–DNJ synthesis. The total synthesis of D–*allo*–1–DNJ and L–*talo*–1–DNJ by employing flash dihydroxylation and reductive lactamisation as key steps from readily available L–tartaric acid was accomplished (*RSC Adv.* **2014**, *4*, 40852).



Enantioselective total synthesis of (*R*) and (*S*) pipecolic acid: The total synthesis of (*R*) and (*S*) pipecolic acid was achieved starting from cis aziridine–2–carboxylate as common synthetic precursor. This synthesis involved regioselective reductive cleavage of aziridine ring and Wittig olefination as the key chemical transformations. The aziridine synthon was derived from renewable starting material i.e. D–mannitol. The (*R*)–pipecolic acid was obtained in 5 purification steps while (*S*)–pipecolic acid in 7 purification steps with 31% and 28% overall yield respectively from the same chiral synthon. This synthetic approach is practically simple and economical (*Tetrahedron-Asymmetr*. **2014**, *25*, 1246).



Healthcare

Natural products and methodology

Metals magic: Total synthesis aided by novel metal-catalyzed reactions

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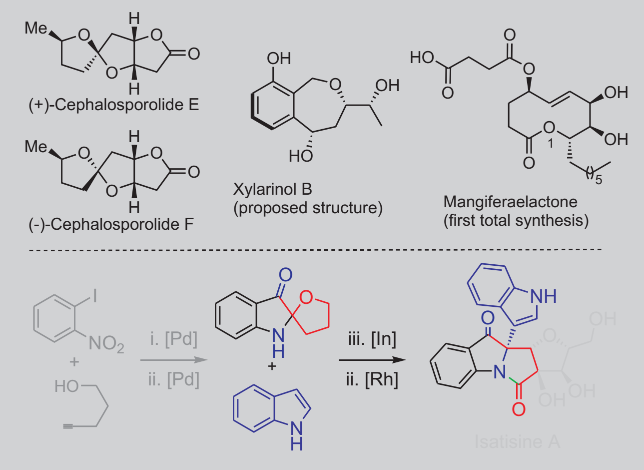
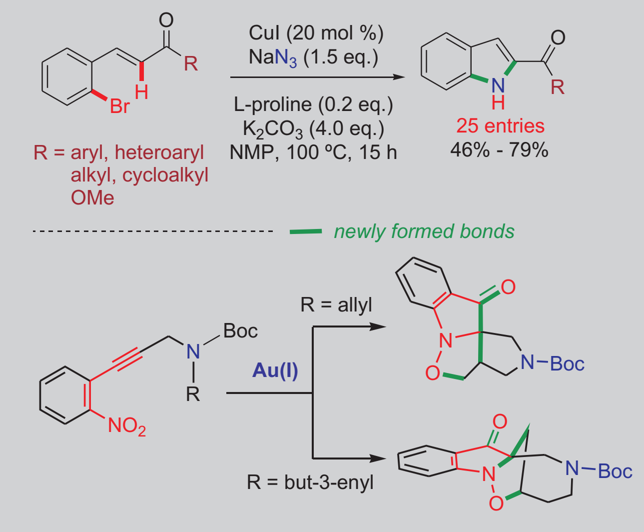
The research was focused mainly on the synthesis of biologically active natural products. It was aided by the discovery of newer methodologies for generating molecular complexity from readily available starting materials with inherent stereochemical specificity.

Total synthesis: A concise and short total synthesis of cephalosporolides E/F, the first total synthesis of mangiferaelactone establishing its absolute configuration and the total synthesis of putative structure of xylarinol B and a sequential metal-catalytic transformations for the synthesis of central tricyclic core of isatisine A were some of the accomplishments in this area.



Catalytic domino processes for complex molecular skeletons: A domino-process involving the Au-catalyzed nitroalkyne redox leading to isatogen and its subsequent [3+2]-cycloaddition with a suitably positioned olefin has been accomplished to construct the central tricyclic core of spiro-pseudoindoxyl class of natural products (*Org. Lett.* **2014**, *16*, 4766).

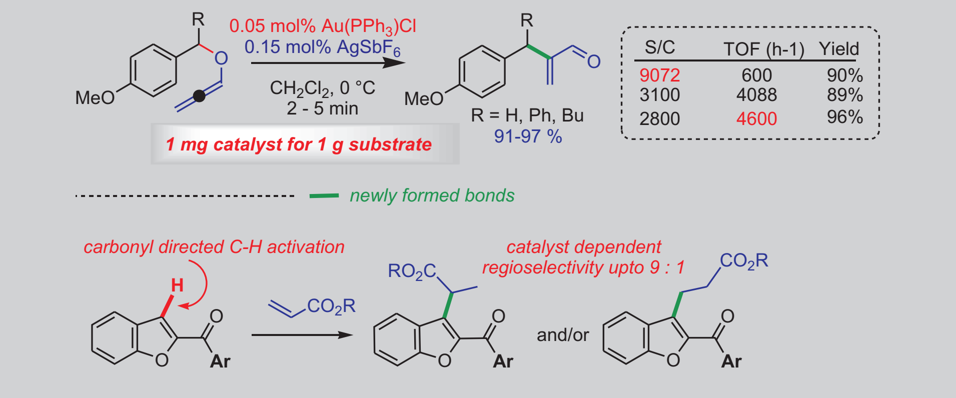
Simultaneously, 2-aroylindole derivatives characterized with diverse biological activities and with exceptional anticancer activity were synthesized from easily accessible *o*-bromochalcones as substrates by employing a Cu-catalyzed domino process comprising SNAr with azide, conversion of azide to nitrene, intramolecular insertion of nitrene across the C–H bond (*Chem. Commun*. **2014**, *50*, 7790).



Natural products and methodology

Catalytic methods for fine chemicals: A simple method for the synthesis of α-substituted acryl aldehydes was developed by employing gold-catalyzed [1,3] – rearrangement of the allenyl ethers. The reaction was almost spontaneous with a record turnover frequency of 4600 h^{-1} in the area of homogeneous gold-catalysis (*Chem. Commun.* **2014**, *50*, 2152).

The pharmaceutically relevant 2,3-disubstituted benzofurans were synthesized by a novel carbonyl-directed ruthenium-catalyzed C–H activation and alkylation with acrylates. Depending upon the catalyst employed the complementary branched and linear alkylation with acrylates was accomplished selectively. It was the first report in the history of metal-catalyzed coupling or alkylation with acrylates in a branched fashion (*Chem.–Eur. J.* **2014**, *20*, 7884).



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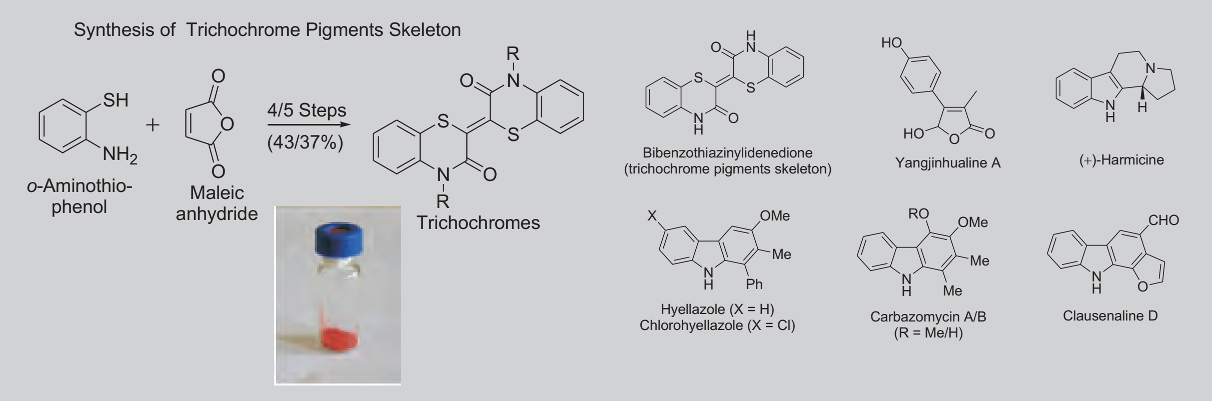
Total synthesis of recently isolated bioactive natural products: The objective was to design the bioactive natural products with highly efficient practical routes. The research group is engaged in total synthesis of several desired, complex bioactive natural and unnatural products, pseudo natural products and natural product hybrids using cyclic anhydrides as potential precursors, employing variety of new synthetic strategies. Trichochromes bearing an indigoid chromophore were isolated from human red hair. The list of natural products synthesized during the past year includes trichochrome pigments skeleton, yangjinhualine A, carbazomycin A, carbazomycin B, hyellazole, chlorohyellazole, clausenaline D and (+)-harmicine. The syntheses were carried out that involved many key steps such as the remarkable selective sulfuryl chloride induced dihalogenation-dehydrohalogenation, regioselective reduction of aryl(alkyl) maleic anhydrides, well designed Grignard reactions, Baeyer–Villiger oxidation and acid catalyzed stereoselective intramolecular cyclization were the involved key steps (*Org. Lett.* **2014**, *16*, 5470; Synthesis 2014, 46, 2591, 2015, 47).



Healthcare

Natural products and methodology

Total synthesis of biologically active compounds and medicinal chemistry

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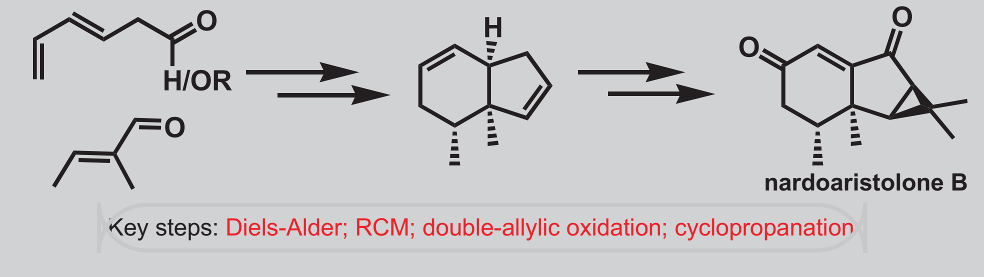
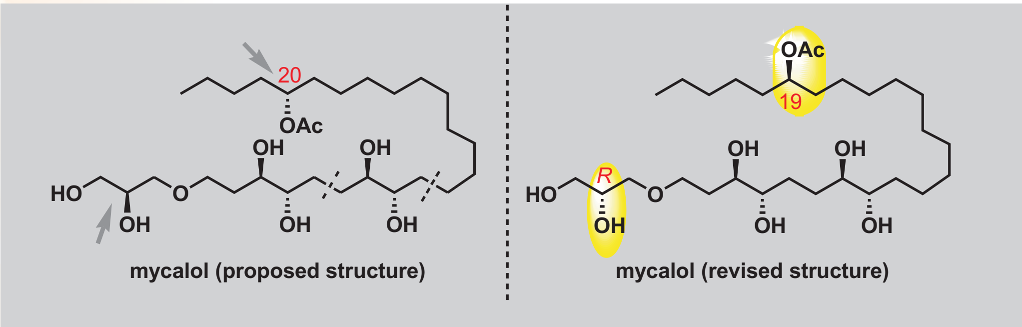
The focus was on the total synthesis of biologically active compounds and medicinal chemistry with an ultimate aim of discovering drugs. Current natural product targets included insect repellents, antibacterial, anti-inflammatory, anti-cancer, anti-TB and neuroprotective agents. The significant progress was made on "Silicon-switch approach".

Total synthesis of (±)-nardoaristolone B: First stereoselective synthesis of (±)-nardoaristolone B using a very short and protecting-group-free sequence was accomplished. The Diels–Alder/Wittig/RCM reaction sequence, double allylic oxidation, and stereoselective cyclopropanations were the highlights of the synthesis. A few novel analogues of nardoaristolone B including an exocyclopropyl containing compound were synthesized (*Org. Lett.* **2014**, *16*, 4252; Patent: 2082/ DEL/ 2014).



Total synthesis and structural revision of mycalol: Mycalol, a novel polyoxygenated ether lipid isolated from a marine sponge attracted attention owing to its promising specific activity against different cell lines derived from anaplastic thyroid carcinoma. The target compound was synthesized successfully but the comparison of NMR spectra of both the synthesized compound and the protected form of mycalol showed subtle variations. Based on careful analysis of high-field 2D NMR spectra, a new structure to mycalol was proposed and synthesized with two changes in the originally proposed structure by Fontana's group (*Org. Lett.* **2015**, *17*, 1652).

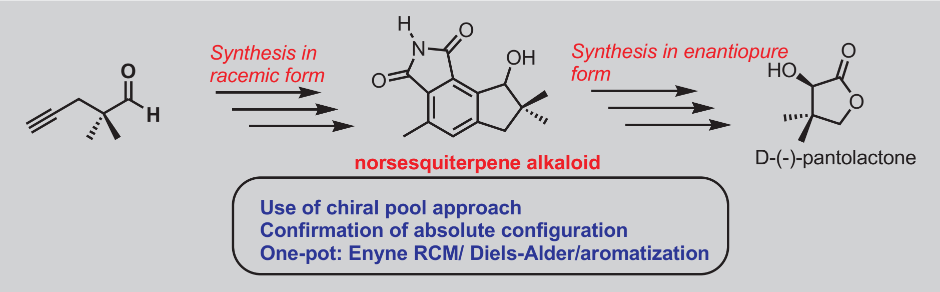


Total synthesis of deoxy-solomonamide B: The total synthesis of deoxy-solomonamide B starting from tryptophan in an efficient manner by mimicking the proposed biogenetic route was undergone. Present synthesis utilized a crotylation, oxidative cleavage of indole moiety and macrolactamization as key steps. The present route was potentially useful in preparing the actual natural products Solomonamide A and B and is suitable for producing analogues around the skeleton. Besides, thepresent method can be used for the synthesis of biologically active natural/ unnatural compounds which contain an orthoacyl aniline moiety (*Org. Lett.* **2014**, *16*, 6148).

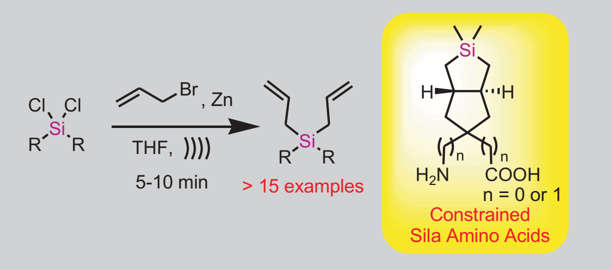
Total synthesis of an anticancer norsesquiterpene: The target natural product was successfully synthesized in both racemic and enantiopure forms. The synthesis featured a one-pot, three-step reaction sequence comprising an

Natural products and methodology

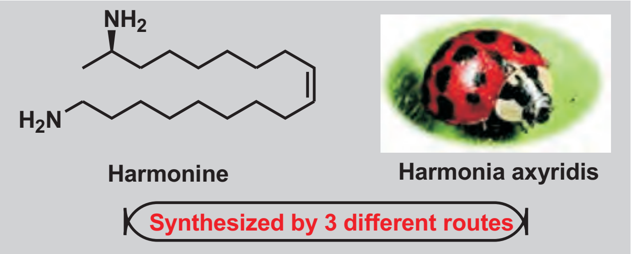
enyne RCM/Diels–Alder/ aromatization sequence to construct the desired indane skeleton present in the natural product (*Org. Biomol. Chem.* **2014**, *12*, 4098, 2015, 13, 970; Patent: 0421/DEL/2014).



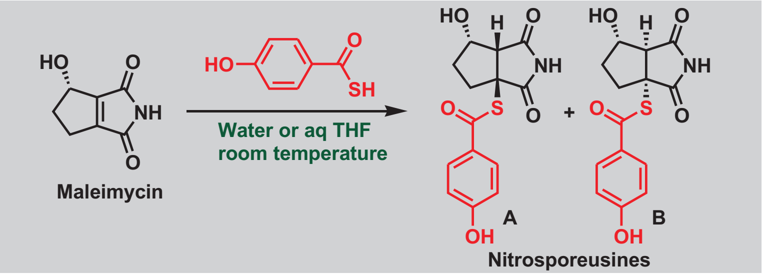
Synthesis of novel constrained sila amino acids: A simple, fast and efficient method was developed as a part of Silicon–switch approach for the allylation and propargylation of chlorosilanes through zinc mediation and ultrasound promotion. Silicon incorporated unnatural α,β and γ–amino acids with unusual 5,5–trans fusion were prepared using allyl–silanes as starting material for the first time. The design and synthesis of the constrained sila analogue of GABA (γ–amino butyric acid) is a highlight of this work (*Org. Biomol. Chem*. **2014**, *12*, 4093; Patent: 3243/DEL/2013).



Synthesis of harmonine, a chemical weapon of ladybird beetles: Three novel and different synthetic routes were developed to access the defense alkaloid harmonine. The developed routes are simple and practical to access harmonine and its analogues (*RSC Adv*. **2014**, *4*, 30923; Patent: 1845/DEL/2014).



First synthesis of nitrosporeusines: The natural products nitrosporeusins A and B were isolated by Lin and co–workers and showed very good inhibitory activity against the H1N1 virus. The unprecedented skeleton with multiple biological activities prompted to take up this molecule as a synthetic target. The total synthesis was accomplished and its library of molecules using very simple and scalable chemistry (*Tetrahedron Lett.* **2015**, *56*, 1252; Patent(s): 2815/DEL/2014, 2816/DEL/2014).



Healthcare

Natural products and methodology

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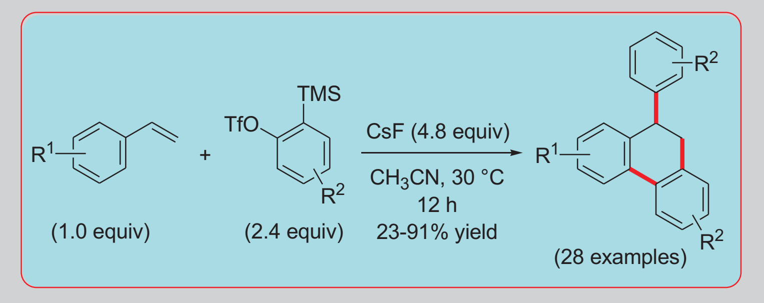
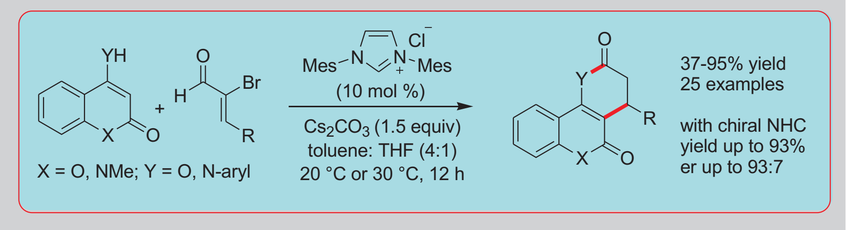
Transition-metal-free carbon-carbon bond-forming reactions using aryne chemistry and N-heterocyclic carbene organocatalysis: The transition-metal-free carbon-carbon bond-forming reactions using arynes resulted in the one-pot construction of molecular complexity, which was applied for the synthesis of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

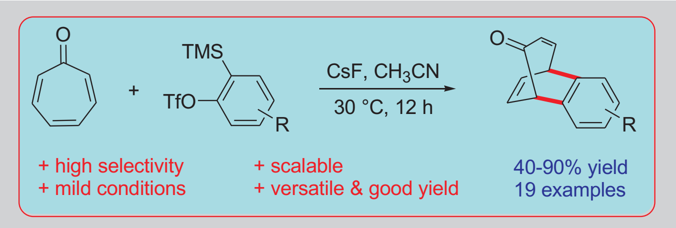
Efficient synthesis of 9-aryl dihydrophenanthrenes by a cascade reaction involving arynes and styrenes: A mild, general and transition-metal-free protocol was reported for the synthesis of 9,10-dihydrophenanthrenes. The aryne generated by the fluoride-induced 1,2-elimination of 2-(trimethylsilyl)aryl triflates undergone an efficient cascade reaction initiated by the Diels-Alder reaction with the differently substituted styrenes leading to the formation of 9-aryl 9,10-dihydrophenanthrene derivatives in moderate to good yields (*Org. Lett*. **2014**, *16*, 676).



Synthesis of functionalized coumarins and quinolinones by NHC-catalyzed annulation of modified enals with heterocyclic C–H acids: The N-Heterocyclic carbene (NHC) catalyzed lactonization and lactamization of 2-bromoenals with heterocyclic C–H acids proceeding via the α, β-unsaturated acyl azolium intermediates were demonstrated. The reaction furnished coumarin- or quinolinone-fused lactone/lactam derivatives (*J. Org. Chem*. **2014**, *79*, 4245).

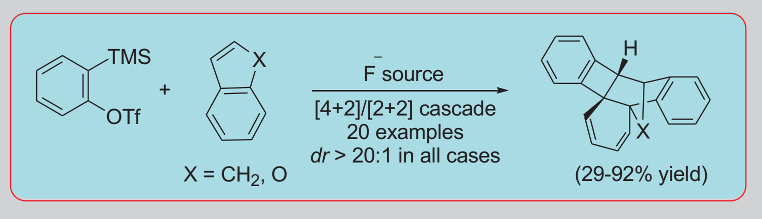


Diels-alder reaction of tropones with arynes: Synthesis of functionalized benzobicyclo [3.2.2] nonatrienones: A new procedure for the mild, practical and scalable Diels-Alder reaction of tropones with arynes was reported. Differently substituted tropones undergone selective [4+2] cycloaddition with arynes generated in situ by the fluoride-induced 1,2-elimination of 2-(trimethylsilyl)aryl triflates, allowing the formation of functionalized benzobicyclo[3.2.2]nonotrienone derivatives in moderate to good yields. In addition, the photophysical properties of the cycloadducts were presented (*J. Org. Chem*. **2014**, *79*, 4757).



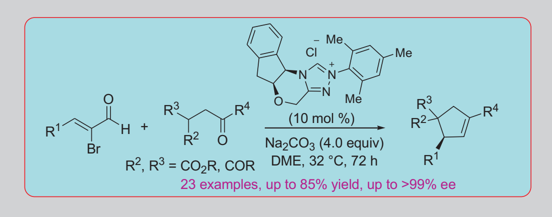
Natural products and methodology

Tandem [4+2]/[2+2] cycloaddition reactions involving indene or benzofurans and arynes: The reaction of arynes with indene/benzofurans was developed. The arynes generated from 2-(trimethylsilyl)aryl triflates by the fluoride induced 1,2-elimination reacted with indene or various benzofurans proceeding via a cascade reaction involving the Diels-Alder reaction and a [2+2] cycloaddition reaction. The tandem process afforded functionalized dihydrobenzocyclobutaphenanthrenes in moderate to good yields. Moreover, the method was utilized for the one-pot synthesis of benzo[b]fluoranthene (*Org. Lett.* **2014**, *16*, 3576).

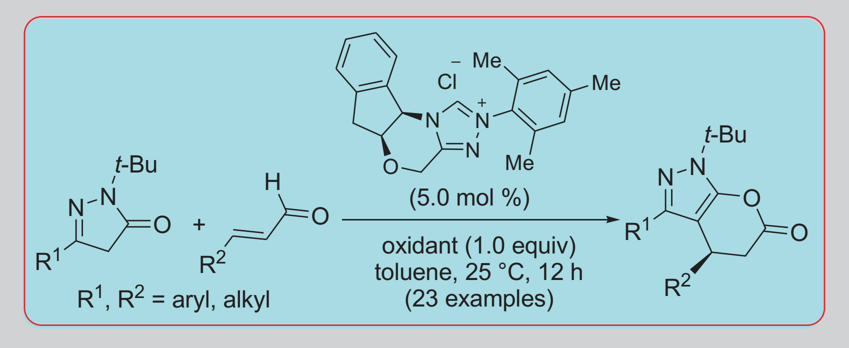


Multicomponent reactions involving phosphines, arynes and aldehydes: The phosphine triggered multicomponent reaction of arynes and aldehydes was reported, which took place via the formal [3+2] cycloaddition of initially generated 1,3-zwitterion from phosphine and aryne with aldehydes. The reaction resulted in the formation of diverse benzooxaphosphole derivatives in good yields (*Chem. Commun*. **2014**, *50*, 11389). Additionally, an operationally simple MCC involving in situ generated arynes from 2-(trimethylsilyl)aryl triflates, phosphines, and various acyclic and cyclic activated carbonyl compounds was developed for direct access to diverse (spiro)benzoxaphosphole derivatives in moderate to good yields (*Org. Lett*. **2014**, *16*, 5132).

NHC-catalyzed enantioselective synthesis of functionalized cyclopentenes: Highly enantioselective NHC-organocatalyzed synthesis of functionalized cyclopentenes proceeding via α, β-unsaturated acyl azolium intermediates was demonstrated. The organocascade reaction of modified enals with malonic ester derivatives having a γ-benzoyl group involved the Michael-intramolecular aldol-β-lactonization-decarboxylation sequence to deliver cyclopentenes in good yields and excellent ee values (*Chem. Commun.* **2014**, *50*, 14539).



Enantioselective synthesis of functionalized pyrazoles by NHC-catalyzed reaction of pyrazolones: The N-heterocyclic carbene (NHC)-organocatalyzed enantioselective annulation reaction of pyrazolones with α,β-unsaturated aldehydes proceeding via the chiral α,β-unsaturated acyl azolium intermediates under oxidative conditions was presented. The reaction afforded dihydropyranone-fused pyrazoles in moderate to good yields and good er values under operationally simple and base-free conditions (*Org. Lett*. **2015**, *17*, 1417).



Healthcare

Natural products and methodology

Asymmetric synthesis of biologically important compounds

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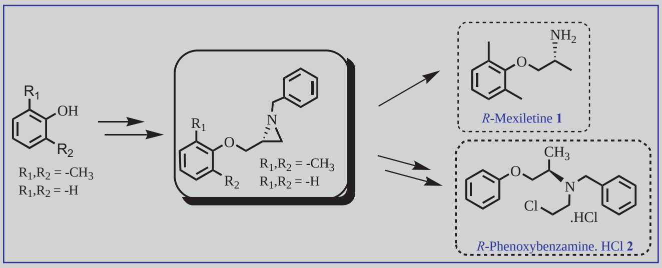
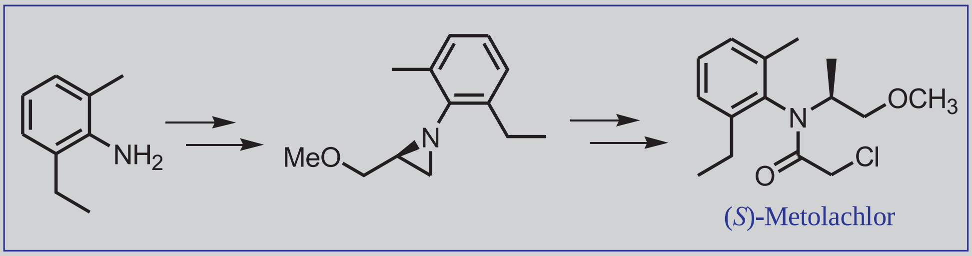
The research was focused on the asymmetric synthesis of biologically important compounds, especially chiral drugs employing newly developed enantioselective strategies.

Synthesis of (*R*)-mexiletine and (*R*)-phenoxybenzamine hydrochloride: Mexiletine (Mexitil®) is an important β–amino aryl ether class of drug used in the treatment of arrhythmia, allodynia and myotonic syndromes. However, (*R*)–isomer of mexiletine (**1**) is more potent than the (*S*)–isomer. Similarly, phenoxybenzamine hydrochloride (Dibenzyline®) is an important drug in the α–blocker series, widely used in the treatment of hypertension. However, the (*R*)–isomer of phenoxybenzamine hydrochloride (**2**) is 14.5 times more potent than its (*S*)–isomer. A new and efficient route for the synthesis of (*R*)–mexiletine (**1**) and (*R*)–phenoxybenzamine HCl (**2**) was developed via controlled reductive ring opening of chiral aziridine intermediate as a key step. Simple procedures, ready availability of the starting materials, good yield and high enantiopurity are some of the salient features of this approach (*Tetrahedron Lett.* **2015**, *56*, 5269).



Synthesis of (*S*)-metolachlor: Metolachlor (Dual®) is one of the most important grass herbicides for use in maize and a number of other crops. It is an *N*–chloroacetylated, *N*–alkoxyalkylated ortho–disubstituted aniline. Enantio–merically enriched form of metolochlor namely Dual Magnum® replaced the racemic mixture in the market, leading to a reduction of the environmental load by ca. 40%. The synthesis of (*S*)–metolochlor (active ingredient of Dual Magnum®) was accomplished in high enantiopurity starting from 2–ethyl–6–methyl aniline (Patent: PCT WO 2014/037962A1).



Applications of NMR spectroscopy

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The research was aimed to address various structural problems in the area of chemical science and material science for structure–property correlation applying methodologies based on solid state and solution state NMR spectroscopy.

Structural chemistry: Structural features of a number of synthetic peptide oligomers mimicking biomolecular structural architectures resulting from non bonding interactions were investigated by modern NMR spectroscopic techniques. It was focused mainly on building blocks containing proline, anthranilic acid or orthanilic acid. The oligomers of these systems were shown to possess different back bone conformations driven by its hydrogen bonding patterns. NMR techniques were used to revise the proposed structure of mycalol, an anticancer marine natural product (*Org. Biomol. Chem.* **2014**, *12*, 774; *RSC Adv.* **2014**, *4*, 13018; *Org. Lett.* **2015**, 1652).

Healthcare

Natural products and methodology

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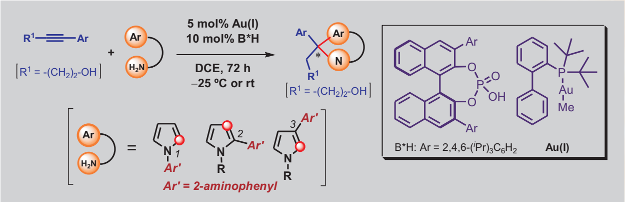
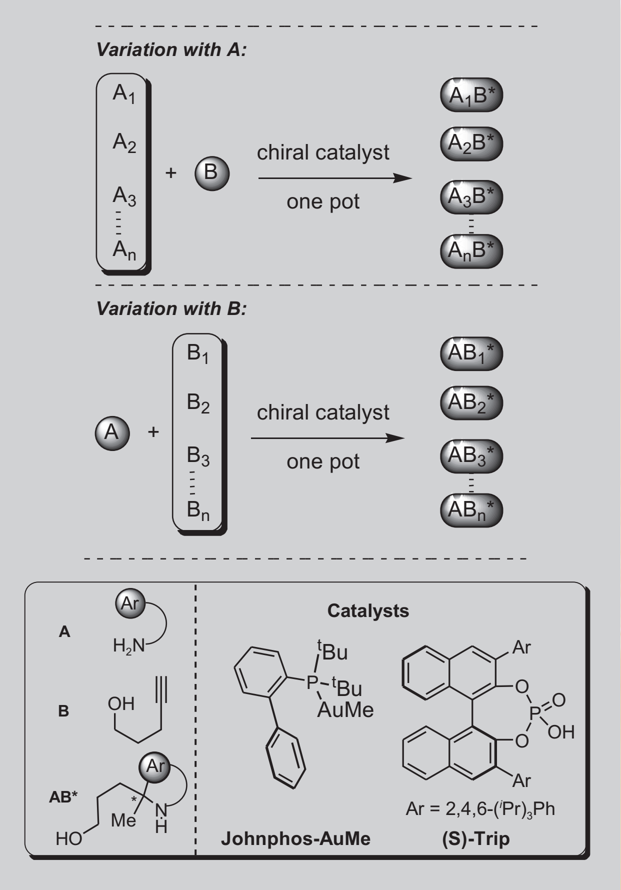
Diversity oriented synthesis: The synthesis of small organic molecules as probes for discovering new therapeutic agents has been an important aspect of chemical-biology. A new form of diversity oriented synthesis (DOS) namely "relay catalytic branching cascade" (RCBC) was introduced by the research group wherein a common type of starting material being reacted with several scaffold building agents (SBAs) to obtain structurally diverse molecular scaffold under the influenceof catalysts. It was reported that catalyst dependant selectivity in RCBC - the reaction of common type of substrate with SBAs gave two different types of the type of catalyst used. The reaction of common type of molecular scaffolds and their formation was essentially dependant on substrates (alkynols, A) with variables (bis-nucleophiles, B) gave two different types of molecular scaffolds (AB^a and AB^b) and their formation was essentially dependant on the type of catalyst used (*Chem. Eur. J.* **2015,** *21*, 2319).

As a part of interest in asymmetric catalysis research group found a catalytic enantioselective hydroamination-hydroarylation of alkynes under the catalysis of (R$_3$P)-Au-Me/(*S*)-TRIP. The alkyne was reacted with a range of three pyrrole-based amino-aromatics to give pyrrole-embedded aza-heterocyclic scaffolds bearing quaternary carbon centers. The presence of hydroxyl group in the alkyne tether was turned out to be very crucial to obtain products in high yields and ee's. The mechanism of enantio-induction was established by carefully conducted experimental and computational studies (*Chem. Eur. J.* **2015**, *21*, 975).



A strategy was reported to access the enantioenriched molecules in a single operation which may find use in combinatorial chemistry. The alkynols B reacted with various scaffold building agents (SBAs) A$_1$, A$_2$, A$_3$...An under Au(I)/chiral Brønsted acid binary catalyst system to give A$_1$B*, A$_2$B*, A$_3$B*...A$_n$B* (Fig 3). Similarly, SBAs A reacted with various alkynols B$_1$, B$_2$, B$_3$...B$_n$ under the same reaction condition to produce AB$_1$*, AB$_2$*, AB$_3$*...AB$_n$*. The approach was very interesting as one can access fairly large number of enantioenriched scaffolds in one-pot. No such technique has been reported to assess the enantioenriched compounds, especially heterocycles of pharmacological interest (*Chem. Eur. J.* **2015**, *21*, 3580).



Healthcare

Natural products and methodology

Development of synthetic methods and total synthesis of natural products

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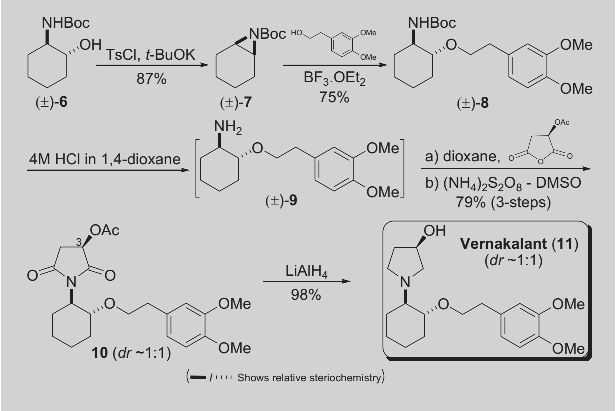
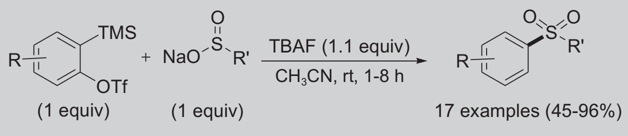
The objective was to develop the novel methodologies and their application in the total synthesis of drugs and bioactive natural products.

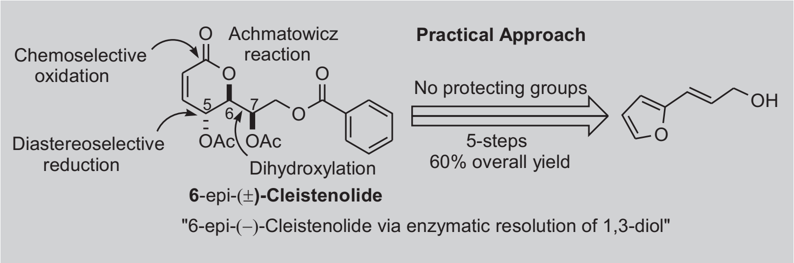
Practical synthesis of vernakalant drug for cardiac arrhythmia: Vernakalant was discovered by Cardiome /Astellas Pharma Inc. and later developed as a novel antiarrhythmic agent for the treatment of atrial fibrillation (cardiac arrhythmia leading to strokes) in collaboration with Merck & Co., Inc. Its intravenous formulation was approved as a drug by the European agency (EMEA) under the trade name of Brinavess (Cardiome/Merck). A concise and practical synthesis method was developed for the drug vernakalant (11) in 5-steps with 51% overall yield (*Beilstein J. Org. Chem*. **2015**, *11*, 1008; Patent: IN 2999/DEL/2014).



Transition-metal-free C-S bond formation: A facile access to aryl sulfones from sodium sulfinates via arynes: An efficient transition-metal-free process was demonstrated, wherein a broad range of alkyl/aryl/heteroaryl sodium sulfinates reacted with varyingly substituted aryne precursors (*o*-silyl aryl triflates) under mild reaction condition to afford structurally diverse sulfones in good to excellent yields (*Org. Lett.* **2014**, *16*, 3836; Patent: WO PCT/IN2014/000772).



Protecting group-free diastereoselective total synthesis of 6-epi-(±)-Cleistenolide and chemoenzymatic synthesis of 6-epi-(–)-Cleistenolide: A short, efficient, practical and protecting group-free diastereoselective total synthesis of 6-epi-(±)-cleistenolide (1) was achieved in five steps with 60% overall yield. The application of the chemoenzymatic approach also furnished 6-epi-(–)-cleistenolide (1) (>99.9% ee). The Achmatowicz reaction, chemoselective oxidation of secondary alcohol, diastereoselective 1,3-anti reduction of β-hydroxy ketone and an enzymatic resolution of 1,3-diol were the key features of this linear total synthesis (*Eur. J. Org. Chem*. **2014**, 8049).



Healthcare

Natural products and methodology

Silver acetate co-catalysis of the Mizoroki-Heck reaction with 1,1-disubstituted olefins

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The objective was to explore the AgOAc co–catalyzed Mizoroki–Heck reaction of 1,1–disubstituted olefins, diarylethenes, atropate and itaconate esters, route to Tamoxifen analogue precursors and benzylidene succinates.

AgOAc catalyzed Mizoroki-Heck reaction of 1,1-disubstituted olefins: Tamoxifen and ferrocifen are important anti breast cancer drugs with high activity. Various analogues were synthesized and tested for anti–cancer activity. The Mizoroki–Heck reaction of stilbenes was used as a good methodology for the synthesis of tamoxifen in high overall yields. The reaction further provided a catalytic methodology for the synthesis of various analogues library of tamoxifen and related drugs. Beller *et al* had showed the use of the Mizoroki–Heck reaction in the synthesis of trisubstituted olefins as important biologically active molecules. Itaconate esters were shown to be good partners for the Mizoroki–Heck reaction with aryl halides and triflates. The resulting 2–(E)–benzylidene succinates were reduced by asymmetric hydrogenation to give chiral benzyl succinates which were important structural motifs for drug molecules. The AgOAc co–catalyzed Mizoroki–Heck reaction of aryl iodides with 1,1–disubstituted olefins like diphenyl ethene, ethyl atropate and itaconate ester provided an expedient route to such trisubstituted olefins.

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Synthesis of squalamine and its analogues and their anticancer activity: Insufficient amounts of squalamine are available from natural resources for mechanistic studies, coupled with clear need for the preparation of analogs prompted research group to undertake the synthesis of squalamine and its analogues.

Synthesis of nine novel bile acid hydrazides was carried out and their gelation properties were studied. Three compounds were found to undergo self–assembly leading to organogelation in certain organic solvents. The properties of one of these gels were thoroughly investigated by conventional methods typical for molecular gel studies. Rheological study of these gels was also carried out. Hydrogen bonding study of the hydrazide group was done with help of IR and temperature and concentration dependent proton NMR. Morphology of the xerogels was studied using the E–SEM images (*New J. Chem*. **2015**, *39*, 453).

New fluconazole analogues containing two units of 1,2,3–triazole (A) and the others containing amide linkage (B) were synthesized and showed very good in–vitro as well as in–vivo antifungal activity. A hemolysis study of the most active two compounds showed that both compounds did not cause any hemolysis at the dilutions tested. These compounds did not exhibit any toxicity to L929 cells at MIC and lower concentrations. In the docking study, the overall binding mode of 6e and 13j appeared to be reasonable and provided a good insight into the structural basis of inhibition of Candida albicans Cyp51 by these compounds (*Org. Biomol. Chem*. **2015**, *13*, 6551).

A new neutral alumina supported copper iodide catalyst was prepared for microwave–assisted synthesis of 1,4–disubstituted 1,2,3–triazoles via three–component reaction in water. The new catalyst was fully characterized by FTIR, solid state NMR, SEM, EDX, TGA, and XRD. The key features of this procedure were use of water as a solvent, recyclability of the catalyst up to eight runs without appreciable loss of activity and high yields of products. Broad scope of this protocol showed by synthesis of a variety of diversely substituted 1,2,3–triazoles and also two component azide–alkyne click reaction (*Asian J. Org. Chem*. **2015**, DOI: 10.1002/ajoc.201500189).

Healthcare

Natural products and methodology

Biosurfactants, self-assemblies, quorum quenching and drug delivery

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Degradation of quorum sensing signals by *Kluyvera-citrophila* penicillin G acylase (KcPGA): A new dimension for amidase activity of KcPGA was reported by demonstrating its ability to cleave bacterial quorum sensing signal molecules, acyl homoserine lactones (AHL) with acyl chain length of 6–8 with or without oxo-substitution at third carbon position. AHL degrading capability of KcPGA was obtained using CV026 based bioassay method based on quantifying the violacein produced. 3-oxo-C6 HSL was the best substrate for KcPGA followed by C6 HSL. Modeling and docking studies on active site of enzyme revealed the fitting of AHLs perfectly within the hydrophobic pocket of the enzyme active site (*Enzyme Microb. Tech.* **2014**, *5*, 1; Patent: PCT/IN 2014/ 000265 WO).

Micron to nano-curcumin by sophorolipid co-processing and its application: Co-sonication of curcumin and acidic sophorolipid in aqueous solution led to a dramatic enhancement of curcumin bioavailability through size reduction and encapsulation. The cytotoxicity effects of curcumin on breast cancer cell lines, MCF-7 and MDA-MB-231 were significantly enhanced by the formation of its complex with sophorolipid. The relative cytotoxicity of curcumin with its SL(A) complex was more due to the presence of the glucose moiety. The results further suggested that sophorolipid based formulations, which solubilized and nanoencapsulated the curcumin after lipid digestion, showed great potential for curcumin cell entry (*RSC Adv.* **2014**, *4*, 60334; Patent: 2076/DEL/2014).

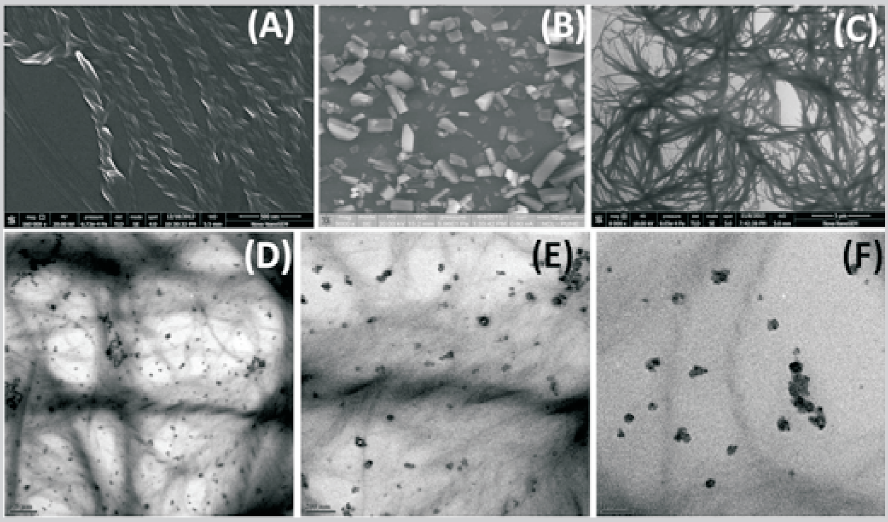

Fig. 1: A) SEM of SL(A) showing ribbon structure; (B) SEM of curcumin showing chunks of. B) undefined structure; and (C) SEM of SL(A) + curcumin exhibiting morphological change vis a vis SL (A); (D–F) high resolution TEM images of SL(A) + Cur (scale bar sizes for A, B, C, D, E, F are 0.5, 10, 5, 0.5, 0.2 and 0.1 mm respectively)

UV-assisted size sampling and antibacterial screening of *Lantana* leaf extract: The silver nanoparticles were synthesized using *Lantana camara* leaf extract. The silver nanoparticles showed very high antibacterial activity against *E coli* (Gram -ve) and S. aureus (Gram +ve), at very low concentrations (50 ppm Ag nanoparticles) (*RSC Adv.* **2015**, 5, 24513).

Sophorolipid assisted tunable and rapid gelation of silk fibroin to form porous biomedical scaffolds: Three dimensional polymer hydrogels are used as scaffolds and drug delivery vehicles for biomedical applications. Silk fibroin (SF) is a promising candidate in this area. However, SF has a long gelation time in weeks that can be reduced only by non-physiological treatments or by addition of chemical and non-biodegradable polymer and/or surfactant. The accelerated gelation of SF under physiological conditions was reported using sophorolipid (SL) as a gelling agent. SL and SF are completely miscible yielding a very clear solution. Interestingly, this clear solution gels in a time span of just a few minutes. The hydrogels so formed showed pore architecture, porosities and mechanical stability which support adheration and extensive proliferation of tissue cultured mouse fibroblast cells (*RSC Adv.* **2015**, *5*, 33955; Patent: 1248/DEL/2014).

Healthcare

Natural products and methodology

Isolation and methodology development

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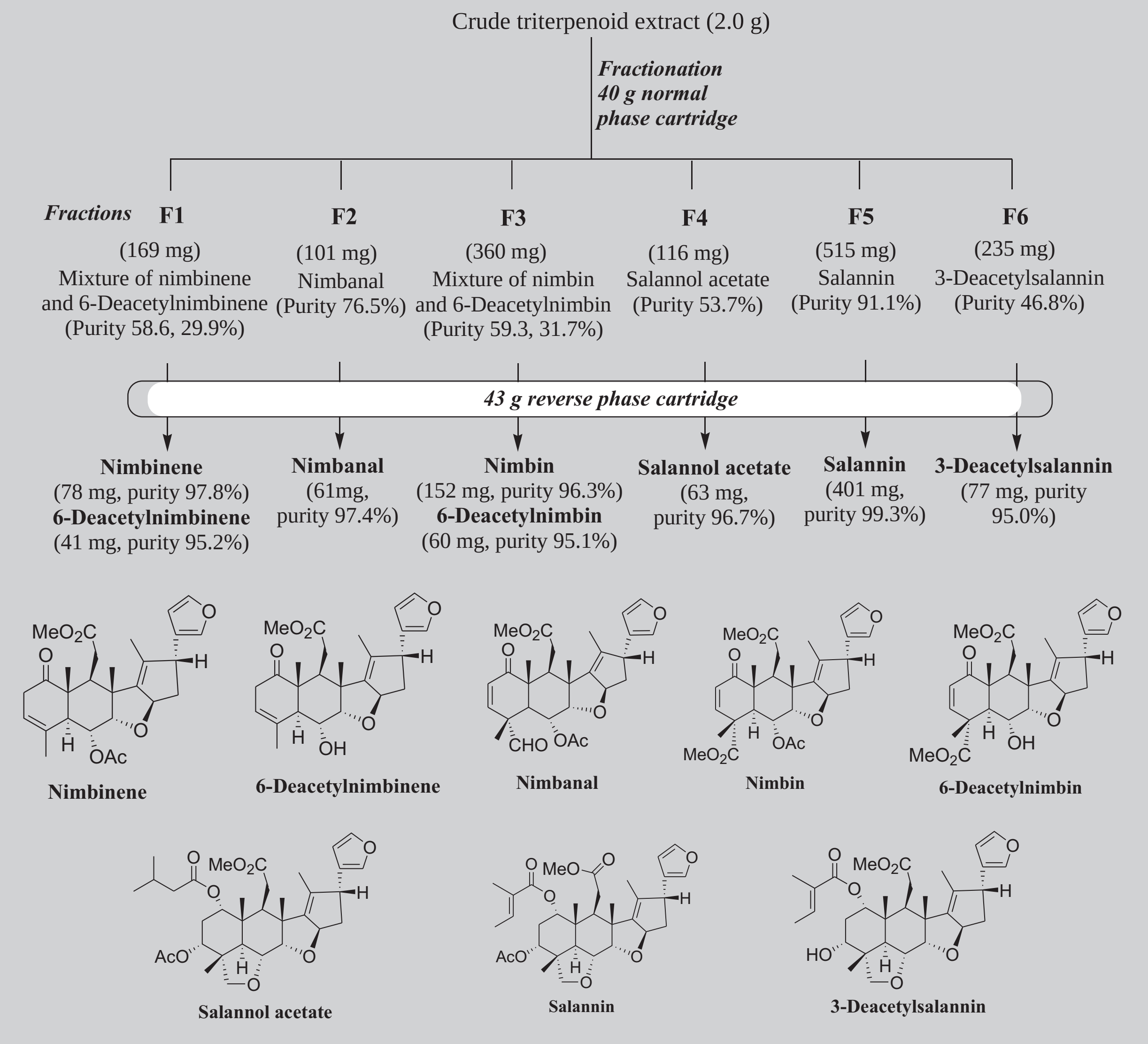
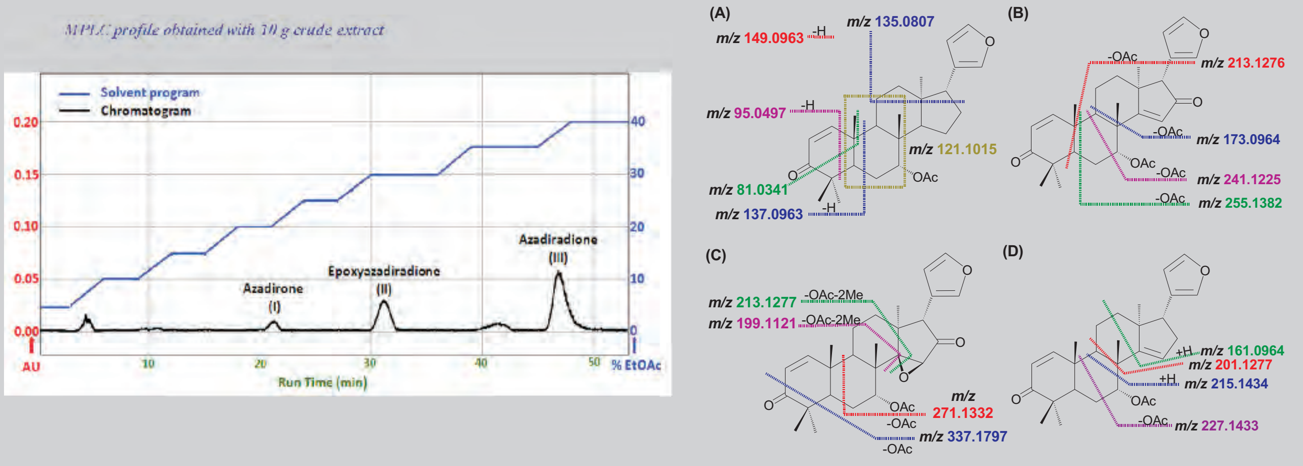
Method development for isolation of Neem limonoids and their characterization: The group has developed a medium pressure liquid chromatography (MPLC) method for the isolation of bioactive Neem Limonoids (triterpenoids) by using normal phase and reverse phase prepacked silica gel columns and were characterized using Ultra performance liquid chromatography-electrospray ionization-quadrupole-MS/MS spectrometry.



The procedure was efficient with respect to rapidity and purity of triterpenoids isolated. Characterization of MS/MS spectra and structure-fragment correlations of the daughter ions (generated from [M+H] + precursor ions) corresponding to isolated triterpenoids were studied using ESI (+)-quadrupole / orbitrap-MS/MS spectrometry with an optimized stepped normalized collision energy. The applicability of developed MS/MS based identification technique, was utilized for the identification of studied triterpenoids in the extracts of stem and bark tissues from Neem. Comparison of the retention time and ESI (+)-MS spectra of pure triterpenoids, presence of individual molecules was done.

Natural products and methodology

Expedient preparative isolation, quantification and characterization of limonoids from Neem fruits: Major basic limonoids from Neem fruits such as azadirone, epoxyazadiradione and azadiradione were isolated in preparative scale using an automated and MPLC-based protocol. They were individually quantified using HPLC. An LC–ESI–MS/MS-based rapid identification technique was developed for the high-throughput screening of these limonoids in phytochemical extracts (*J. Chromatogr. A* **2014,** 1366).



MPLC profile obtained with 10 g crude extract, structure–fragment relationships of common m/z obtained for basic limonoids (I, II and III) (A); structure–fragment correlations of diagnostic peaks for (B) azadiradione III, (C) epoxyazadiradione II and (D) azadirone I

Healthcare

Screening methods and bioassays

Development of rapid analysis methods for profiling of metabolite disease markers

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The objective was to develop and validate high throughput methods for rapid identification and quantification of metabolites with clinical relevance. The developed methods showed potential use in disease diagnostics and in investigations to employ large population cohorts to understand the molecular basis of disease.

Mass spectrometry and metabolite profiling: Profiling and measurement of metabolites from human biological fluids has significance in disease diagnostics and therapeutics. Mass spectrometry (MS) allows accurate molecular profiling of metabolites at trace quantities and has become the most important tool in metabolomics research, and more recently in diagnostics laboratories. However, currently used gas and liquid chromatography coupled MS methodologies have severe throughput limitations. Matrix assisted laser desorption ionization mass spectrometry (MALDI MS) presents a rapid and high throughput alternative. Recent advances that have made high resolution MS (HRMS) systems accessible as a routine technique allow direct analysis of established metabolite markers using MALDI MS.

Cost efficient, rapid, and high throughput MALDI MS analysis: Research group used MALDI MS previously for the quantitative detection of triazine contaminants from milk and water. The results were validated using existing HPLC MS methods. About 288 samples were analyzed within a few hours resulting in significant throughput increase over HPLC methods. Direct MS analysis using MALDI MS also required much less solvent consumption and instrumental maintenance when compared to electro spray ionization (ESI) methods. A user friendly algorithm, 'MQ' was also developed for batch processing of sample raw data and seamless accurate mass-based unknown determination (*Anal. Methods* **2011**, *3*, 2360).

Direct determination of isomeric dimethyl arginine metabolites from human urine: Isomeric asymmetric and symmetric dimethyl arginine (ADMA and SDMA) are metabolic markers of cardiovascular and chronic kidney diseases. ADMA and SDMA were determined using MALDI MS simultaneously with no prior chromatographic separation. The DMA isomers yielded unique product ions at m/z 46 and m/z 172 that were used for HRMS quantitation. Calibrations yielded good linearity and reproducibility along with excellent recoveries for QC samples. ADMA and SDMA determined in urine from healthy subjects (n = 11) were found to be in agreement with previously reported physiological levels (Fig. 1). Efforts are underway to implement the method in clinical analysis (*Anal. Methods* **2014**, DOI:10.1039/C4AY00309H).

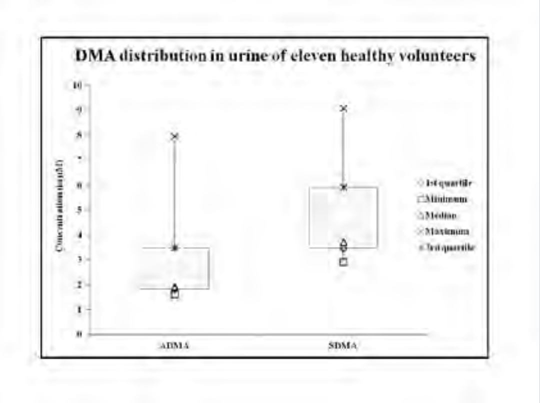

Fig. 1: Box whisker plot representing absolute quartile distribution of ADMA and SDMA in urine of eleven individual healthy human subjects

The analysis showed that ADMA and SDMA were present in the range of 1.6–8 μM and 2.9–9.1 μM, respectively. Quartile distribution showed the majority of distribution (area in box bordered by 1st and 3rd quartiles). Majority distribution of the analytes was in the range of 2-3.5 μM and 4-6 μM for ADMA and SDMA, respectively.

Healthcare

Screening methods and bioassays

Advanced glycation end products

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Development of diagnostic fragment ion library for quantification of glycated peptides of albumin: Human serum albumin (HSA), a highly abundant plasma protein, readily undergoes glycation and suggested as an alternative diagnostic marker to HbA1c for monitoring glycemic status in diabetes. Therefore, quantification of glycated HSA is of utmost clinical significance. Fragment ion library was constructed for quantification of glycated peptides of albumin (Fig. 1). Targeted SWATH analysis of diabetic clinical plasma led to identification and quantification of 13 glycated peptides of albumin. Five lysine sites namely K549, K438, K490, K88 and K375 were observed to be highly sensitive for glycation modification. The peptides involving these lysine sites could be potential novel markers to assess the degree of glycation in diabetes (*Mol. Cell. Proteomics* **2015,** *14*, 2150).

Reduction of AGEs and activation of DAF-16 by Rifampicin in *Caenorhabditis elegans*: It was showed that rifampicin reduced the glycation of important cellular proteins *in vivo*, and increased *C. elegans* life span by using mass spectrometry. Genetic studies using mutants suggested that rifampicin requires DAF–18 for eliciting longevity in worms. Interestingly, the drug translocated DAF–16 to the nucleus and transcribed its target genes. Together, the data suggested that the dual ability to reduce glycation *in vivo* and activate prolongevity processed thorough DAF–16 made rifampicin effective life span–extending interventions (*Aging Cell* **2015**, *14*, 463).

Investigation of phosphoproteome in RAGE signaling: Receptor for advanced glycation end products (RAGE) is implicated in pathogenesis of diabetes and its complications. It interacts with various ligands including AGE, amyloid β, S100 etc., and activates several signal transduction pathways through involvement of various kinases. RAGE activated kinases can phosphorylate multiple substrates depending upon their expression and localization, leading to altered cellular responses in different cell types and conditions. One such example is, glycogen synthase kinase 3 beta which is known to phosphorylate glycogen synthase, acts downstream to RAGE, and hyperphosphorylates microtubule–associated protein tau causing neuronal damage. The known substrates of RAGE activated kinases were analyzed, and the role of some of the important substrates involved in diseases was studied.

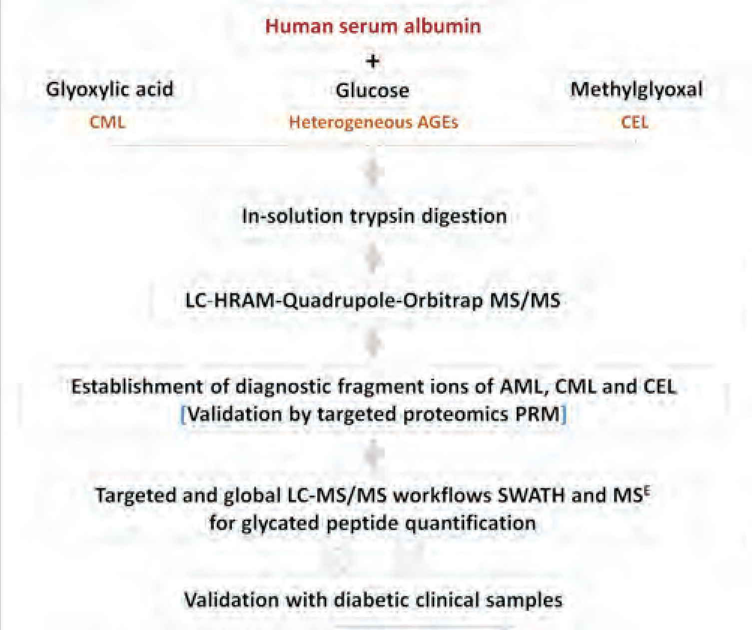

Fig 1: Workflow for targeted quantification of glycated peptides of albumin

Healthcare

Screening methods and bioassays

Human associated microbes

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Genome sequencing insights into human gut bacteria: Human stomach harbors trillions of microbes of various lineages across various geographies. *Helicobacter pylori* are a urease positive, gastric pathogen that causes gastric diseases. There is little information of prevalence of non–*H. pylori* bacteria. Isolation and genome sequencing of two strains of *Ochrobactrum intermedium* were undergone. It was isolated in urease positive gastric from Indian individual. Comparative genomic analysis of 2 strains revealed functional similarities with virulence related gene clusters present in *H. pylori* genomes, which probably might aid in its ability to persist in the human gastric mucosa (*FEMS Microbiol Lett*. **2014**, *359*, 12).

Detection of *Streptococuus tigurinus* from human oral cavity; a new and emerging player in oral health: *Streptococcus tigurinus* is a new member of the *Streptococcus viridians* group that was originally reported in infective endocarditis. A strain of *S. tigurinus* was isolated from subgingival plaque of a patient with periodontitis identified by 16S rRNA gene analysis, which was originally identified as *S. pluranimalium* by Vitek 2. This is the first report of isolation of *S. tigurinus* from the oral cavity of a periodontitis case. The oral cavity could be an ecological niche of *S. tigurinus* as well (*FEMS Microbiol. Lett*. **2014**, *357*, 131).

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Biotechnological applications of systematics and poly-phasic approaches: The classification of microorganisms on the basis of traditional microbiological methods (morphological, physiological and biochemical) creates a blurred image about their taxonomic status and thus needed further clarification. Hence, the methods now employed for bacterial systematics include, the complete 16S rRNA gene sequencing and its comparative analysis by phylogenetic trees, DNA–DNA hybridization studies with related organisms, analyses of molecular markers and signature pattern(s), biochemical assays, physiological and morphological tests. Collectively these genotypic, chemotaxonomic and phenotypic methods were applied to determine the taxonomic position of bacteria. Many novel bacterial species were proposed with this approach that include *Deinococcus enclensis* sp. nov., *Bacillus encimensis* sp. nov., *Nonomuraea indica* sp. nov., and *Exiguobacterium enclense* sp. nov (*Anton. Leeuw. Int. J. G.* **2015**, *107*,141, 433; *Int. J. Syst. Evol. Micr.* **2015**, *65*, 692; *J. Antibiot.* **2015**, *68*, 491).

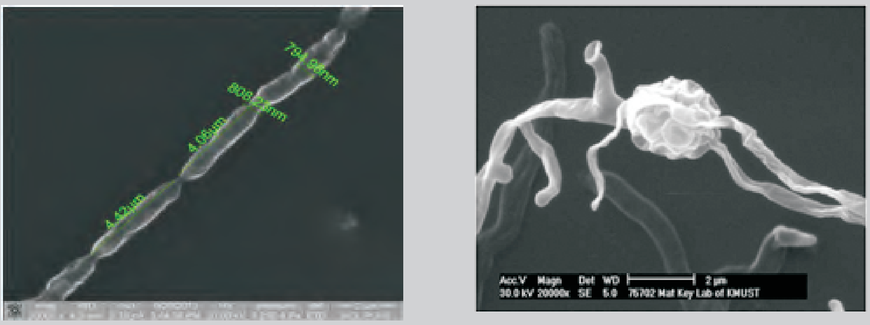

Fig. Scanning electron microscope images

Healthcare

Chemical biology

Development of novel molecular transporters for cargo delivery to skin

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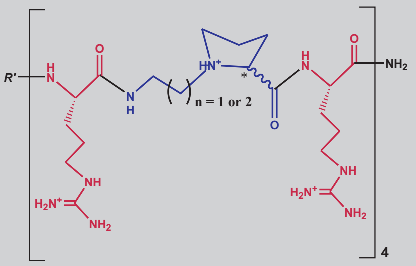
The objectives of the project were to design and synthesize novel molecular transporters enabling enhanced cargo delivery, with special focus on skin as the target. Polycationic (R–X–R)–motif oligomers were the most successful at cell penetration and cargo delivery. This study dealt with the effect of controlled constraint and stereochemistry of the spacer (–X–) on the cell–penetrating properties.

(R-X'-R)-motif α-ω-α-cell-penetrating peptides: Novel *N*-aminoalkyl-proline-derived spacers (X') were incorporated in (R-X'-R)-motif cell-penetrating α-ω-α-peptides. It resulted in molecular transporters with superior efficiency at transporting pDNA into cells. The chirality together with the hydrophobicity and flexibility derived from the spacer chain showed influence on their cell–penetrating and cargo delivery properties. The peptides containing *N*–(3–aminopropyl)–D–proline spacers were found to be the best at cell penetration and cargo delivery in the study (*Bioorg. Med. Chem. Lett.* **2014**, *24*, 4198).



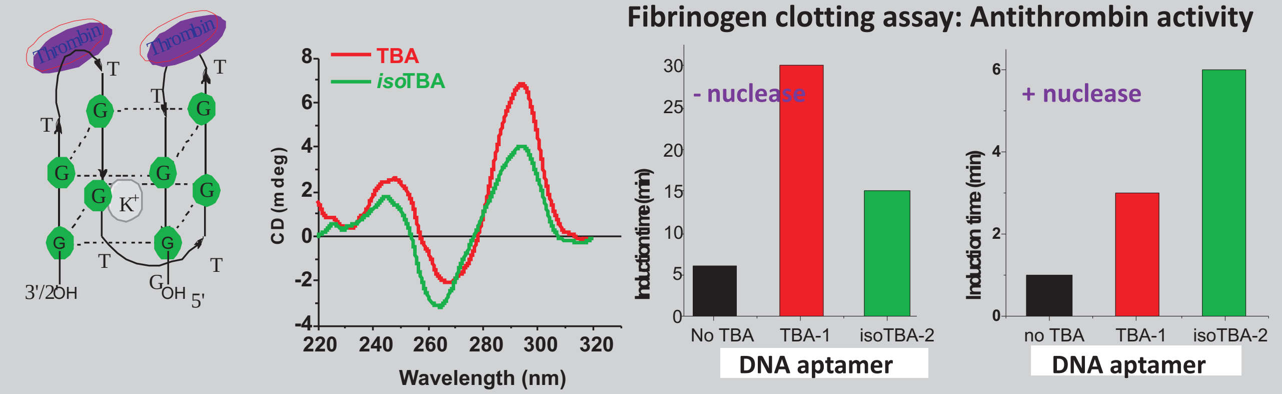
(**R**-**X'**-**R**)-motif α-ω-α-CPPs

cf-(R-aeLP-R)$_4$-NH$_2$ (**I**)
cf-(R-aeDP-R)$_4$-NH$_2$ (**II**)
cf-(R-apLP-R)$_4$-NH$_2$ (**III**)
cf- (R-apDP-R)$_4$-NH$_2$ (**IV**)
cf-(R-Ahx-R)$_4$-NH$_2$ (**V**)
Ac-Phe-(R-aeDP-R)$_4$-NH$_2$ (**VI**)
Ac-Phe-(R-apDP-R)$_4$ -NH$_2$ (**VII**)
Ac-Phe-(R-Ahx-R)$_4$ -NH$_2$ (**VIII**)

Fig. 1: Synthesized peptides of the study

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

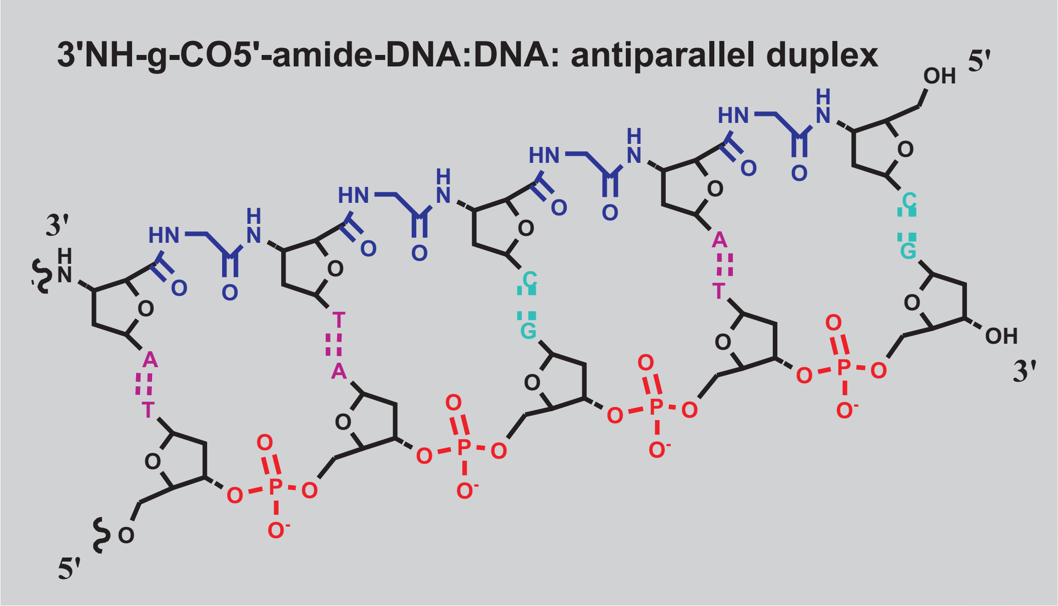
2'-5'-Linked isoDNA G-quadruplexes: Replacement of the 3'–5'–phosphodiester linkages in the DNA thrombin–binding aptamer (TBA) by 2'–5'–phosphodiesters led to a topologically similar antiparallel G–quadruplex that not only bound to thrombin but was also able to perform the designed function of clotting inhibition. In the presence of nucleases, the inherently resistant 2'–5'–phosphodiester backbone was advantageous and could delay clotting and display an anticoagulant effect even better than the native TBA (*Chem. Commun*. **2014**, *50*, 605).



Chemical biology

β,γ-Substituted PNA: Stereochemistry-dependent switchable binding to target DNA and RNA were achieved. The PNAs with (R,R)-β,γ-bis-methoxymethyl substituted thymine were significantly improved the access of PNA to intracellular space. The poor water-solubility and cell uptake were significant shortcomings of the native unmodified aminoethylglycyl (aeg) PNA that improved the modification/substitution reported (*Chem. Commun.* **2015**, *51*, 7693).

Glycine-linked nucleoside-β-amino acids: Amide-linked sugar-amide DNA was designed and its challenging synthesis was achieved. Oligomers were found to display sequence-specific binding to DNA and RNA with better binding to RNA than DNA. It presented large scope for further development using different natural L-/D-amino acids (*Bioconjugate Chem*. **2015**, DOI: 10.1021/acs.bioconjchem.5b00296).



Membrane effects in receptor organization

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Membrane lipids, especially cholesterol play an important role in G protein-coupled receptor (GPCR) function. The molecular dynamics simulations were performed to explore the effect of cholesterol on several receptors and a general consensus molecular view is emerging. Several cholesterol interactions sites were identified on the receptor that were highly dynamic. The results suggested that the energy landscape of cholesterol-GPCR interactions corresponded to a series of shallow minima interconnected by low barriers. It was shown that these cholesterol effects modulate GPCR dimer structures. The lipid effects on receptor structure and organization represent a new frontier in GPCR research (*Biophys. J.* **2015**, *106*, 1290; *BBA Biomembranes* **2015**, *1848*, 1775; *Adv. Exp. Med. Biol.* **2015**, *842*, 247).

Diverse cellular functions are supported by membrane protein assemblies associated with the cell membrane. Although considered to be protein-mediated, membrane components are now being recognised as critical in modulating and dictating function. The effect of the lipid bilayer was studied in particular its composition on the association of transmembrane proteins. A new method based on ensemble of simulations was proposed and tested to analyse the association. The method on the polyalanine peptides was used to show that it is computationally more tractable. The group is now extending the methodology to study association in the growth factor receptors (*Phys. Chem. Chem. Phys*. **2015**, *17*, 1390; J. Chem. Theory Comput. **2015**, *11*, 2278).

Healthcare

Chemical biology

Biotransformation of natural products

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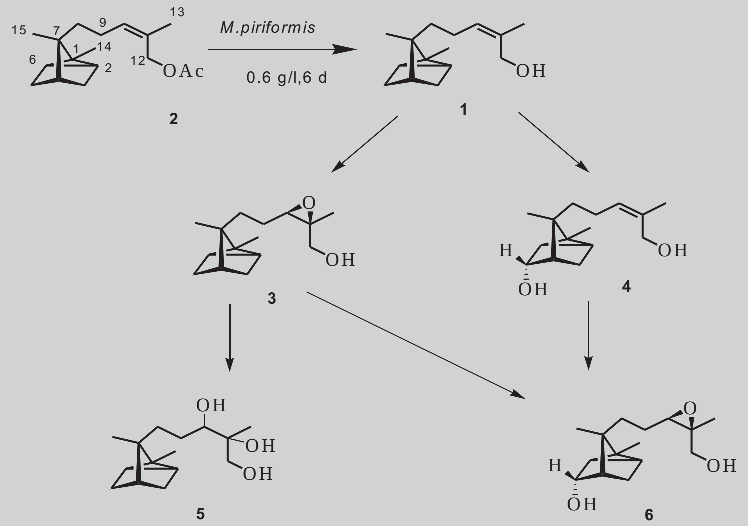
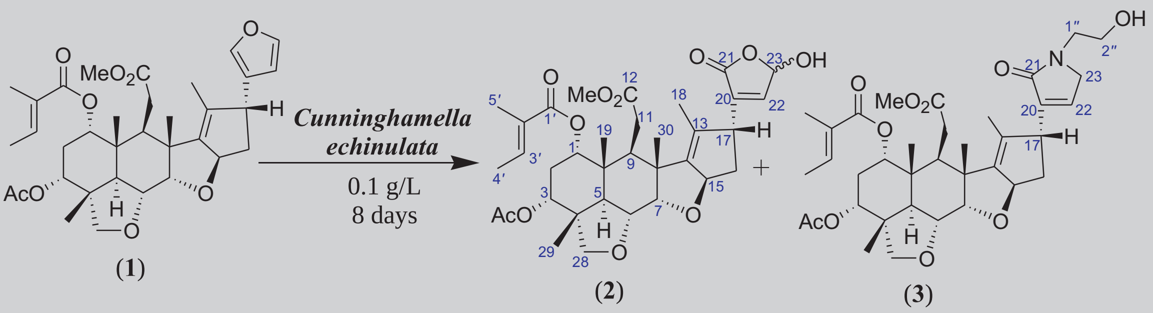
The focus of research group was on biotransformation of natural products mediated by fungus to obtain either novel metabolites of medicinal value or metabolites that acts as an intermediate in the biosynthetic pathway thereby aiding in the elucidation of biosynthetic pathway in its natural source.

Regio- and stereo-selective hydroxylation and epoxidation on (Z)-α-santalol: Four novel metabolites were characterized as 10,11–cis–β–epoxy–α–santalol, 5α–hydroxy–(Z)– α–santalol, 10,11–dihydroxy–α–santalol and 5α–hydroxy–10,11–cis–β–epoxy–α–santalol after biotransformation of (Z)–α–santalol using fungal strain *Mucor piriformis*. α- and β-isomers of 10,11-cis-epoxy-α-santalol were resolved efficiently using Amano PS lipase from *Burkholderia cepacia* (*Org. Biomol. Chem.* **2014**, *12*, 1048).



A pathway for biotransformation of α-santalyl acetate (2) into 10,11-cis-β-epoxy-α-santalol (3), 5α-hydroxy-(Z)-α-santalol (4), 10,11-dihydroxy-α-santalol (5) and 5α-hydroxy-10,11-cis-β-epoxy-α-santalol (6) with Mucor piriformis

Functionalization of salannin, a insecticidal limonoid from Neem: Rare and novel bioconversion of Salannin was efficiently converted by fungal system, *Cunninghamella echinulata* into two metabolites, where the C–17 furan moiety was transformed into γ–hydroxybutenolide (salanninolide) and N–(2–hydroxyethyl)–α,β–unsaturated–γ–lactam (salanninactam) analogues. Present studies indicated salanninolide to be a metabolite in the C–secolimonoid biosynthetic pathway (*RSC Adv.* **2014**, *4*, 27661).

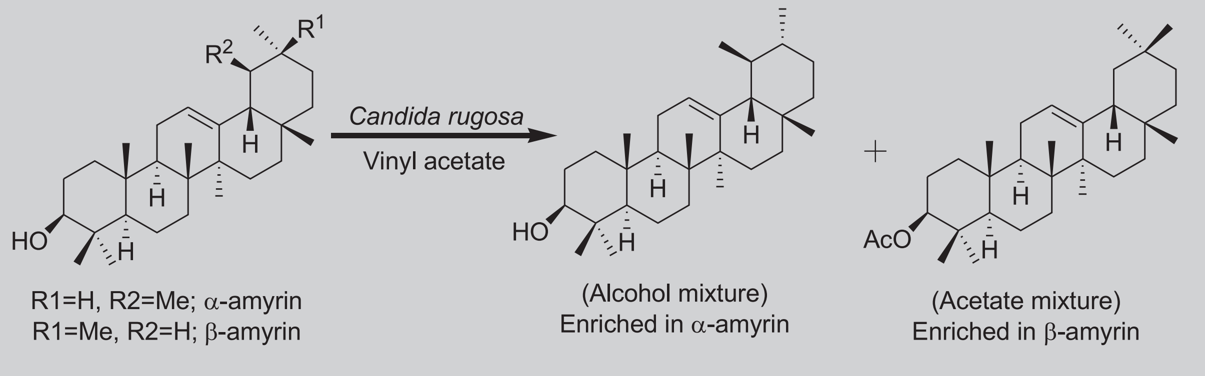


Biotransformation of Salannin (1) by Cunninghamella echinulata into salanninolide (2) and salanninactam (3)

Lipase mediated separation of triterpene structural isomers, α- and β-amyrin: Pentacyclic triterpenoids α–and β–amyrin from the latex of *Plumeria obtusa* possess a wide range of biological and pharmacological activities but high

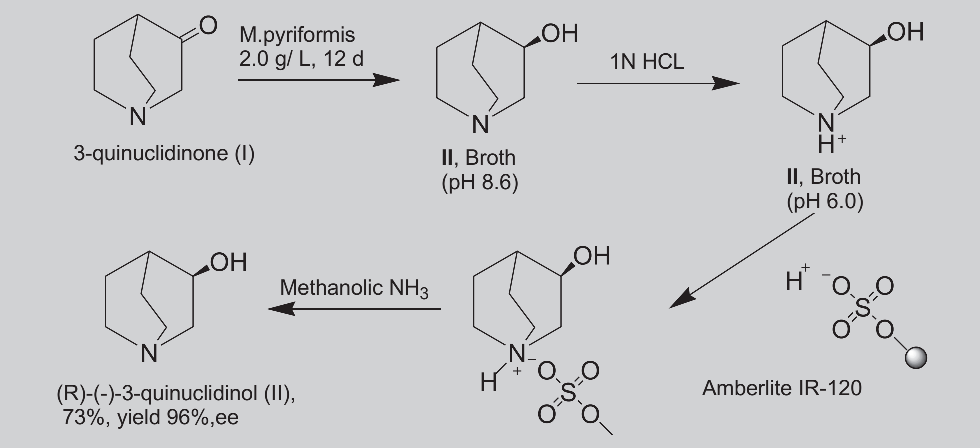
Chemical biology

structural similarity between these two structural isomers made their chromatographic separation ineffective. In the presence of vinyl acetate as the acyl donor, *Candida rugosa* lipase carried out acetylation of β–amyrin more efficiently as compared to α–amyrin leading to a kinetic separation of individual isomers (*Tetrahedron Lett.* **2014**, *55*, 3122).



Kinetic separation of α- and β-amyrin mixture by Candida rugosa (CRL)

Fungi mediated production and practical purification of (R)-(-)-3-quinuclidinol: Asymmetric reduction of a prochiral ketone, 3–quinuclidinone (I) in an efficient manner to produce an important pharmaceutical precursor (R)–(–)–3–quinuclidinol (II) with 96% enantiomeric excess was performed by the fungus *Mucor piriformis.* (R)–(–)–3–quinuclidinol (II) is an important precursor for the syntheses of muscarinic receptor ligands which were used frequently in the treatment of Alzheimer's disease. The efficiency of the process was improved by developing a cation exchange resin (Amberlite IR–120) that assisted the purification of water soluble metabolite II from fermentation media (*Tetrahedron Lett.* **2014**, *55*, 5911).

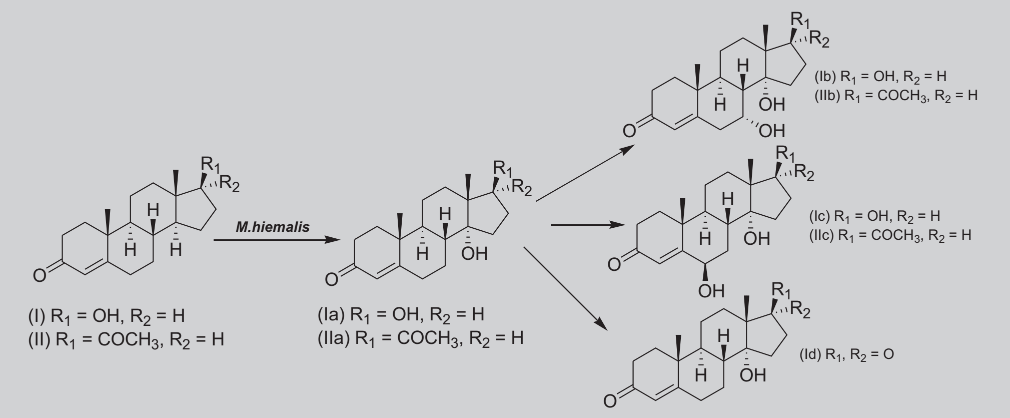


Biocatalytic reduction and Amberlite assisted isolation of 3-quinuclidinone (I) using *M. piriformis*

Hydroxylation of steroids by mucor hiemalis: Transformation of testosterone and progesterone into synthetically challenging 14α–hydroxy derivatives was achieved by using fungal strain *Mucor hiemalis*. Incubation of *M. hiemalis* with testosterone initiates its biotransformation by hydroxylation at 14α– position, prolonging which led to the formation of corresponding 6β/7α, 14α–dihydroxy metabolites. While in the case of progesterone,

Chemical biology

all three metabolites were formed with no alteration in the level of metabolites on prolonged incubation beyond the initial 4 days. Studies using cell-free extracts suggested that the 14α-hydroxylase activity was NADPH dependent and belonged to the cytochrome P450 family (*Steroids* **2014**, 85).



Isolation and characterization of the genes involved in iridoid biosynthesis in vinca: Monoterpene indole alkaloids (MIAs) are a multifarious class of natural products with distinct chemical and biological properties 1–3. Over 3000 MIAs are known today with diverse structures and biological activities. The *Apocynaceae* family plant, *C. roseus* is a rich source of the iridoid-derived MIAs and is known to contain over 200 alkaloids in various tissues. Two MIAs from this plant, vincristine and vinblastine, are widely prescribed as potent anti-cancer agents.

Cascaded enzymatic activity in iridoid biosynthesis in Catharanthus roseus: A key enzyme involved in the biosynthesis of MIAs is an NAD(P)+ dependent oxidoreductase system, 10-hydroxygeraniol dehydrogenase (Cr10HGO), which catalyses the formation of 10-oxogeranial from 10-hydroxygeraniol via 10-oxogeraniol or 10-hydroxygeranial. Cloning and functional characterization of 10- hydroxygeraniol dehydrogenase (Cr10HGO) system from *C. roseus* indicated that Cr10HGO showed broad substrate specificity for 10-hydroxygeraniol, 10-oxogeraniol or 10-hydroxygeranial over monohydroxy linear terpene derivatives. Concerted enzymatic function in the biosynthesis of cis-trans-nepetalactol was demonstrated using 10-hydroxygeraniol and NADP1 with Cr10HGO and CrIDS combined assay system. The stereochemistry of the enzymatic product was determined and was (1R, 4aS, 7S, 7aR)-nepetalactol, which was a key intermediate in the biosynthesis of iridoids and MIAs. Further *in vitro* formation of (1R, 4aS, 7S, 7aR)-nepetalactol was demonstrated when geraniol was incubated with CrG10H, Cr10HGO and CrIDS (*Sci. Rep.* **2015**, 5).

Healthcare

Chemical biology

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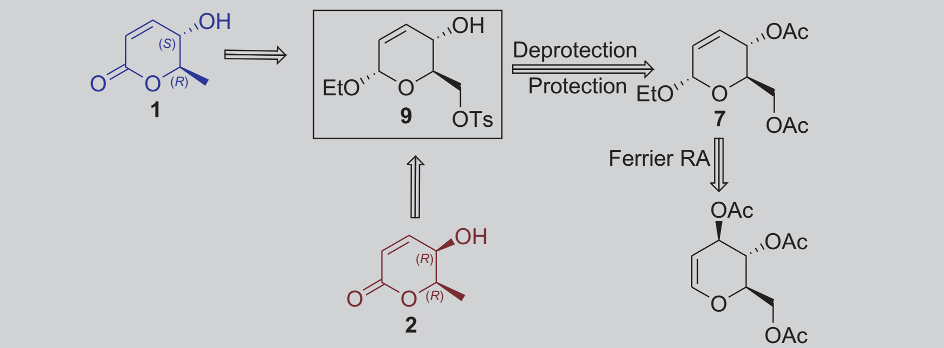
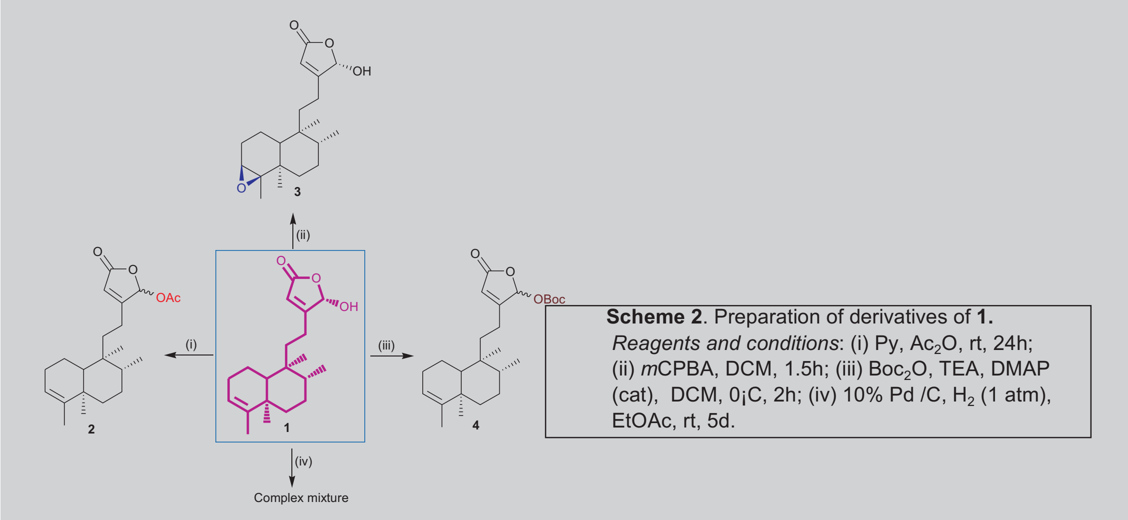
Chiral pool approach for the synthesis of bioactive molecules: Osmundalactone **1** isolated from Paxillus showed antifeedantactivity against *Plutella xylostella* and *Heliothis virescens*. Bioactive molecules such as (+)–osmundalactone **1** and 4–epi–(+)–osmundalactone **2** from a easily available carbohydrate template, D–glucal **6** (Scheme 1) were synthesized. A common intermediate 9 for the synthesis of both compounds **1** and **2** was envisaged. Compound **9** was easily obtained from D–glucal **6** by Ferrier rearrangement followed by deprotection of acetyl groups and protection of primary hydroxyl with tosyl group (*Tetrahedron Lett.* **2015**, *56*, 2783).



Scheme 1.

Clerodane type diterpene from *Polyalthia longifolia*: Bioactivity–guided chemical examination of methanolic extract of leaves of *Polyalthia longifolia* var. *pendula* led to the isolation of the active constituent, a diterpene **1** which was identified as 16–hydroxycleroda–3,13(14)Z–dien–15,16–olide.



Scheme 2. Preparation of derivatives of **1**.
Reagents and conditions: (i) Py, Ac_2O, rt, 24h; (ii) *m*CPBA, DCM, 1.5h; (iii) Boc_2O, TEA, DMAP (cat), DCM, 0¡C, 2h; (iv) 10% Pd /C, H_2 (1 atm), EtOAc, rt, 5d.

Initial, structure–activity–relationship (SAR) data generated by synthesizing some derivatives revealed that the double bond between C3–C4 and the free hydroxyl group at C16 were crucial for the antifungal activity of the diterpene **1**. The mode of action of **1** in *C. albicans* was due to compromised cell membrane permeability and disruption of cell wall structures. Interestingly, compounds (**1-4**) did not show any haemolysis of red blood cells. All the tested compounds inhibited Y–H transition in dimorphic *C. albicans* NCIM3557 at much lower concentration than their MIC90 values. Determination of ROS generation by diterpene **1** using DCFH–DA and DHR123 (dihydrorhodamine) staining of *C. albicans* NCIM3557 indicated production of intracellular ROS as a mechanism of antifungal activity (*Eur. J. Med. Chem*. **2015**, *94*, 1; Patent: 2114/DEL/2014).

Healthcare

Chemical biology

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Structure-function, substrate-specificity and evolution of cholylglycine Ntn-hydrolases: An improved method (BSS: Binding Site Similarity based scoring system) for the annotation of the pharmaceutically and therapeutically important BSH/PVA enzymes incorporates substrate specificity, binding site (Fig. 1) and phylogenetic information. Sequences from gram-positive, gram-negative bacteria and archaea were accurately annotated using BSS scores as BSH/PVA enzymes. Based on the clustering that separated gram-positive from gram-negative bacteria and detailed sequence analysis of CGH enzymes, supporting evidence was provided for the hypothesis that the diderms and archaea were evolved from monoderms (*Microbiology* **2014**, *160*, 1162).

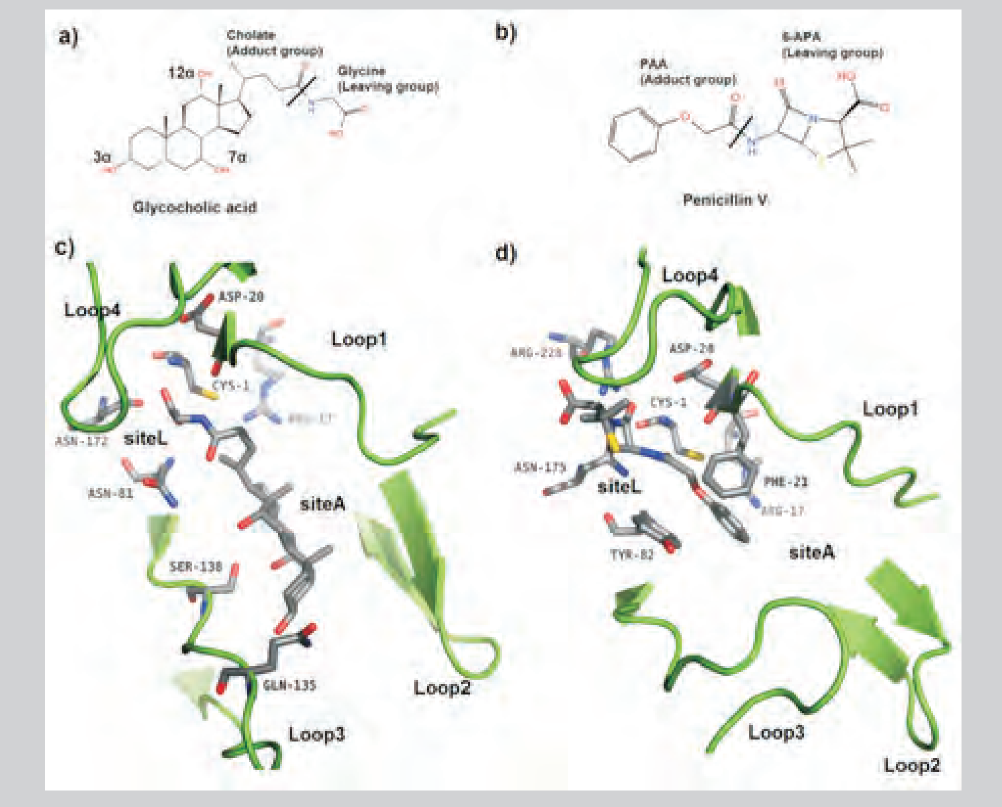

Figure shows are the substrates (a) Glycocholic acid (GCA; a bile salt) and (b) Penicillin V (penV), respectively. The scissile amide bonds that are hydrolyzed by the CGH enzymes are marked with a line. The leaving and adduct groups of each substrate along with the three polar hydroxyl groups (3α, 7α and 12α-OH) of GCA are labeled. (c) Mode of binding of GCA in BSH enzyme BlBSH (d) Mode of penV binding to PVA enzyme BsuPVA. In both complexes, the adduct groups occupy siteA while directing the leaving groups towards the active site (siteL), positioning the scissile amide bond just inside the cleft of the enzyme, close to the N-terminal Cys residue, in an orientation favorable for the nucleophilic attack. The four substrate binding loops are shown in cartoon representation.

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The mechanism of cold denaturation in proteins is often incompletely understood due to limitations in accessing the denatured states at extremely low temperatures. Using atomistic molecular dynamics simulations, structural and solvation properties of yeast frataxin were compared at its temperature of maximum stability and the experimentally observed temperature of complete unfolding. The results indicated that the surface exposed beta-sheet domains are more susceptible to cold denaturing conditions (*J. Chem. Phys.* **2014**, *141*, 205103).

Healthcare

Chemical biology

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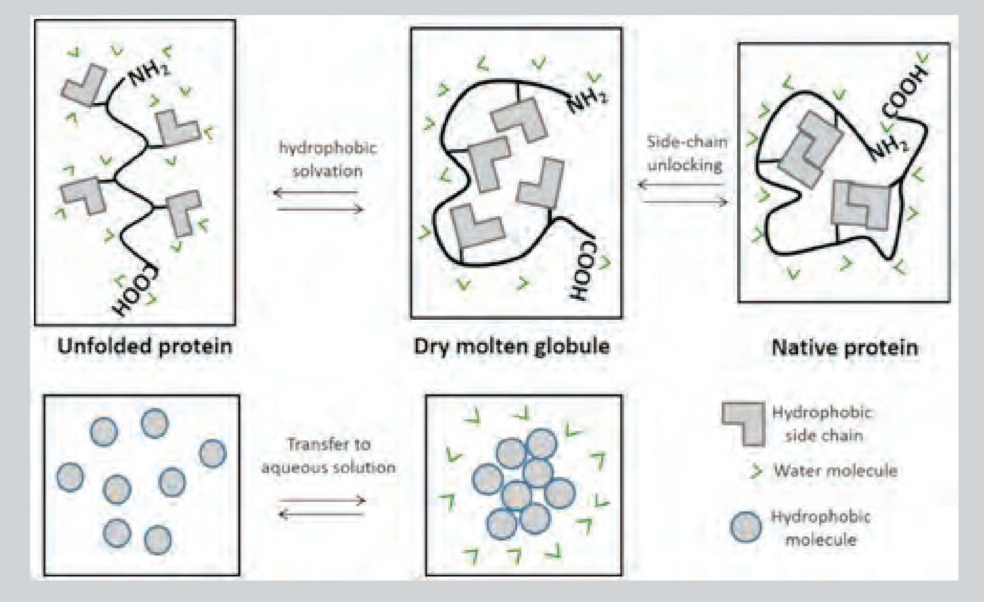
Protein stability and folding: The nature of physical forces which contributes to the stability of protein molecules is poorly understood. It is commonly believed that hydrophobic forces are the sole contributor to the protein stability. The pH induced unfolding of a multi–domain protein, Human Serum albumin was investigated using a battery of spectroscopic methods, including fluorescence resonance energy transfer, time–resolved fluorescence and solvent accessibility methods. The results allowed the group to dissect out the contribution of different forces and it indicated that side chain packing (Vander wall forces) also contributed significantly to protein stability, in addition to the hydrophobic effect. The role of chemical chaperones like TMAO, in modulating the protein stability was also investigated (*P. Natl. Acad. Sci. USA* **2014**, *111*, 4856).



Structural and functional transitions of kinetically stable protein

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Acid stability of the kinetically stable alkaline serine protease possessing polyproline II fold: The kinetically stable alkaline serine protease from *Nocardiopsissp.*; NprotI, possessing polyproline II(PPII) fold was found to be functionally stable when incubated at pH 1.0, even after 24 h. It showed enhanced activity after incubation at 50^{o}C–60^{o}C. Acid tolerant and thermostable NprotI served as a potential candidate for biotechnological applications (*Protein J.* **2015**, *34*, 60).

Tryptophan environment and functional characterization of a kinetically stable NprotI: The single tryptophan residue from *Nocardiopsissp*. serine protease (NprotI) was studied for its microenvironment using steady state and time–resolved fluorescence. Maximum quenching was observed with acrylamide. The fluorescence lifetime of 5.13 ns was observed indicating one conformer of the trp. No inhibition was seen with soybean trypsin and limabean inhibitors, while, CanPIun competitively inhibited NprotI indicating unusual stability of the protein (*J. Fluoresc.* **2014**, *24*, 1363).

Healthcare

Medicinal chemistry

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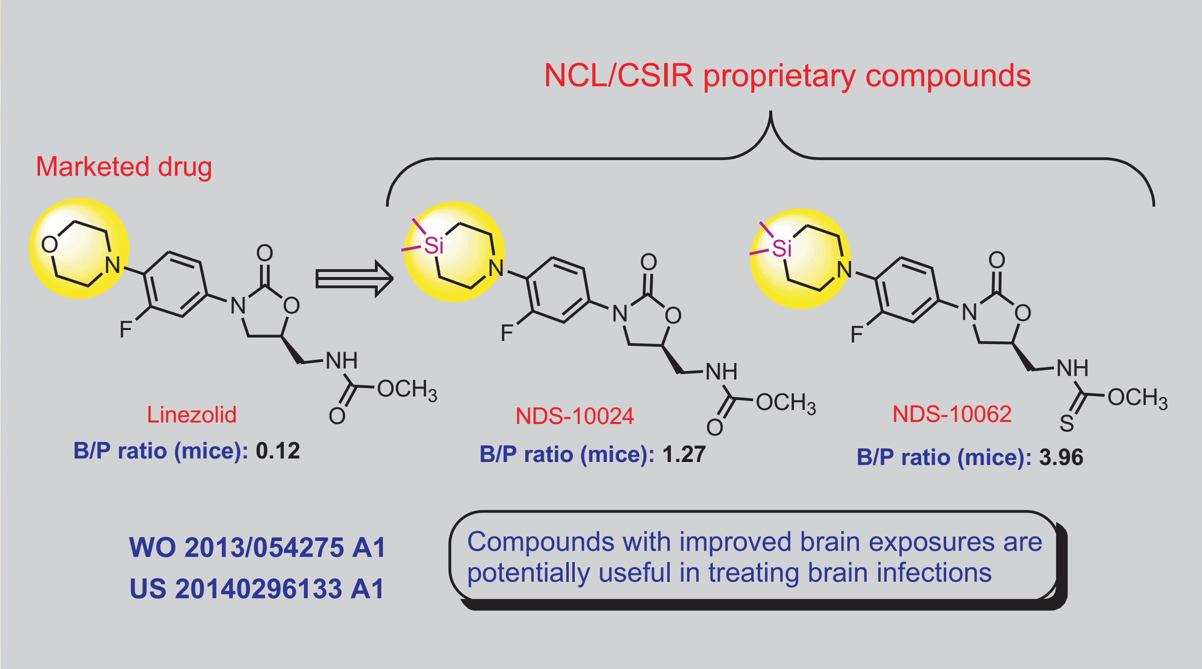
Medicinal chemistry using silicon switch approach: A medicinal chemistry program on “Silicon switch approach” with multiple projects under this theme was initiated. The increased lipophilicity of organosilicon molecules often enhances cell and tissue penetration which can be an attractive feature in the design of drugs targeting bacteria and central nervous system (CNS). This approach has minimum risk and provides clear patent space. It is a relatively new concept in drug discovery with very few companies and academic groups currently working on it. Significant contributions were made to identify three different series. Therapeutic options for brain infections caused by pathogens with a reduced sensitivity to drugs are limited. The approach showed the potential for treating brain infections caused by bacteria as the silicon incorporated compounds are expected to cross blood–brain–barrier (BBB). Recent reports on the potential use of linezolid in treating brain infections prompted us to design novel compounds around this scaffold. The findings in pre–clinical species suggested that silicon incorporation was highly useful in improving brain exposures. Interestingly, three compounds from this series showed up to a 37–fold higher Brain: Plasma ratio when compared to linezolid thereby indicating their therapeutic potential in brain infections (meningitis). The same strategy was applied for the development of potent anti–TB agents. That led to the identification of two different series of compounds based on diarylpyrrole and diarylpyrazole with nanomolar MIC values. Various other medicinal chemistry programs are under way in the group. The current specific areas are antibacterial, antiinflammatory, antidiabetic and antimalarials.



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2D–IR spectroscopy has evolved as one of the ideal experimental techniques to study ultrafast structural and conformational dynamics in proteins and enzymes. The article reviewed the 2D–IR experimental methodology and provided a qualitative understanding of the spectral signatures of the various ultrafast dynamic processes in the 2D–IR spectrum to provide molecular level understanding of the structure – dynamics – function relationship of bio–molecules (*Sci. Lett.* **2015**, *4*,173).

Healthcare

Medicinal chemistry

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Inter-individual differences in drug response: The human β_2-adrenergic receptor (β_2AR) is an important member of the GPCR family and its mutation, Arg16Gly, is linked to differential (good/bad) response to the asthma drug, albuterol. The dynamics of the variants was studied to address this issue. The N-terminal region of the Gly variant is more dynamic than the Arg variant and long-range effects at the binding site lead to preferential docking of albuterol to the Gly variant. This work provided a molecular mechanism linking the Arg16Gly variation to the differential response to albuterol in asthma patients (*Plos Comput. Biol.* **2014**, e1004006).

Antimicrobial peptides: Synthetic antimicrobial peptides (AMPs) are natural peptides with anti–bacterial and anti–fungal properties. These peptides are emerging as important candidates to counter antibiotic resistance. Three peptides belonging to the cationic, helical AMP family were rationally designed with high bacteriocidal and ant–fungal activity (Patent: 2320/DEL/2014).

Synthesis of API

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Ntn hydrolases and related enzymes: Penicillin acylases are the enzymes involved in the industrial production of 6–aminopenicillanic acid and the synthesis of semisynthetic β-lactam antibiotics. The cloning and characterization of PVA enzyme was reported from the gram–negative plant pathogen, *Pectobacterium atrosepticum*. The recombinant strain exhibited very high yield (250 mg/l) and a high specific activity (430 IU/mg). The enzyme kinetics is significantly different from the previously reported PVAs, displaying positive co–operativity and substrate inhibition. Sequence analysis and characterization revealed the distinctive nature and underscore the need to study PVAs from gram–negative bacteria (*Int. J. Biol. Macromol*. **2015**, *79*, 1).

Healthcare

Identification of lead molecules

Asymmetric synthesis of bioactive molecules and novel synthetic methodologies

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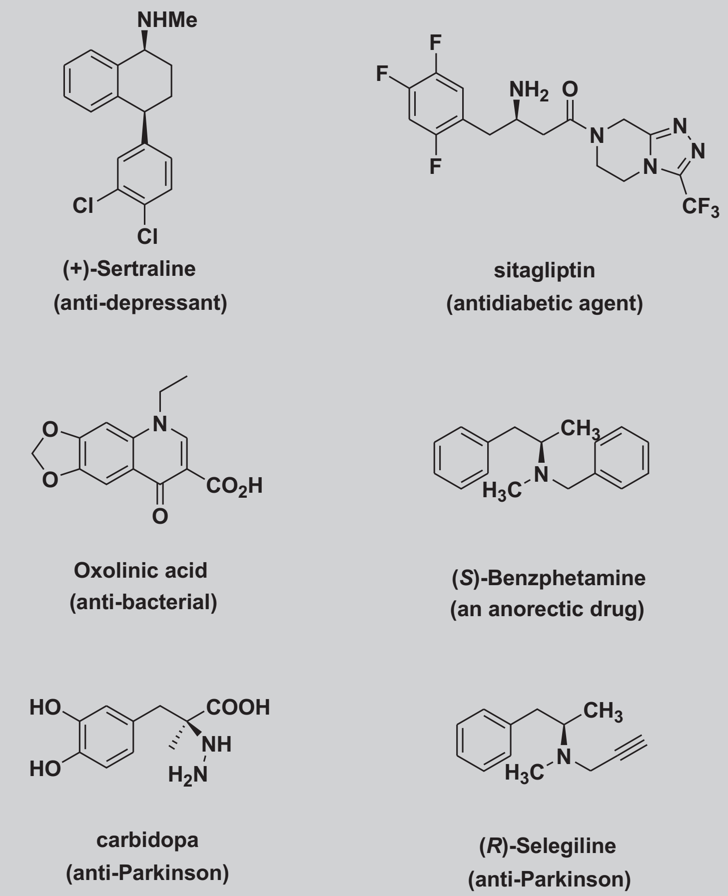
The research included development of new synthetic methodologies using organocatalysis and transition metal catalysis, newer synthetic methods for C–C and C–N bond formations, and their application in multi-step asymmetric synthesis of pharmaceuticals, large number of bioactive natural products from readily available non-chiral sources, utilization of CO_2 and metal-free processes for key organic transformations.

Asymmetric synthesis of pharmaceuticals and bioactive molecules: New methods were developed for the synthesis of important life-improving and life saving chiral drugs under the category of anti-malarial, anti-Parkinson, anti-Alzheimer's, anti-hypertensive, anti-depressants etc in an efficient and cost effective manner (Fig. 1). The synthesis of optically active drugs was meticulously planned and executed that include Sertraline (anti–depressant), Sitagliptine (anti-diabetic agent), Oxolinic acid (anti-bacterial), Benzaphetamine (an anorectic drug), Carbidopa and Seligiline (anti-Parkinson), Amprenavir and Saquinavir (anti-HIV), Tamiflu (anti-influenza), Sitagliptin (anti-diabetic), Rasagiline (anti-Parkinson), ICI-118,551 (anti-hypertensive), and a large number of bioactive natural products such as (+)-Neopeltolide, (-)-Aspinolide A, Tanikolide, Herbaric acid, Isocladosporin, guggultetrol, D-ribo-phytosphingosine tetraacetate, (2S,3S)-3-hydroxy-L-arginine, (2S,3S)-3-hydroxypipecolic acid, (S)-3-Hydroxypiperidine, 3-epi-jaspine B, yashabushidiols A and B and the lactone unit of compactin and mevinolin (*Tetrahedron-Asymmetr*. **2015**, *26*, 24, 67, 118, 548, 571; *Synlett* **2014**, *25*, 102; *Synthetic Commun*. **2015**, *45*, 1559; *RSC Adv*. **2014**, *4*, 49770).



(+)-Sertraline (anti-depressant)

sitagliptin (antidiabetic agent)

Oxolinic acid (anti-bacterial)

(*S*)-Benzphetamine (an anorectic drug)

carbidopa (anti-Parkinson)

(*R*)-Selegiline (anti-Parkinson)

Fig 1 : Important drugs synthesized in the lab

Identification of lead molecules

Synthetic methodologies involving organocatalysis and iodine catalysis: The research included the development of new synthetic methodologies for the synthesis of biologically active molecules using organocatalysts (Fig. 2). Novel synthetic methods were developed using proline as catalyst for the synthesis of bioactive 4–hydroxy pyrrolidine derivatives through syn–Mannich/ Corey–Chaykovsky reaction cascade via [4+1] annulations, Kainic acid derivatives through syn–Mannich/wittig/N–alkylation /Michael addition reaction cascade via [4+1] annulations. Proline catalysis was also used for the synthesis of amino diols. N-heterocyclic carbenes (organocatalyst) were used for oxidative coupling of styrene/α-bromoacetophenones with aromatic aldehydes for the synthesis of α, β-epoxy ketones. I$_2$-catalyzed alkene functionalization reactions were performed for the synthesis of α- acyloxyketones, esters, diol derivatives and divergent azido alcohols (*J. Org. Chem*. **2015**, *80*, 2024; *Synlett* **2015**, *26*, 355; *RSC Adv*. **2015**, *5*, 21803; *Chem. Commun*. **2015**, *51*, 10276; *Org. Lett*. **2014**, *16*, 5674).

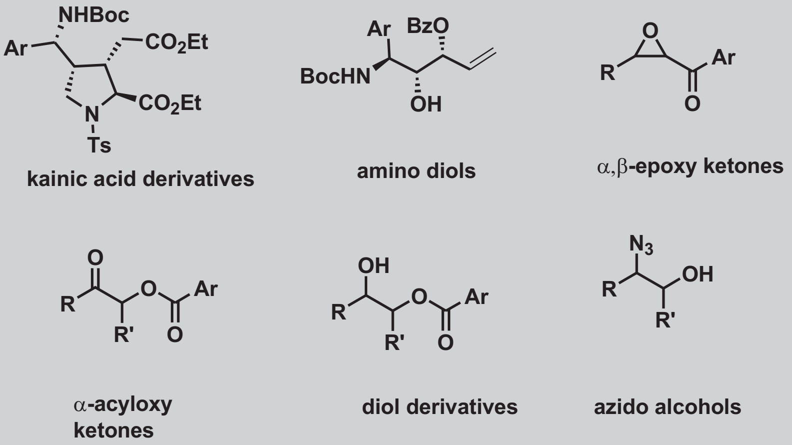


Fig 2: Key organic frameworks synthesized using organocatalysis and iodine catalysis

Synthetic methodologies involving transition metal catalysis: A simple methodology afforded substituted quinoline esters and isocoumarins, important building blocks for the synthesis of pharmaceuticals and polycyclicaromatic electronic materials via Rh–catalysed ortho–C–H activation in high yields. A flexible, novel single–step method was reported that employed the Cu–catalyzed debrominative cyanation of gem–dibromoolefins for the synthesis of α,β–unsaturated nitriles. Additionally, a highly practical, novel method was demonstrated for the oxidative esterification of aromatic aldehydes with methyl arene and alcohols using Ti-superoxide as a heterogeneous catalyst. A copper bromide (I) catalyzed carbonylative coupling reaction was developed for the synthesis of carboxylic acid derivatives with sodium cyanide as a C1 source. A review on NaIO$_4$ was also published (*Org. Biomol. Chem.* **2015**, *13*, 5918; *Adv. Synth. Catal*. **2014**, *356*, 2231).

Healthcare

Identification of lead molecules

Study of genome to pathway-level complexities in biological systems

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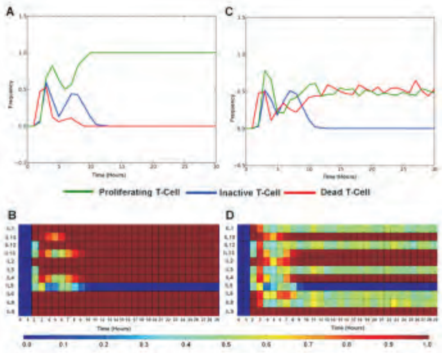
The aim was to study the biological systems across different levels like genome to population. The mathematical modeling, computational approaches and optimization techniques were employed to understand the complexities of gene regulation, metabolic and signaling pathways, their cross-talks and cellular interactions holistically. It helped to understand the progression of complex diseases, identify potential treatment strategies, bring out many potential drug targets to counteract and control the disorders, which constitutes a basis for system level understanding and has potential application in pharmaceutical industry.

Modeling and computational study of immune cell signaling pathways: Immune system is constituted by different cell types, such as, T and B lymphocytes, macrophages etc. T-cells play a pivotal role in combating intracellular pathogens and cancer. The functions of these T lymphocytes depend on the delicate regulations of the T-cell signaling cascades regulating the cytokine expression profile of the lymphocyte and the phenotypic responses of the cell. T-cell signaling pathway study was carried out in the research. It was hypothesized that the temporal protein expression patterns of various T-cell signaling component proteins as well as the phenotypic responses (such as proliferation, inactivation, cell death, interleukin production etc.) can be regulated by tuning various co-stimulatory and co-inhibitory molecules including Ca^{+2} signaling pathway.

Reconstruction and analysis of T-cell signalling pathway: In order to capture all the regulations of signaling cascade, a comprehensive T-cell signaling pathway was manually reconstructed, coupled with other intracellular important signaling pathways (e.g. MAPK, Ca^{+2} signaling pathway etc.) and other co-stimulatory and co-inhibitory pathways. The model of T-cell signaling network was analyzed (Fig. 1) using the data and the concept of semi-dynamic Boolean or logical equations to study various temporal protein expression patterns, generated through different stimulation and co-stimulation signal (*Database-Oxford* **2015**, DOI:10.1093/database/bau126).



Changes in Cell Phenotypes and corresponding Interleukin Expression pattern due to CD27 and LTBR mutation. (A) and (B) normal condition; (C) and (D) CD27 and LTBR mutated condition.

In silico identification of key T-cell regulatory molecules: The simulations highlighted the importance of the CRAC channel in the regulation of T-cell proliferation. The necessity of the different co-receptor molecules in T-cell (OX40, CD27 and LTBR), became clear in different mutations in these simulation. The impact of co-receptors CD27 and LTBR mutation clearly showed the role in maintaining the T-cell functionalities and regulation of interleukin production, and their prime target molecules (Fig. 1), and also revealed the precise route of signal propagation and changes in the behavior of interleukin production due to mutations (*J. Biosciences* **2015**, DOI 10.1007/s12038-015-9561-1).

Comparative analysis of codon usage bias across leishmania and other trypanosomatids: *Leishmania* (kinetoplastid protozoans) cause widespread neglected tropical disease leishmaniasis in humans and are responsible for different disease complicationswithin the host due to a distinct species specific heterogeneity observed among different *Leishmania* species. *Leishmania* genome is highly intact and does not display major variations in gene organization or nucleotide content between species. This poses complexity in finding probable reasons for species-specific differences in clinical manifestations. A large scale analysis of codon usage patterns between *Leishmaniaand* other Trypanosomatid species was performed to understand the variations in gene organization and its effect on the phenotype (*Data in Brief* **2015**, 4, 269).

Identification of lead molecules

Causes and consequences of codon usage bias in *Leishmania* genomes: Codon usage bias (CUB) was investigated at different levels to understand the influence of different factors like mutational pressure, translational selection and amino acid composition bias. The GC bias at wobble position governed codon usage bias across *Leishmania* species, rather than amino acid composition bias. The influence of CUB on formation of folded structures within the mRNA was studied. The presence of non-random genome-specific codon usage patterns was demonstrated within each *Leishmania* genome, as codons that avoid secondary structure formation are preferred within the *Leishmania* coding sequences. The putative differences in global expression between genes belonging to specific pathways across *Leishmania* were predicted. It explained the role of evolution in shaping the otherwise conserved genome to demonstrate species-specific function-level differences for efficient survival of the parasite within the host (*Genomics* **2015**, *106*, 232).

Chemoinformatics for drug discovery

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Chemoinformatics assisted methods for virtual screening: The group is engaged in the area of chemoinformatics activities for the past two decades especially in developing open source tools and problem solving platforms for academic and industrial pharmaceutical research. In the past year, as part of innovative research, ten papers were published in two special thematic issues dedicated to Chemoinformatics for Virtual Screening in Drug Designing. The role of Chemoinformatics data and methods, along with software code and case studies were written in a book entitled *Practical Chemoinformatics*.

Design and development of new chemoinformatics tools for virtual screening: Virtual screening (VS) is the backbone of computational drug discovery workflow, an indispensable component in all drug design programs. The present volume is a compilation of distinct, logically organized research papers presenting original ideas supported with specific case studies highlighting the new in house developed virtual screening tools and their specific applications. The tools relate to computational handling of chemical structures, properties and development of integrated workflows and application of high performance computing platform as a problem solving environment for major chemoinformatics tasks (ChemInfoCloud). The use of chemoinformatics approach was demonstrated for the design of new molecules inspired by molecules from marine organisms to develop an interactive marine database named MIMMO (Medicinally Important Molecules from Marine Organisms). The virtual screening tools presented possess state of the art modules for similarity searching, diversity selection, scaffold analysis, library generation, annotation and pharmacophore mapping to find diverse chemotypes from the vast chemical space (*J. Comb. Chem. H. Thr. Scrn.* **2015**, *18*, 528; Patents: WO 2014/207670 A1, US 14/901151, EP 14755415.8).

Role of data and methods in chemoinformatics for virtual screening: Efficient smart filters were developed that enabled prioritizing and screening of large molecular libraries prior to synthesis. Though the techniques, algorithms computational time etc for virtual screening have increased by leaps and bounds it is surprising that most of the research still focuses on limited number of targets and chemotypes. It became evident from these studies that a lot of target, ligand space is unchartered and an integrated approach is indispensable for the discovery of new lead molecules for combating diseases (*J. Comb. Chem. H. Thr. Scrn.* **2015**, *18*, 624).

A collaborative effort with organic synthesis group led to the discovery of a new series of spirochromone annulated chalcone conjugates that possessed anti-tubercular activity against Mycobacterium tuberculosis H37Rv strain. Quantitative structure activity relationship (QSAR) modeling revealed a quantitative relationship between biological activities and frontier molecular orbital energies of synthesized compounds. The predictive model can be employed further for virtual screening of new compounds in this series (*RSC. Adv.* **2015**, *5*, 106448).

Healthcare

Identification of lead molecules

Asymmetric synthesis of biologically active compounds

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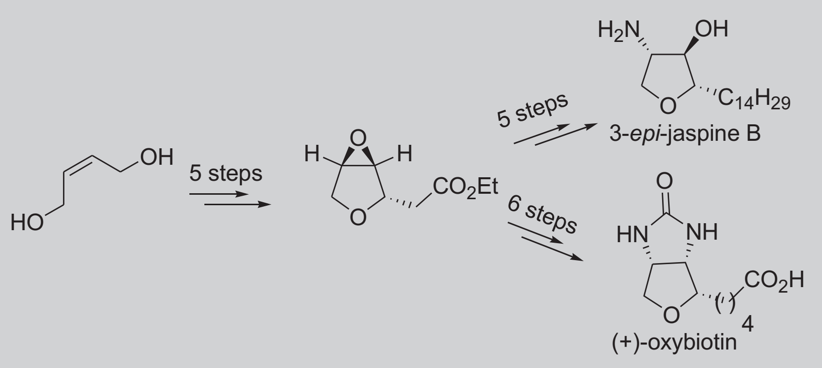
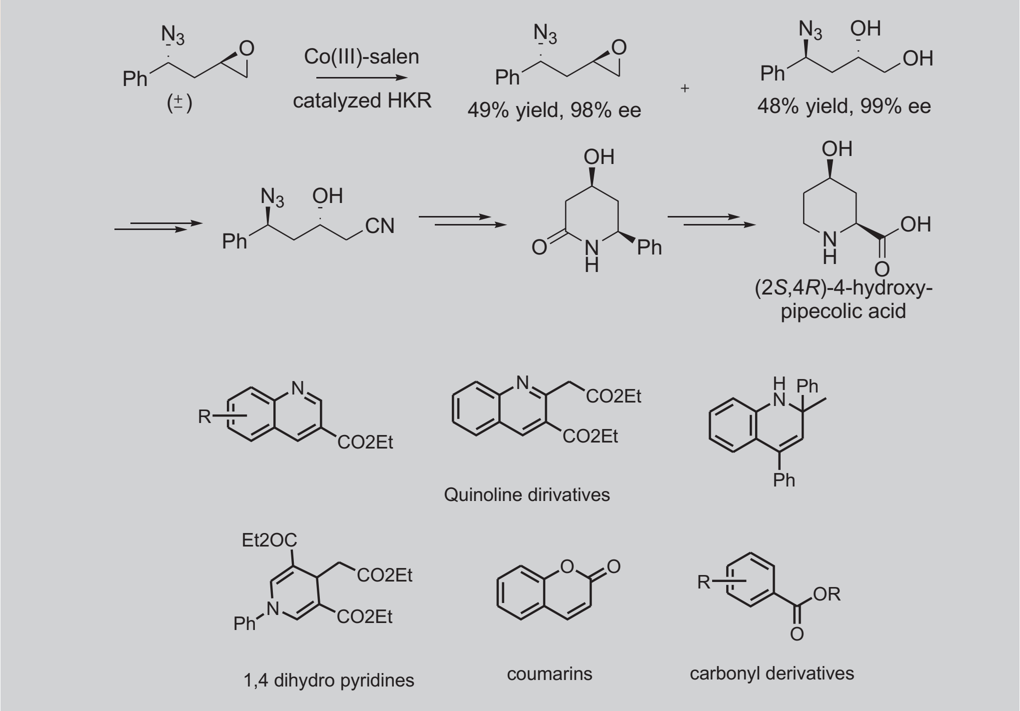
The research was focused on the use of metal or organocatalysts in the development of novel methodologies and their applications in the asymmetric synthesis of drugs and bioactive natural compounds.

Synthesis of 3-epi-jaspine B and (+)-oxybiotin: A new synthesis of cytotoxic anhydrophytosphingosine 3–epi–jaspine B (34.7% overall yield; 97% ee) and (+)–oxybiotin (21.2% overall yield; 97% ee) bioactive oxygen analogue of biotin was described starting from commercially available cis–2–butene–1,4–diol. The key reactions employed in the synthesis included Sharpless asymmetric epoxidation and a novel tandem desilylationoxa–Michael addition reaction strategy to construct tetrahydrofuran core (dr>99%).



Asymmetric synthesis of (2S,4R)-4-hydroxypipecolic acid : An efficient formal synthesis of (2S,4R)–4–hydroxypipecolic acid was achieved in high optical purity (99% ee) from readily available benzaldehyde. The strategy employed an iodine–induced intramolecular cyclization of a carbonate and Co–catalyzed hydrolytic kinetic resolution of two stereocentered racemic azido epoxide as the key reactions to construct chiral 1,3–amino alcohol functionality.



Key organic frameworks synthesized under transition metal catalysis

Sustainable Chemical Industry

Process intensification and engineering

Design of flow reactors

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The group works in the area of design of flow reactors for variety of chemical reactions. The multiphase reactive flow in small channels was studied and the interest aspects that are very different from conventional non-reactive flows were explored. The approach was extended for the synthesis of API, dyes, intermediates and nanomaterials.

Continuous flow nitration of *o*-Xylene: Continuous flow nitration of variety of aromatic substrates is a foray of the group. The nitration of o-xylene over a wide range of conditions was demonstrated recently. The fuming nitric acid as the nitrating agent, the selectivity for isomer 2,3-dimethyl-4-nitrobenzene was always higher than 2,3-dimethyl-3-nitrobenzene as compared with the conventional mixed acids. The nitration of 3-nitro isomer formed some impurities due to its higher reactivity with nitric acid. An economic analysis of the continuous flow reactor for production of 100 kg/hr and 500 kg/hr of 2,3-dimethyl-4-nitrobenzene in a jacketed tubular reactor showed that numbering-up is a more economical approach for higher production capacity. A combination of large and small sized tubes depending upon the relative rates of heat generation during a reaction will achieve more profit and less payback period than having the entire reactor made of single tube size (*Org. Process Res. Dev.* **2015**, DOI: 10.1021/acs.oprd.5b00064; *J. Flow Chem.* **2014**, *4*, 210).

Modeling and scale-up approach for diazotization in flow reactor: A scale-up approach for diazotization reaction was developed. A specific case of diazotization of aniline was considered and explored using Central Composite Design. On the basis of the parameters obtained from RTD experiments isothermal axial dispersion model was validated and used for scale up. The model was used for successful scale-up from tubular reactor (1.78 mL) to AmAR3 reactor (28.96 g/hr) for synthesis of diazonium salt.

Flow pattern with fractal impellers: Fractal Impeller (FI) is useful for distribution of energy throughout the stirred tank reactor in a relatively uniform manner. Flow generated by FI in the stirred tank was investigated experimentally using Ultrasonic Velocity Profiler. All the three velocity components and turbulent kinetic energy were mapped in the entire stirred tank. The contribution of tangential velocity component was found maximum in comparison with that of radial and axial components. The RMS velocities of all the components showed that the FI generates non-homogeneous and non-isotropic turbulence (*Proc. Eu. Mix. Conf.* **2015**).

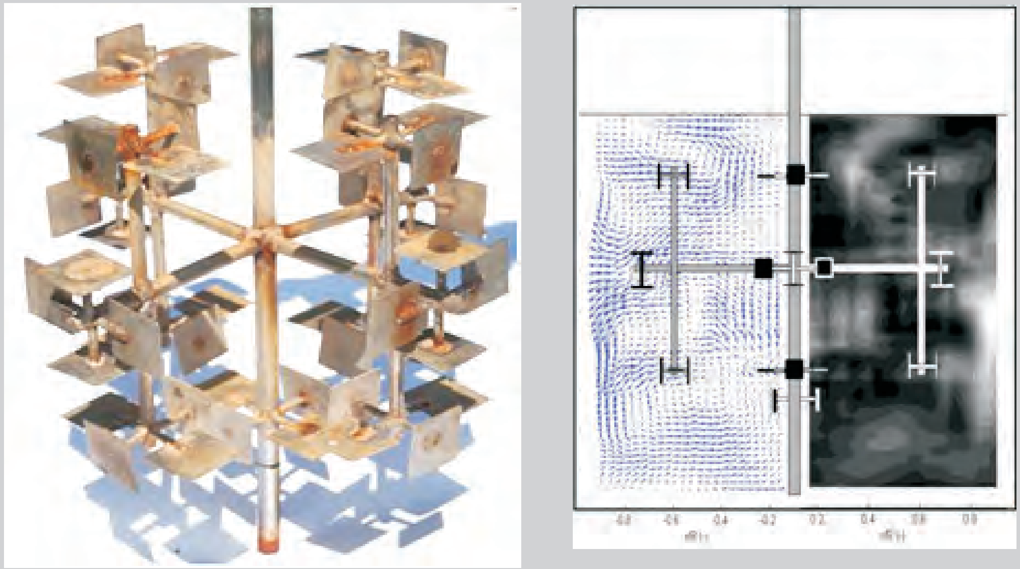

Fig: (Left) Fractal Impeller, (Right) Mean velocity distribution in r-z plane between two baffles, vector plot of left half plane and velocity magnitude contour plot in the right half plane

Sustainable Chemical Industry

Process intensification and engineering

Slurry erosion wear test rig

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The objective was to develop a slurry erosion test rig and create an infrastructure for erosion wear testing to investigate the erosion wear behavior of different engineering materials and the erosion wear resistance of different hard surface coatings.

Slurry Erosion wear test rig as shown in Fig. 1 was designed and developed for erosion wear testing of engineering materials. The dominant parameters namely, orientation angle, solid concentration, particle size and velocity was controlled to understand the erosion wear behavior.

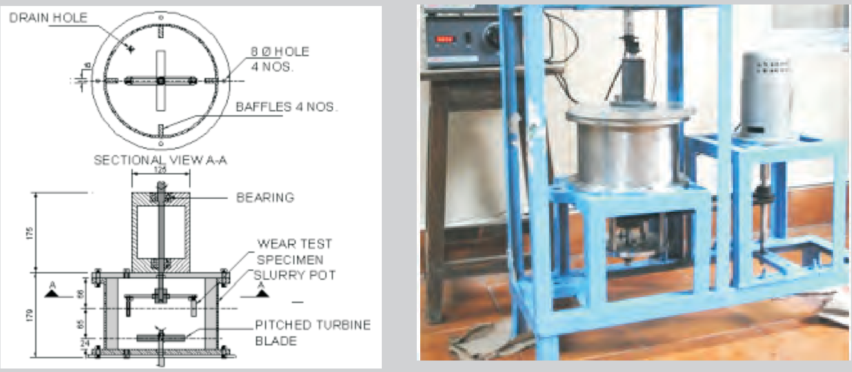

Fig. 1: Experimental set up for Slurry Erosion Testing

Field Study: The Pump at “Girana Pumping Station” at village Savkheda was dismantled and the impeller (Fig. 2) of the pump was examined with necked eyes, it was observed that the diffuser vanes of the impeller were worn out unevenly and material was removed due to either parallel flow wear or erosion wear.

Fig. 2: Worn out impeller of Gordanrich 200 HP 5 stage pump

Based on the preliminary survey and impeller of the pumps the material identification was done and its mechanical properties were investigated. Work was done for the sample preparation and erosion wear testing. The material removal mechanism was identified for the prediction of its life.

Novel eco-friendly and autocatalytic process for the synthesis of tributyl citrate

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Organic esters assumed to be important intermediates in chemical and pharmaceutical industries mostly produced by acid-catalyzed esterification reactions. The esters of bio-based organic acids fall into the category of benign or green solvents and proved to be promising replacements for halogenated petroleum-based solvents in a wide variety of applications. In the conventional manufacturing of tributyl citrate, various catalysts are used for esterification process. However the catalytic processes showed limitations in the separation of catalyst (H_2SO_4 and *P*-TSA) from reaction mixture and its reuse is difficult.

Many impurities were formed in the presence of catalyst (H_2SO_4 and *p*-TSA). The catalytic process gives yellowish and brownish colored TBC product. Hence an eco-friendly autocatalytic reactive distillation process was developed for the synthesis of TBC where citric acid was used as a catalyst for the reaction. TBC obtained in the laboratory scale process showed 99.9% purity and colorless product was achieved. The advantage of autocatalytic reaction is the absence of separation step and regeneration of catalyst. Further, the overall cost of the process is low as compared to heterogonous catalyst (Patent filed: 2015-NF-0115).

Sustainable Chemical Industry

Process development and scale-up

Scaling-up nanomaterials

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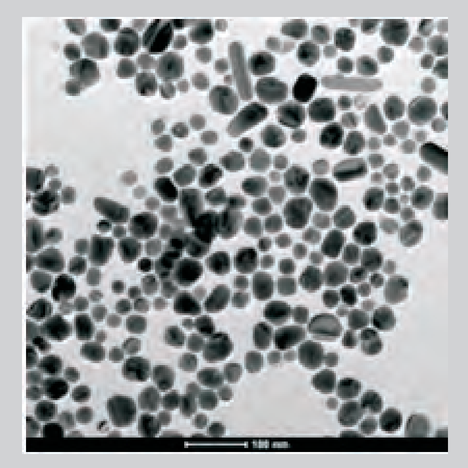
In recent years there has been growing interest in the application of silver nanoparticles. Well-controlled synthesis of AgNPs can be achieved through chemical synthesis; however these methods are restricted to very small scale synthesis. A scalable approach was developed using Turkevich method with a detailed analysis of the reaction kinetics and mechanism behind the synthesis of AgNPs. The effect of relative rates of nucleation and growth kinetics on the particle size distribution, shape variation and overall yield of the process was quantified. The process was demonstrated for synthesizing a few hundred grams of Ag NP per day with consistent particle size distribution (Patent: NCLI-INV-2015-59).



Process development for the synthesis of p-methoxy acetophenone

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Conventional *p*-methoxy acetophenone was produced by Friedel–Crafts reactions, with acid chlorides or anhydrides. It often requires excess quantities of Lewis acid (i.e., $AlCl_3$), and the process produces significant amount of corrosive vapor and aqueous aluminum waste. Acetanisole is an aromatic chemical compound with an aroma described as sweet, fruity, nutty, and similar to vanilla. It is used as an intermediate for pharmaceuticals, agrochemicals and polymerization catalyst for the manufacture of olefins. It is also used as a cigarette additive, a fragrance and flavoring agent in food. An eco-friendly process was developed for the synthesis of *p*-MAP using anisole, acetic acid and new catalyst. The advantage of present method is that the process is environmental-friendly and cost-effective. The demonstration of the process for the manufacture of *p*-MAP at pilot scale was given to M/s. Hariom Chemical, Bhavnagar, Gujarat at CSIR-NCL. During the demonstration more than 99% pure *p*-MAP was obtained. It minimized the potential environmental impact of Friedel–Crafts acylation (Patent filed: 0416/DEL/2015).

Process development studies for hydroquinone from phenol

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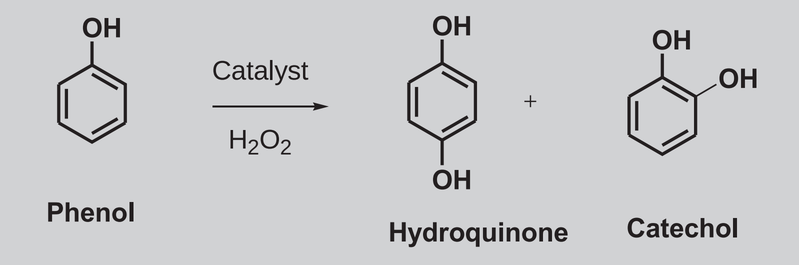
The project involved the production of hydroquinone and catechol using phenol under catalytic reaction condition. The advantage of this method is that the process is environmental-friendly and cost-effective.



Scheme : Hydroxylation of Phenol

Sustainable Chemical Industry

Process development and scale-up

Development of low temperature demulsifier

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Stable water in oil emulsions is encountered commonly in the oil industry. The stability of water in oil emulsions said to be attributed to the presence of surface active materials such as asphaltenes, resins, naphthenic acids and clays. These materials form a rigid interfacial film at the oil or water interface that hinders the coalescence of emulsified water droplets. Chemical demulsification is an economic, convenient and efficient method for breaking water in oil emulsions. The function of the demulsifier is to modify the interfacial properties and displace the asphaltenic stabilized emulsion film from the oil or water interface. Amphiphilic block copolymers contain hydrophilic EO and hydrophobic PO blocks are commercially available and widely used as demulsifiers. The structure of a demulsifier can influence the interfacial properties and cause displacement of the emulsion film. However, ethylene oxide (EO) or propylene oxides (PO) are toxic, explosive and deadly carcinogens. Hence, in terms of cost, safety and general ease, pyridines or salts of carboxylic acids were preferred for the synthesis of demulsifier. These salts of carboxylic acids are far better in terms of synthesis, handling and storage.

Different carboxylic acids-styrene based demulsifier were developed for separation of water from simulated as well as actual crude oil. It was found theses demulsifier showed excellent demulsification efficiency of more than 95%. The actual demulsification of ONGC crude was performed at Bombay high ICP platform using developed demulsifiers. It was observed that the developed demulsifier gave excellent results [water content in crude oil 1% and oil content in water 175 ppm, organic chloride = 0 ppm; demulsification efficiency 99.14 (%v/v)] at 40C, demulsifier dose 100-1000 ppm, and curing time 6 min. The major advantages of developed demulsifier include cost of demulsifier is very low as compared to commercial one. For the synthesis of demulsifier moderate process conditions are required [60-80C and atmosphere pressure] and reactor setup required for synthesis of demulsifier is very simple. The developed demulsifier worked efficiently at low temperature. The curing time required for demulsification of crude was very low. The developed demulsifier was insoluble in water and therefore it will not create the effluent problem (Patent filed: 3437/DEL/2014).

Sustainable Chemical Industry

Process separations

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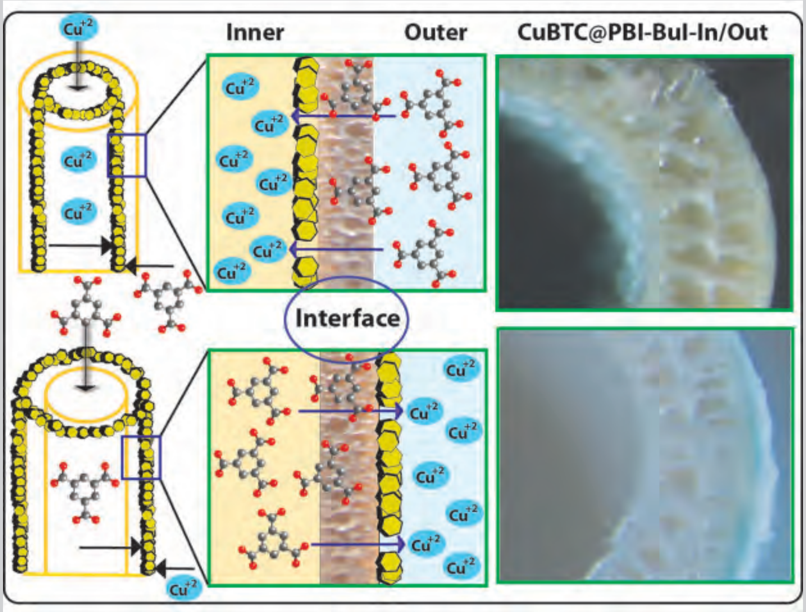
MOF@PBI hollow fiber membranes for gas separation: MOF based membranes are gaining increasing attention for separation of gases and liquids. Finding an easy and scalable method to control the in-situ growth of the MOF crystals on hollow polymeric membranes was a key challenge. A new, convenient, scalable room temperature interfacial MOF (ZIF-8 and CuBTC) synthesis approach was demonstrated. It tuned the conditions in such a way that the MOF coating was preferentially obtained either on inner or outer surfaces of polybenzimidazole based hollow fiber (PBI-BuI-HF) membranes. The growth of MOFs on hollow fibers was continuous, uniform and showed appreciable gas separation performance. This methodology was easily scalable, as it was developed by using membrane module of 1 feet length (*Nanoscale* **2015**, *7*, 7291; Patent: 3324/DEL/2014).



Synthesis of CuBTC@PBI-BuI-In (inner) and CuBTC@PBI-BuI-Out (outer) *via* interfacial approach

Sustainable Chemical Industry

Catalysis

Supported noble metals for catalytic conversion of furfural and benzyl alcohol to industrial chemicals

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The objective was to develop efficient and selective noble metal catalysts for reduction of furfural and oxidation of benzyl alcohol to industrial chemicals and further explore the factors governing catalytic activity in these transformations.

Catalytic reduction of furfural: Reduction of furfural (FAL) produced the furfuryl alcohol through C=O hydrogenation, tetrahydrofurfurylalcohol by both ring and C=O hydrogenation, 1,2– and 1,5–pentanediols by hydrogenation followed by ring opening, n–butanol (by decarbonylation followed by hydrogenation and ring opening), 2–methylfuran (2–MF, by hydrogenolysis of C=O), furan (by decarbonylation) and tetrahydrofuran (THF, by decarbonylation followed by hydrogenation), (Fig. 1). The palladium or platinum supported on γ-Al_2O_3 exhibited high catalytic activity at mild to moderate conditions. The above products could be achieved with high selectivity by tuning reaction conditions like temperature and hydrogen pressure. These catalysts were reusable in several recycling experiments (*J. Catal*. **2015**, *327*, 65).

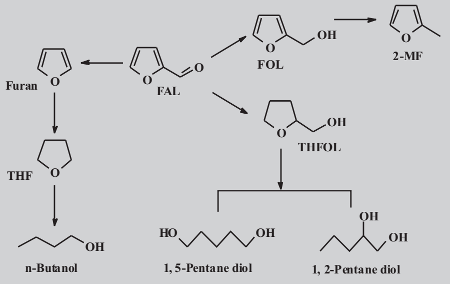

Fig. 1: Furfural and its reduced products

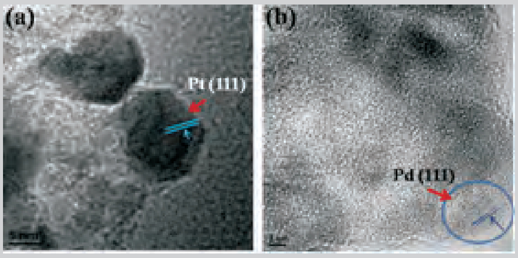

Fig. 2: HRTEM of (a)Pt and (b) on Al_2O_3

The supported Pt catalyst was selective (100%) for FOL in the liquid-phase hydrogenation at room temperature, whereas the Pd catalyst was selective for THFOL at those conditions. Differences in structure and mode of FOL adsorption were the causes for variation in selectivity of the supported Pt and Pd catalysts. At a given loading (ca., 1 - 5 wt%), HRTEM revealed that the particles of Pt were bigger in size than Pd (Fig. 2). The exposed (111) planes of Pt facilitated adsorption/activation of the carbonyl group of furfural at Pt atoms yielding higher amount of FOL. The Pd on Al_2O_3 was richer in electron-density and hence, facilitated ring rather than carbonyl group activation. FOL was reformed at 240°C into furan and 2-MF simply in water medium and without having hydrogen supply. Pentanols and butanol were formed in good selectivity when the reaction was performed in presence of external hydrogen. Furan was hydrogenated into THF (100% yield) at room temperature. Acidity of the support showed a major influence on the catalytic activity and product selectivity. Differences in d-band width and repulsive interactions between ring and metal electrons, particle size, support acidity and mode of activation of FAL on metal surfaces were the causes affecting the catalytic activity.

Selective oxidation of benzyl alcohol: Au supported on sodium titanate nanotubes (NaTNT) was found highly active for oxidizing benzyl alcohol selectively to benzaldehyde under solvent and base-free conditions. When Pd was co-added, the activity of Au enhanced significantly. The particle size of Au decreased in presence of Pd. When the support basicity was changed by exchanging Na^+ with other alkali and alkaline earth metal ions (A = Li^+, K^+, Cs^+, Mg^{2+}, Ca^{2+}, $Sr^{2+}$and Ba^{2+}), significant changes in molecular electronic structure and catalytic activity of Au were noted. Au/BaTNT with higher basicity, smaller Au particles and higher metal dispersion showed the highest catalytic activity. Catalytic activity (turnover frequency (TOF) = moles of benzyl alcohol converted per mole of exposed Au per hour) decreased with increasing Au particle size (Fig. 3) (*Catal. Commun.* **2015**, *58*, 149; *RSC Adv.*, **2015**, *5*, 47740).

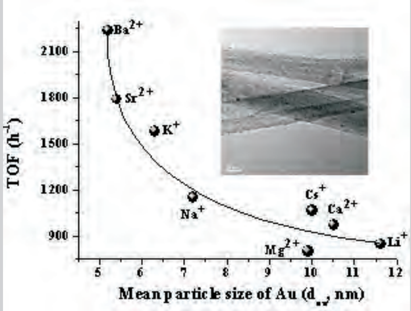

Fig. 3: Correlation of alcohol oxidation activity with the mean particle size of Au supported on ATNT

Sustainable Chemical Industry

Catalysis

Multifunctional novel catalysts of industrial importance

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Research was focused on designing multifunctional catalyst systems for hydrogenation of levulinic acid to γ‐valerolactone (GVL) with and without external hydrogen, furfural to tetrahydrofurfuryl alcohol and liquid phase oxidation of lignin model compounds such as veratryl, vanillyl, sinapyl and coumaryl alcohols. Non‐noble metal multifunctional catalysts were also developed for Water Gas Shift Reaction (WGSR).

Levulinic acid hydrogenation to GVL without external hydrogen: Levulinic acid was completely and selectively converted to GVL, in the presence of formic acid over Ag-Ni-ZrO_2 catalyst [Fig. 1]. The synergism of Ag and Ni for transfer hydrogenation eliminated the need of external hydrogen that made the process safer. The magnetic nature of the catalyst offered its easy recovery for efficient recyclability. The approach was standardized for hydrogenation of several C3- C6 platform molecules in aqueous medium (*RSC Adv.* **2014,** *4*, 9730).

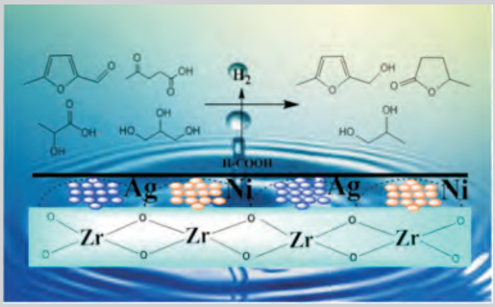

Fig. 1: Catalytic transfer hydrogenation of LA to GVL

Tailoring the product distribution with batch and continuous process options in catalytic hydrogenation of furfural: A novel approach was developed for direct conversion of furfural (FFR) to tetrahydrofuran (THF) over carbon supported Pd catalyst [Fig. 2]. CSIR‐NCL catalyst showed complete FFR conversion with a total of 80% selectivity to ring hydrogenated products including THF. Selectivity to THF alone was enhanced > 40% with complete FFR conversion in a continuous operation with on stream activity of ~ 100 h. The reaction pathway elucidated from some control experiments revealed that the decarbonylation of FFR to furan over Pd/C catalyst is a prerequisite for THF formation (*Org. Process. Res. Dev*. **2014**, *18*, 1434).

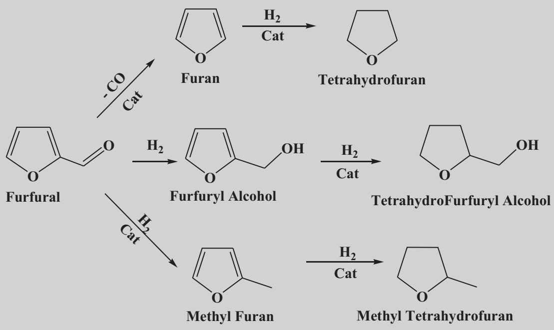

Fig. 2: Direct conversion of furfural to THF

Triple nano-composites of $CoMn_2O_4$, Co_3O_4 and reduced graphene oxide for liquid phase oxidations: A triple composite of reduced graphene oxide (RGO) with Mn and Co was developed. It exhibited an excellent activity for the selective liquid phase aerobic oxidation of aromatic alcohols under base-free condition to give the corresponding aldehyde (>85%). HR-TEM of RGO–MnCoO revealed that it was a composite material having uniform nanotubes of ~ 25nm length and 6 nm diameter with a fringe pattern showing (103) and (004) planes and a lattice space of 0.26 nm and 0.22 nm, respectively, for the spinel $CoMn_2O_4$. The detail studies by XRD, XPS, N_2-adsorption/ desorption isotherm and O_2–TPD techniques of the as prepared RGO-MnCoO nanocomposite were used to understand the role of RGO in the enhancement of catalytic activity for oxidation reaction (*Catal. Sci. Technol.* **2014**, *4*, 1771; *Appl. Catal. A: Gen.* **2014**, *487*,130; *Catal. Commun*. **2014**, *44*, 29).

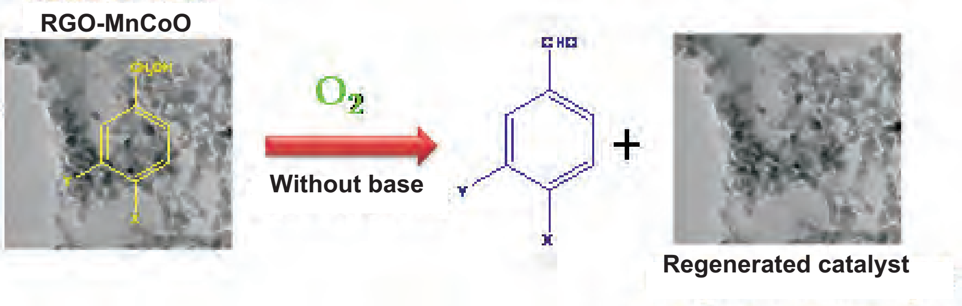

Fig. 3: Triple nano-composite catalyst for liquid phase oxidation

Catalysis

Mesoporous manganese oxide was developed by solvothermal method for liquid phase oxidation of veratryl alcohol with 96% conversion and almost completed selectivity to veratraldehyde. HR–TEM images revealed that solvothermal method generated the mesoporous manganese oxide with perforated hexagonal nanoplates while, co–precipitation method gave octahedron manganese oxide. FE–SEM images revealed that, MnOx–ST catalyst was highly porous and aggregate of hexagonal nanoplates exhibited flower like appearance (*RSC Adv*. **2014**, *4*, 19450).

Cu-Al catalysts for water gas shift reaction: A novel Cu–Al oxide catalyst was developed had various Cu species responsible for highly efficient water gas shift reaction (WGSR). Cu–Al composition of 70:30 was the best for WGSR using reformate gas composition. In addition, the Cu-Al (70:30) catalyst reduced under 100% H_2, was quite stable with time on stream of 100 h, at higher gas hourly space velocity (GHSV) of 36,201 h^{-1}. The structural investigation of our co-precipitated catalysts with varying Cu-Al compositions revealed the presence of non-zero copper as well as metallic Cu forming an essential aspect for the observed WGSR activity. The highest activity and stability of Cu-Al-7 catalyst reduced under 100% H_2 at lower temperature was found to be due to particle size stabilization and lower extent of Cu aggregation by Cu_2O and boehmite phases respectively, along with formation of various Cu species during activation protocol for 12 h. Complete CO_2 selectivity without methanation was observed for all the Cu-Al compositions irrespective of their pretreatment conditions (*ChemCatChem*. **2014**, *6*, 1698; *RSC Adv*. **2015**, *5*, 1430).

Scale-up of CSIR-NCL process for selective hydrogenolysis of glycerol to 1,2-PDO: The project was undertaken as Phase II program of previous NMITLI project for scaling up of the NCL process at pilot level. The project was successfully completed on 30th September 2014. The specific objectives were to design the high pressure pilot plant for continuous hydrogenolysis of glycerol with a scale of operation of ~ 1kg of catalyst, to undertake stepwise scale up of preparation of the proven catalyst and to evaluate the industrial bioglycerol as a feed.

Catalyst preparation scale up: The lab scale preparation of a non–noble metal (Cu–Al) catalyst developed at CSIR–NCL was scaled up to 1 kg successfully. Reproducibility of the catalyst preparation scale up at various stages ranging from 6g lab scale to max. 1Kg pilot scale was established by the repeated activity testing experiments for batch glycerol hydrogenolysis. The catalyst powder was formulated into tablets (5x5 mm) by optimizing the binder composition and was successfully tested for pilot scale trials (400 g catalyst scale).

Pilot scale glycerol hydrogenolysis: CSIR–NCL catalyst was then tested with 60% bio–glycerol (procured from Praj) loading which gave an average conversion of ~ 68 % with ~92 % selectivity to 1,2–PDO. In–situ activation of the catalyst was also optimized gives the performance results similar to previous bench mark experiment (Fig. 4). Bio–glycerol procured from another commercial source (Malaysia) was first pre–treated with Amberlite ion exchange resin to remove chloride ions. The pre–treated 60% aqueous glycerol was used as a feed. The continuous run was initially taken for ~100 h, the results of which also gave > 70% bio–glycerol conversion with ~ 80 % selectivity to 1,2–PDO.

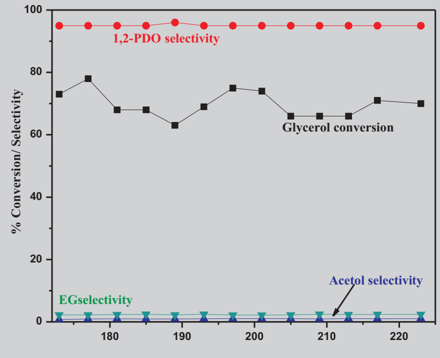

Fig. 4: 60% bioglycerol loading 20NL/h,

Product separation and recovery was done using ASPEN simulation. Based on the pilot scale data process economics has been also completed. CSIR–NCL Catalyst preparation was also done for a test purpose from the commercial catalyst supplier and the negotiations are on with some industries for commercialization of the process (*Org. Process Res. Dev.* **2012**, *16*, 1043; Patent(s): US 8,809, 593 B2, 2014, WO 2011/138643 A2).

Sustainable Chemical Industry

Catalysis

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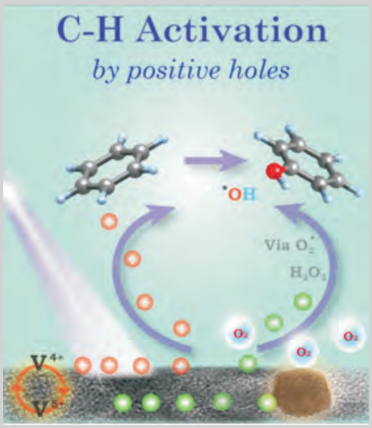
C-H activation by light at room temperature: The electron–hole pair is produced upon light absorption by semiconductors and the holes are responsible for oxidation. The usability of such energetic and positive holes at ambient temperature was checked applying heterogeneous catalysis. The concept of C–H activation was evaluated which was a difficult task to achieve at room temperature. Isolated vanadium ions incorporated in TiO_2 lattice ($Ti_{0.98}V_{0.02}O_2$) and deposited a small amount of gold on it ($Au/Ti_{0.98}V_{0.02}O_2$) to achieve it. The surrounding benzene molecules were oxidized to phenol on shining UV light on these catalysts, which was one of the demanding reactions (Fig. 2) (*ACS Catal*. **2014**, *4*, 2844).



Green catalysis with air for ethyl benzene to styrene conversion: The aim was to design a suitable catalyst providing high ethyl benzene conversion and styrene selectivity at lower temperature with sustainable activity using heterogeneous catalysis. Present industrial catalyst i.e., potassium promoted iron oxide suffers from coking as it operates at 700°C due to endothermic nature and requirement of latent heat. Efforts were made to find a suitable alternate catalyst. It led to manganese incorporated in titania ($Mn_xTi_{1-x}O_2$), which catalysed ethyl benzene to styrene around 525°C with high yield and sustainability in the presence of air as oxidant (*RSC Adv*. **2014**, *4*, 57087).

Possibility of ambient temperature catalysis: The objective was to make a catalyst for common reactions to work in a wide temperature window, right from room temperature to high temperatures. Catalysis involves the fundamental steps of bond breaking and bond making from reactants to products and electronic nature of the surface plays an important role. Demonstration was done for the CO oxidation that occured from room temperature to high temperatures on palladium surfaces (Fig. 1) by modifying the electronic nature. Changes in electronic nature and evolution of product were directly observed by the cutting edge tool known as ambient pressure photoelectron spectroscopy (*ChemCatChem* **2015**, *7*, 588).

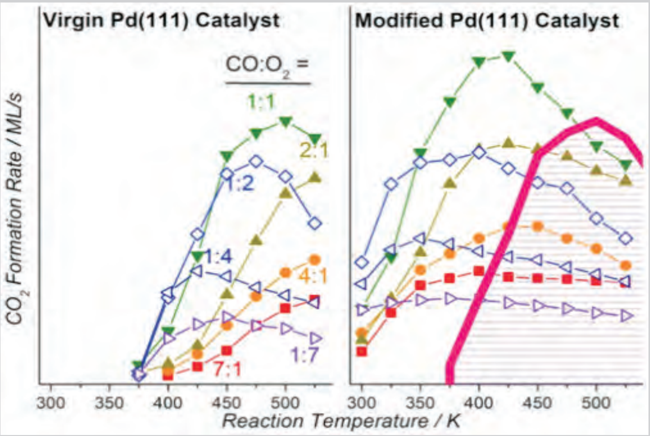


Fig. 1: Rate of CO_2 formation from virgin and modified Pd (111) catalyst surfaces

Catalysis

Uncomfortable co-existing neighbors on the surface for ambient CO oxidation: Defects sites such as oxygen vacancy were neighbored with Ce^{3+} and Cu^{2+}/Cu^{+} led to a cosmopolitan nature of different metal-ions in close proximity in Cu-doped ceria-zirconia. It facilitated the charge fluctuation of different metal-ions in redox environment and hence near ambient oxidation of CO to CO_2 (Fig. 2). A tiny amount of gold on the above catalyst enhanced the heterogeneity and further enhanced CO oxidation. The mixed nature of ions in the neighborhood on the surface with defects was in resonance with the fundamental nature of heterogeneous catalysis, which permitted different elementary reactions to occur in a tandem manner (*ChemCatChem* **2014**, *6*, 3116).

Fig. 2: A representative arrangement of Cu-doped ceria-zirconia surface with oxygen vacancies

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Applications of NMR spectroscopy

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The research was aimed to address various structural problems in the area of chemical science and material science for structure–property correlation applying methodologies based on solid state and solution state NMR spectroscopy.

Materials chemistry: Structural features of magnesium chloride and alcohol adducts as a support material for Ziegler–Natta polyolefin catalysts, adducts of 9–fluorenemethanol and isobutanol were investigated by solid state NMR (*Dalton T.* **2014**, 9143).

Sustainable Chemical Industry

Catalysis

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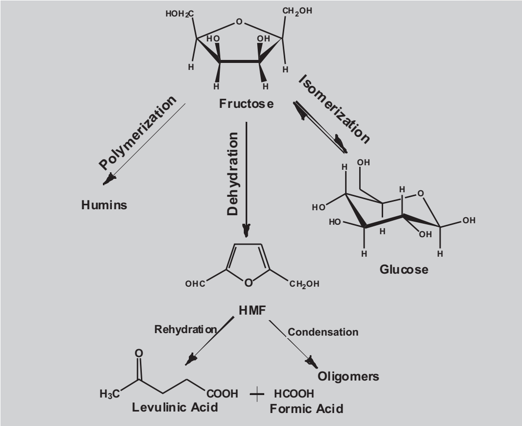
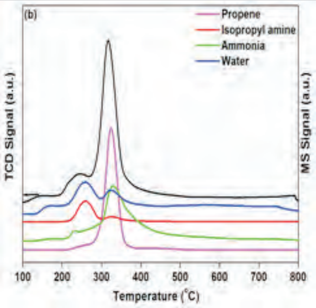
Carbohydrates from biomass are a renewable feed stock for green and sustainable future. The aim of the research was to develop the catalytic processes for the utilization of the renewable feed stock like carbohydrates from biomass to obtain 5–hydroxy methyl furfural (HMF), Levulinic acid and 2,5–dimethylfuran (DMF) a potential additive for gasoline with high octane number (*J. Chem. Sci.* **2014,** *126,* 403).

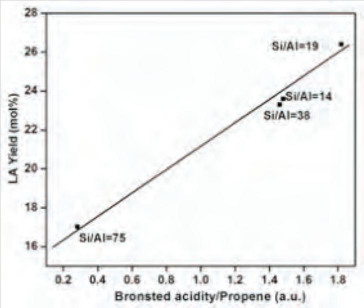
HMF from C6 sugars using AlSBA-15 catalysts: The development of two catalyst systems, one based on clay and the other based on the mesoporous SBA-15 for the dehydration of fructose to HMF in biphasic conditions was done. Various catalyst compositions were developed by incorporating aluminium into SBA-15 by post treatment with $AlCl_3$. The increase in the aluminium content led to increase in extra-framework aluminium species and optimum acidity was found for a sample with Si/Al ratio of 40. A good linear correlation between the moderately strong acidity to total acidity ratio and B/B+L ratio against HMF yield was obtained (*Micropor. Mesopor. Mat.* **2013,** *181*, 38).



Levulinic acid from C6 and C12 sugars using beta zeolites: Beta zeolites with four SiO_2/Al_2O_3 ratios (Beta-28, Beta-38, Beta-75 and Beta-150) were used to study the effect of acidity on the conversion of C6 and C12 sugars to yield Levulinic acid. The TPD of NH_3 was used to probe acidity and Brönsted acidity was investigated by TPD-MS using isopropyl amine as a probe. Isopropyl amine reacted with Brönsted acid sites led to the formation of propylene and NH_3. It was a good probe for the estimation of Brönsted acidity. Beta–38 gave good yield of levulinic acid among the four beta zeolites as its acidity was optimum for the formation. It was observed that beta zeolites lost its crystallinity and hence catalytic activity, when reactions were carried out repetitively in aqueous medium. It was attributed to the byproduct formed during the reaction, as it leached out Al from the zeolites and affected the crystallinity. The catalyst was stable and recyclable while carrying the rehydration–dehydration reaction.



Various TPD-MS traces from Beta-38 zeolite after reaction with isopropylamine

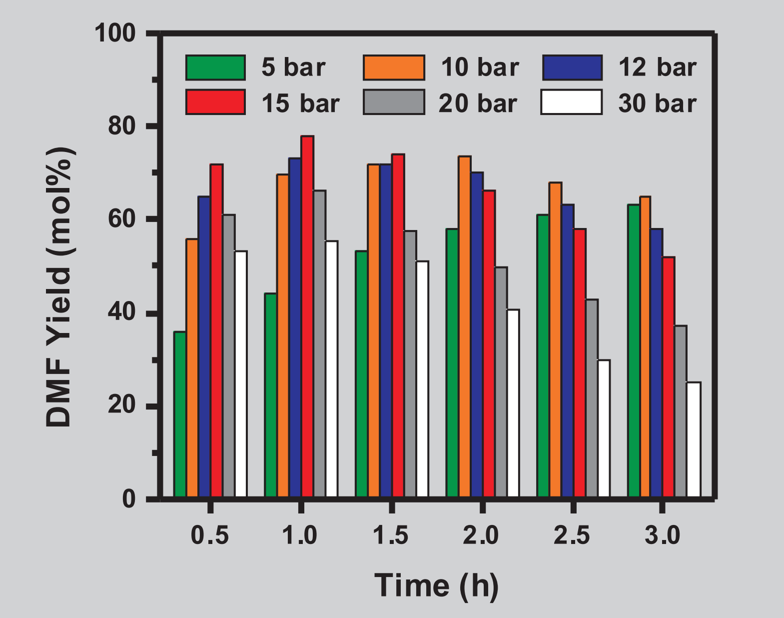


Correlation between Brönsted acidity obtained from propene formed and LA yield

Liquid fuel 2,5-dimethylfuran from biomass derived 5-HMF over supported Ru catalysts: The hydrogenolysis of biomass–derived HMF to DMF was carried out using series of catalysts with different Ru content. The effect of various reaction parameters on the performance of the catalysts was also investigated. Two catalysts systems; (i) Ru supported on hydrotalcite (HT) precursor derived oxides and (ii) Ru supported on NaY zeolite (CBV–100, Si/Al ratio = 2.5) were prepared and used for the preparation of DMF from HMF. The hydrotalcite oxide supported Ru catalyst with only 0.6 wt% of Ru showed very good catalytic activity among the three HT supported Ru catalysts in terms of HMF hydrogenolysis to yield 58 mol% DMF at 100 mol% HMF conversion at 220^{0}C temperature after four hours. The catalyst was found to be recyclable, as its performance was consistent even after 5 repeated uses for the reaction.

Catalysis

When Ru was transformed into NaY zeolite, metal dispersion and metal surface area of 2wt%Ru-NaY catalyst was 53.2% and 3.86 m^2/g respectively. The catalyst showed superior activity comparing to 1wt% and 3wt%Ru-NaY, giving 78 mol% DMF yield at 100 mol% HMF conversions within an hour at 220°C and at 15 bar H_2 pressure (*Catal. Sci. Technol*. **2015**, *5*, 1463).



Effect of H_2 pressure on DMF yield over 2wt%Ru-NaYcatalyst at various reaction times

A scheme of reaction network for the hydrogenolysis of HMF to DMF over supported Ru catalysts was proposed based on the product pattern at different time intervals during the reaction. The yield of DMF was dependent on the solvent used for the reaction with 2-propanol giving the highest DMF yield. The higher yield of DMF in 2-propanol was attributed to transfer of hydrogen from it to HMF to form DMF under reaction conditions. The Ru-NaY catalysts were found to be highly stable even after many recycles (*ACS Sustain. Chem. Eng. DOI* 10.1021/ acssus-chemeng.5b00857).

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It was the first ever experimental proof of the electrostatic preorganization hypothesis by AriehWarshel. The group has shown that extreme electric fields drive enzyme catalysis and this was an effective approach to quantify any catalytic reactions and play an important role in targeted drug design for affordable medicine (*Science* **2014**, *6216*, 1510).

Sustainable Chemical Industry

Catalysis

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Bimetallic catalysts for the conversion of sugars to sugar alcohols: Sugar alcohols (sorbitol, xylitol) find use as low calorie sweetener and are often synthesized from sugars using supported metal catalysts under high pressures (~100 bar H_2). A new low pressure (16 bar) method was developed using $PtSn/\gamma\text{-}Al_2O_3$ (AL) and PtSn/C bimetallic catalysts for efficient conversion of variety of saccharides. It included C5 sugars (xylose, arabinose), C6 sugars (glucose, fructose, galactose), hemicelluloses (xylan, arabinogalactan), inulin and agricultural wastes (bagasse, rice husk, wheat straw) into sugar alcohols (sorbitol, mannitol, xylitol, arabitol, galactitol). PtSn/AL showed enhanced yields of sugar alcohols (40-90%) by 1.5 to 3 times than Pt/AL (20-50%) in all these reactions. Catalysts characterized by various techniques (XRD, TEM, ICP) revealed its stability. XPS study disclosed formation of electron deficient Sn species which helped in polarizing carbonyl bond to achieve enhanced hydrogenation activity (*Green Chem.* **2014**, *16*, 4944; *Bioresource Technol.* **2015**, *178*, 36).

Brønsted acidic ionic liquids for the synthesis of sugars: Hemicellulloses, a hetero-polysaccharide made up of several C5 and C6 sugars is the 2nd largest plant derived renewable polysaccharide available on earth. Brønsted acidic ionic liquid (BAIL) catalyzed hydrolysis of hardwood hemicelluloses was carried out to achieve 87% yield for C5 sugars (xylose+arabinose) in a one-pot method, at 160°C and in water media. The efficiency of the ILs and acid strength both followed the similar trend; $[C_3SO_3HMIM][HSO_4]$ > $[C_3SO_3HMIM][PTS]$ > $[C_3SO_3HMIM][Cl]$ > [BMIM][Cl]. The ion-dipole type interaction present between BAIL and substrate proposed by ^{1}H NMR study suggested help to achieve better activity with BAIL compared to mineral acid, H_2SO_4. These catalysts overcame the diffusion limitations generally observed with solid acid catalysts and provided better activity (*Catal. Sci. Technol.* **2015**, *5*, 531).

Valorization of hemicelluloses to xylose and furfural: An environmentally benign process for furfural synthesis from diversified real substrates using SAPO-44 catalyst was reported. Selective conversions of hemicelluloses from raw biomass (bagasse, rice husk & wheat straw) to extraordinarily high yields of furfural of about 93% were attained at 170°C and in the presence of biphasic solvent system in an efficient one-pot methodology. 82% yield of furfural was also achieved directly from isolated hemicelluloses under similar reaction conditions. Hydrophilic SAPO-44 having higher hydrothermal stability showed similar activity for all the substrates minimum up to 8 times in recycle runs. Various physico-chemical characterizations (XRD, TGA-DTG, TPD-NH_3, solid state NMR) of fresh and spent catalysts were studied on the SAPO-44 stability (*RSC Adv.* **2014**, *4*, 26215).

Depolymerization of lignin to aromatic monomers under milder conditions: The depolymerisation of six different types of lignins by solid acid catalysts under inert atmosphere yielded aromatic monomers with high selectivity (>90%) and good mass balance (95±10 %). The GC, GC-MS, HPLC, LC-MS, and GPC analysis of products confirmed the formation of aromatic monomers. Confirmation of functional groups in products was done by FT-IR, ^{1}H and ^{13}C NMR studies. Isolation of major products by column chromatography and their further characterization by NMR was carried out to show a way for isolation of these products. Detailed characterization of all lignins obtained from various sources helped in substantiating the catalytic results obtained in these reactions. Meticulous study on fresh and spent catalysts revealed that the amorphous catalysts are preferred to obtain reproducible catalytic results (*ACS Catal.* **2015**, *5*, 365).

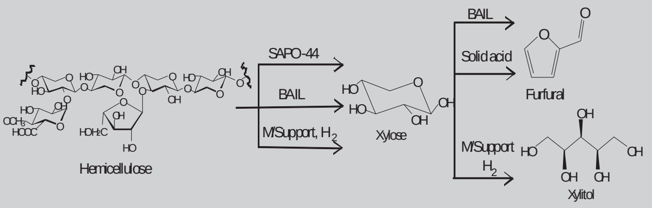

Fig. 1: Conversion of hemicelluloses into sugars, furfural and xylitol

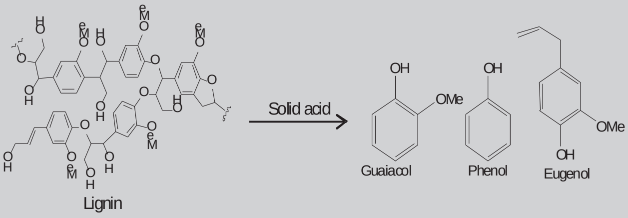

Fig. 2: Depolymerizationof lignin into aromatic monomers using solid acid catalysts

Sustainable Chemical Industry

Catalysis

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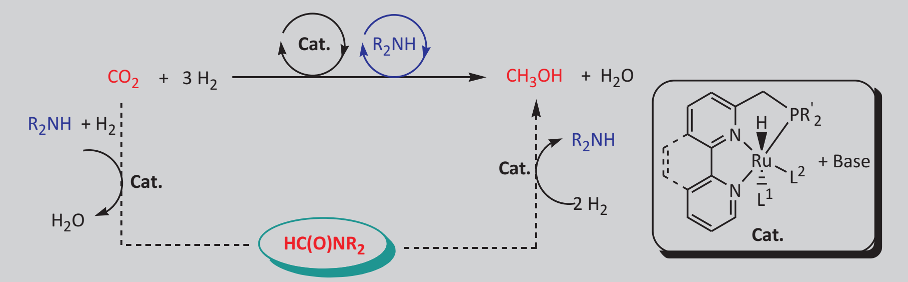
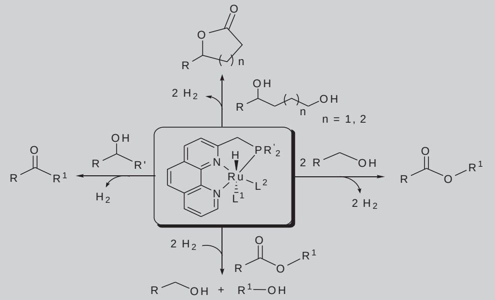
The research was aimed to develop well-defined homogeneous catalysts for hydrogenation, and dehydrogenation reactions.

Catalytic conversion of CO_2 to methanol: A cascade approach: The development of a catalytic system for effective conversion of CO_2 to methanol to serve as an energy carrier and a versatile basic chemical is the need of the time to meet the growing energy demands of the current society avoiding environmental issues, resource depletion and CO_2 emission. Owing to rational tuning of reactivity and selectivity of homogeneous catalysts much attention was paid for its utility in selective hydrogenation of CO_2. The research reported a cascade hydrogenation of CO_2 to methanol under mild reaction conditions catalyzed by well-defined homogeneous ruthenium(II)-complexes (Scheme 1).



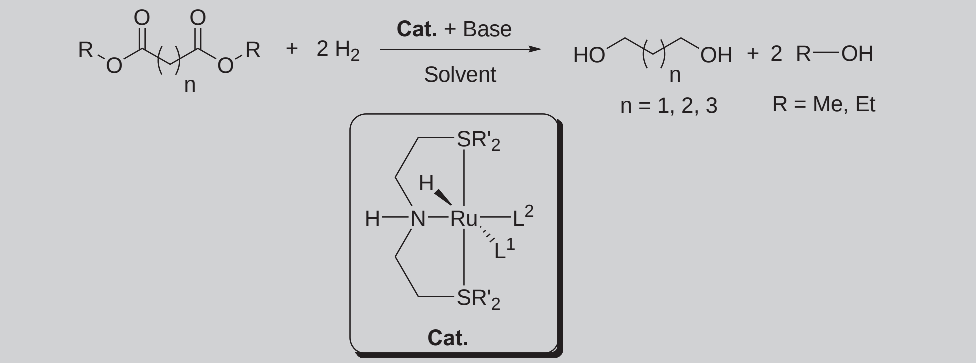
Scheme 1. A cascade hydrogenation of CO_2 to methanol

Catalytic process for the formation and hydrogenation of esters including lactones: A series of Ru(II)-pincer complexes pertaining phenanthroline moiety were synthesized and its synthetic utility was investigated in sustainable catalysis. The direct and selective conversion of alcohols to value-added products like primary alcohols to esters, secondary alcohols to ketones and diols to lactones respectively with liberation of hydrogen gas and efficient hydrogenation of esters including lactones to the corresponding alcohols under very mild, solvent-free conditions was observed (Scheme 2).



Scheme 2. Catalytic process for the formation and hydrogenation of esters

Catalytic process for the synthesis of terminal diols from dialkyl aliphatic esters: A new chemical process for the synthesis of 1,3-propanediol (1,3-PDO) from renewable dialkyl malanotes using soluble SNS-Ru(II)-pincer complexes under mild condition like low hydrogen pressure and low temperature was established (*J. Organomet. Chem.* **2014,** *48,* 19; 2014-INV-0120; 0358/DEL/2015; 0417/DEL/2015).



Scheme 3. Catalytic process for the synthesis of terminal diols from dialkyl aliphatic esters

Sustainable Chemical Industry

Catalysis

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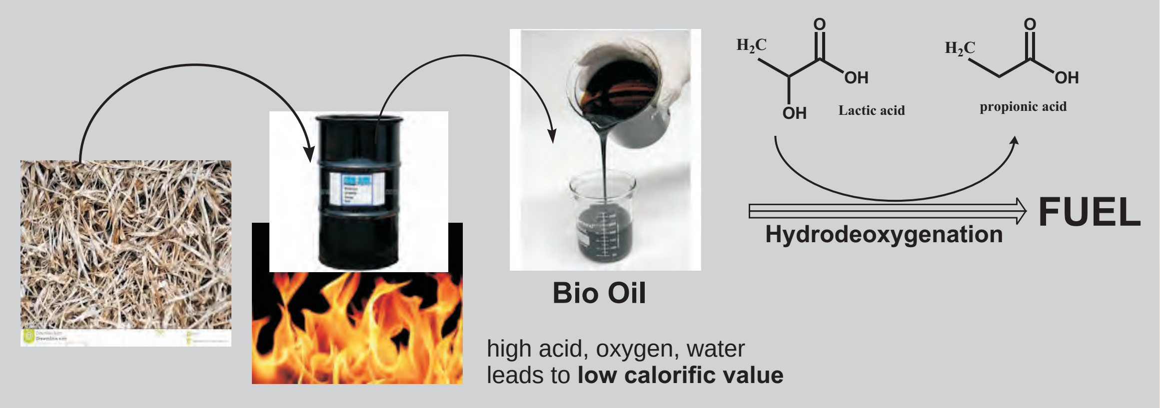
Molybdena modified calcium pyrophosphate for deoxygenation of bioderived lactic acid: Direct deoxygenation was preferred over hydrodeoxygenation to increase the energy of biomass and reduce its transportation costs of biomass due to the atom economy. Calcium pyrophosphate (CP) modified by molybdenum oxide was used for catalytic deoxygenation of lactic acid as model bioderived substrate. The deoxygenation of lactic acid was carried out at 375°C using 50% (w/w) aqueous solution of lactic acid. Acidity of the catalyst played a crucial role in product selectivity. Only support showed very high selectivity for acrylic acid whereas under identical reaction conditions molybdena supported CP showed 26% selectivity for propionic acid with 100% conversion. Acidic supports like γ-Al_2O_3 yielded acetaldehyde as a major product. It is a promising catalyst for deoxygenation of various other bioderived oxygenates.



Hydrogenation of nitro and carbonyl compounds under atmospheric pressure and room temperature using Pd/MgF_2 catalysts: Palladium supported on magnesium fluoride prepared by very simple one pot precipitation method showed surprisingly high catalytic activity for hydrogenation of carbonyl and nitro compounds at room temperature and atmospheric pressure. The unusually high activity was found to be due to metal support interaction which tuned the properties of palladium for hydrogen activation when supported on MgF_2. The acidic properties of the support contributed for very high dispersion of Pd and in turn hydrogen activation. Pd supported on MgF_2 led to the room temperature, atmospheric pressure hydrogenation of carbonyl and nitro compounds. It showed the 96% conversion for acetophenone with 88% selectivity for 1-phenyl ethanol, while 99% conversion for nitrobenzene with 100% selectivity for aniline was observed. The strong metal support interaction helped the efficient recycle of the catalyst with no palladium leaching during hydrogenation. The in situ FTIR studies helped to determine the mechanism of the catalytic reaction and the exact role of palladium and metal fluoride support in the catalytic cycle. This work was carried out in collaboration with Prof. Erhard Kemnitz, Humboldt University, Germany as a part of CSIR–BMBF project.

Fig. 1: Catalytic activity of palladium supported on metal fluorides

Sustainable Chemical Industry

Catalysis

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The aim was to develop a facile route for the optimization of the synthesis variables and also explore the use of cheaper precursors for the synthesis of promising materials for its enhanced performance in organic transformations and environmental application.

Development of facile route for the synthesis of Sn-BEA molecular sieve: Sn-Beta (Sn-BEA) molecular sieve exhibited excellent performance in various heterogeneous organic reactions where Lewis acid sites played a major role. A facile route for its synthesis by hydrothermal crystallization in the fluoride medium using unseeded Aluminium-free hydrogel containing a source of oxyanion was developed. The effectiveness of an oxyacid in decreasing the synthesis time was found to follow the trend as: $HClO_4$ >H_3PO_4 >H_2SO_4. The molar ratios of $TEAOH/SiO_2$, HF/SiO_2 and SiO_2/SnO_2 in initial gel composition were found to influence not only the nature of the phases but also the crystallization periods. The enhanced cyclohexanone conversion was showed by Sn-BEA catalyst prepared by this route under identical set of conditions (*Adv. Porous Mater.* **2014,** *2*, 1).

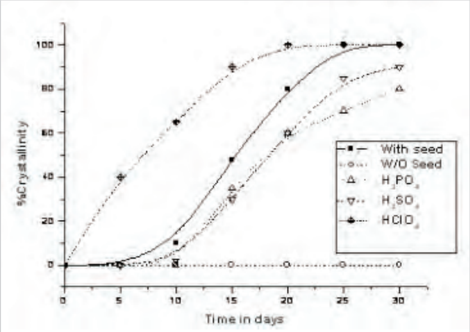

Fig. 1: Kinetics of crystallization of Sn-Beta synthesis in presence or absence of the seed and different oxyacids

Optimization of the synthesis variables for zeolite-based micro-mesoporous composites: Zeolitic bimodal micro– and meso– porous composites were prepared by post–synthesis modification by alkali treatment and direct synthesis by different methods such as two–stage crystallization, seeding and desilication followed by crystallization. Optimized liquid to solid ratio (alkali volume/g. of zeolite) is a crucial parameter in post–synthesis treatment to synthesize the bimodal micro–and meso–porous LTL zeolite. The evaluation of these materials for their performance in Knoevenagel condensation and xylose hydrogenation reactions was also done. Optimization of the pre–crystallization period for the initial formation of LTL–zeolite seeds in the direct synthesis of LTL/MCM–41 composites via two–step process was done. Compositionally different Al–SBA–15 and K–LTL/MCM–41, TS–1/MCM–41, MFI/SBA–15 composites were synthesized directly by optimizing parameters viz. the gel composition, crystallization temperature and time.

Synthesis of fly ash composites for the removal of congo red: A series of fly ash/$NiFe_2O_4$ composites were prepared by varying the percentage mass ratio of fly ash: $NiFe_2O_4$ in the range of 0:100 to 100:0. The spinel nickel ferrite phase was found capable of getting anchored with the fly ash surface and which exhibited more crystalline nature as compared to pure $NiFe_2O_4$ phase. The composite having percentage mass ratio of fly ash: $NiFe_2O_4$ = 50:50 exhibited maximum Cr adsorption from the aqueous solution on account of the higher BET surface area, more porous character, favorable condition for diffusion of dye molecules and combined effect of chemisorptions and physisorption. The recyclability with adsorption capacity of the magnitude was shown to be 23.33 mg g^{-1} which was much higher than individual fly ash, $NiFe_2O_4$ and other composites under the optimum conditions (*Mater. Chem. Phys.* **2014,** *148,* 371).

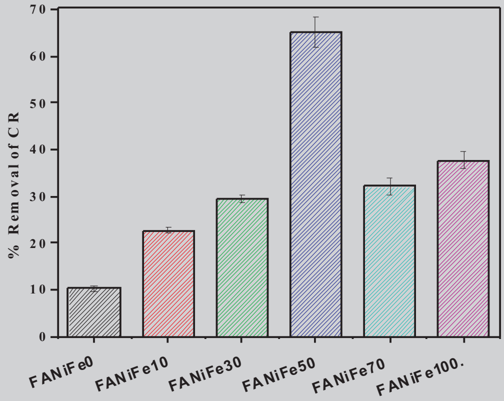

Fig. 2: Comparison of CR adsorptive removal by $FANiFe_0$, $FANiFe_{10}$, $FANiFe_{30}$,$FANiFe_{50}$, $FANiFe_{70}$ and $FANiFe_{100}$

Sustainable Chemical Industry

Catalysis

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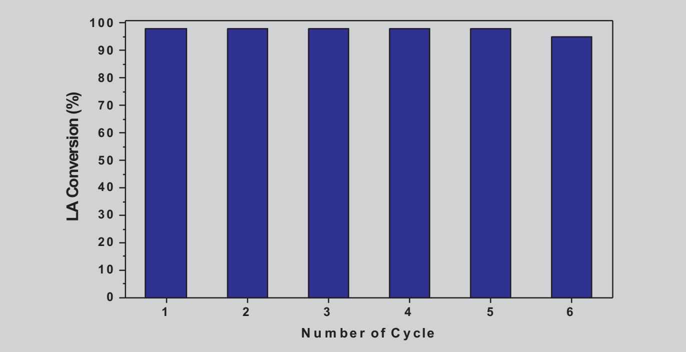
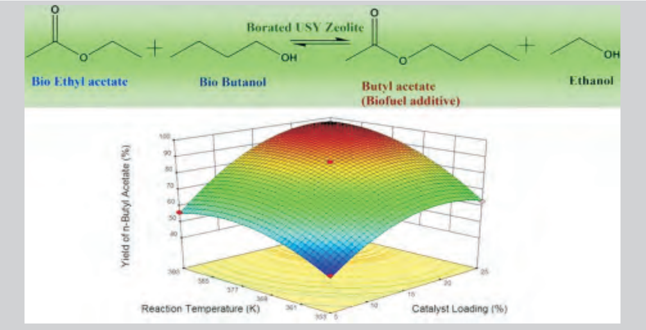
The renewable feedstock such as microcrystalline cellulose; levulinic acid; acetic acid; citric acid; butyl acetate and phenol was systematically converted into valuable renewable chemicals and fuels using various heterogeneous catalysts. The reaction kinetics studies were done using different kinetic models.

Esterification of levulinic acid to ethyl levulinate: The use of desilicated H-ZSM-5 (DH-ZSM-5) as heterogeneous acid catalyst for EL production in a closed system was studied. Maximum Levulinic acid conversion obtained to 95% and the catalyst was reusable for up to six cycles. A pseudo-homogeneous (P-H) kinetic model was also proposed. The activation energy decreased from 73.14 to 21.08 kJ mol^{-1} after increasing the catalyst to LA ratio from 0.10 to 0.25 that indicated a kinetically controlled reaction.



Transesterification of renewable ethyl acetate to butyl acetate: Butyl acetate, a renewable biofuel additive was synthesized by transesterification of ethyl acetate with butanol via a renewable and sustainable route. The synthesis of butyl acetate by this route was more advantageous over conventional Fischer Esterification. Heterogeneous zeolite catalyst such as Ultra Stable Y (USY) and its modified versions obtained by borating (B) on parent USY were used for the synthesis of butyl acetate.

Response surface methodology was employed to optimize the process parameters for transesterification of butanol with ethyl acetate over a 4% (w/w) B–USY catalyst. The influences of three crucial process variables such as catalyst loading, molar ratio, and reaction temperature on yield of butyl acetate were addressed by Box–Behnken experimental design (BBD). 4% (w/w) B–USY was proved to be a potential catalyst with 96% yield of butyl acetate at optimum process parameters. The 4% (w/w) B–USY catalyst was found to be reusable for 6 catalytic cycles.



Catalytic upgrading of citric acid to tri-butyl citrate plasticizer: The synthesis of tributyl citrate (TBC) a non–toxic compound used as a plasticizer was aimed. Easy to separate and environmentally friendly, reusable heterogeneous catalysts were used for its synthesis. The use of renewable citric acid (CA) and butanol makes the process “completely sustainable”. This work found that phosphonated USY zeolite is more effective with 100% CA conversion and 93% TBC yield. This study opens new avenues of research in the development of a sustainable and industrial benign catalytic process for the synthesis of environmentally friendly and non-toxic TBC plasticizer (*Chem. Eng. Res. Des*. **2015**, *98*, 212).

Sustainable Chemical Industry

Biochemical processes and engineering

Glycosylation of recombinant IgG produced in Chinese Hamster ovary cells

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Manufacturing of biosimilars is identified as a significant contributor to the bioeconomy opportunity in India. Many biosimilar proteins, such as erythropoietin and monoclonal antibodies are produced in animal cells due to the requirement of post translational modifications like glycosylation. Biosimilar manufacturing requires mimicking the glycoform profile of the innovator drug without access to the original clone and process conditions for such therapeutics. Knowledge of how process and medium factors affect glycosylation is necessary to design processes to achieve a pre-defined glycoform profile of the recombinant protein product. The effect of medium supplements on glycosylation of IgG was investigated and showed a higher proportion of high mannose M5 glycans when cells were cultured with the alternate sugars. Supplementation of galactose with glucose maintained at low concentrations allowed both lower accumulation of lactate, a waste metabolite, and reduction of high mannose glycans. Surprisingly, substantially higher M5 glycan percentages were found in cultures supplemented with Mn^{2+} when glucose was absent or limiting, both in the presence and absence of galactose, but not when glucose was available in abundance. This was the first report linking the effect of Mn^{2+} on high mannose glycan content to glucose availability (*Biotechnol. Progr.* **2015**, *31*, 460).

A process for the production of lactose free proteins from milk whey

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A process was developed for the separation of proteins from milk whey. The modified **c**ellulose fiber under this project showed 3437.91 ± 52.7 (mg/ m^2) milk whey protein adsorption in comparison to commercial membrane Sartobind®, which was given 2753.12 ± 42.5 (mg/ m^2) milk whey protein adsorption under the laboratory condition. The developed process showed a very high economical impact as the preparation Cost/m^2 of modified cellulose fiber is ₹ 15,340 and Flux 17910 L/hr/m^2 with negligible decrease in buffer flux after 30 consecutive runs; whereas Sartobind® has Purchase Cost/ m^2: ₹ 21,88,292 and Flux 3464 L/hr/m^2 with 77% decrease in buffer flux after 8 consecutive runs. The product obtained using developed process was lactose free whey protein (Fig.), which is not possible using conventional ultrafiltration process that is generally being used at industrial level operations.

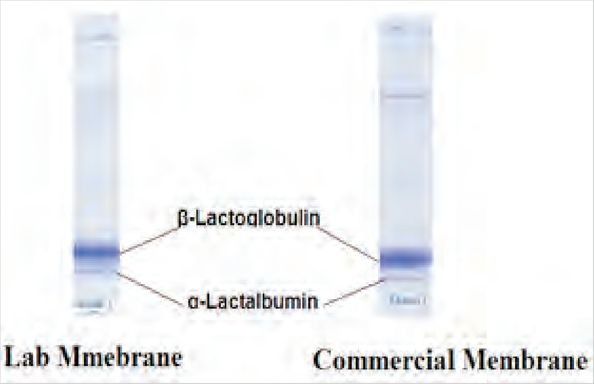

Fig: SDS-PAGE pattern of eluted protein obtained at pH 7.0

Sustainable Chemical Industry

Multiphase reactors and flow processes

Artificial intelligence based modeling of chemical and chemical engineering systems

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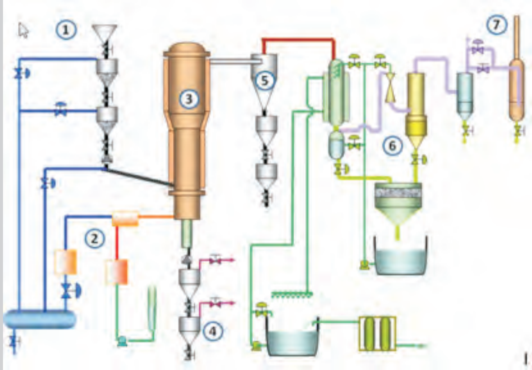
The Genetic programming (GP) based symbolic regression offers an attractive avenue to extract correlations, explore candidate models and provide optimal solutions to the data–driven modeling problems. Its novelty is that it searches and optimizes both the form and parameters of an appropriate linear/ nonlinear function that best fits the given process data. Despite its novelty and effectiveness, GP has not been applied widely in chemical sciences and engineering. The Artificial Intelligence Systems Group (AISG) at CSIR–NCL developed a number of GP–based strategies for modeling chemical and chemical engineering systems.

Artificial intelligence based modeling of high ash coal gasification: The data collected from these experiments was used in the mathematical modeling of FBCG, which was conducted by utilizing two artificial intelligence (AI) strategies namely genetic programming (GP) and artificial neural networks (ANNs). A comparison of the GP and ANN–based models revealed that their FBCG performance prediction accuracies and generalization capabilities vary from good to excellent. The models developed gainfully utilized to design Indian coal based gasifiers. Artificial intelligence based models were developed for the experiment. The pilot plat comprised various processes such as coal feeding system, gasifying agent feeding system, fluidized bed gasifier, ash extraction system, cyclone separator, syngas cooling and cleaning system and Flare stack (*Ind. Eng. Chem. Res.* **2014**, *53*, 18678).



Fluidized bed coal gasification pilot plant at CSIR-CIMFR, Dhanbad

Prediction of reactivity ratios in free radical copolymerization from monomer resonance–polarity (Q–e) parameters: Exclusively data–driven, Q–e parameters based new models were developed for the reactivity ratio prediction in free radical copolymerization using AI–based GP formalism. The GP based models exhibited superior reactivity ratio prediction accuracy and generalization performance (with correlation coefficient magnitudes close to or greater than 0.9) when compared with the Alfrey–Price (AP) and artificial neural network–based models and therefore possessed the potential of replacing the widely used AP models (*Int. J. Chem. React. Eng.* **2015**, DOI 10.1515/ijcre–2014–0039).

Computational intelligence based models for prediction of elemental composition of solid biomass fuels from proximate analysis: Computational intelligence based models were proposed for the accurate prediction of the elemental composition (carbon, hydrogen and oxygen) of coals from their proximate analysis (volatile matter, ash, fixed carbon). These models obviated the need to perform ultimate analysis of coals which is tedious and costly to perform when compared with the proximate analysis (*Int. J. Syst. Assur. Eng. Manag.* **2014**, DOI: 10.1007/s13198–014–0324–4).

Pharmaco-kinetic modeling of caco-2 cell permeability using genetic programming (GP) method: An accurate prediction of the pharmacokinetic properties of orally administered drugs is of paramount importance in pharmaceutical industry. Caco–2 cell permeability is a well established parameter for assessing the drug absorption profiles of lead molecules. Due to the restrictions on animal testing, prohibitive *in situ* models and ethical issues, the development of predictive models are essential. A GP–based approach was proposed for the *in silico* prediction of Caco–2 cell permeability using a diverse set of molecules. The predictions yielded a high magnitude for the training and test set correlation coefficients with low values for root–mean–square–errors, indicating an excellent Caco–2 permeability prediction and generalization performance by the GP model (*Lett. Drug. Des. Discov.* **2014**, *11*, 1112).

Sustainable Chemical Industry

Mathematical and computational modeling

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Relativistic extended coupled cluster method for magnetic hyperfine structure constant: The general implementation of the four-component spinor relativistic extended-coupled-cluster (ECC) method was implemented to calculate first-order property of atoms and molecules in their open-shell ground-state configuration. The implemented relativistic ECC was employed to calculate hyperfine structure constants of alkali metals (Li, Na, K, Rb, and Cs), singly charged alkaline-earth-metal atoms (Be+,Mg+,Ca+, and Sr+) and molecules (BeH, MgF, and CaH). The group has compared the ECC results with the calculations based on the restricted active space configuration interaction (RAS-CI) method. The results are in better agreement with the available experimental values than those of the RAS-CI values.

Relativistic equation of motion coupled method for the double ionization potentials of closed shell atoms: The relativistic equation-of-motion coupled-cluster method for double-ionization spectra (DI-EOMCC) of the closed-shell atomic systems was implemented. The principal valence double-ionization potential values of He and alkaline-earth-metal (Be, Mg, Ca, Sr, and Ba) atoms were calculated. These results were compared with the results available from the NIST database and other ab initio calculations. The group has achieved an accuracy of 0.1%, which was an improvement over the first-principles T -matrix calculations. The group presented the results using the second-order many-body perturbation theory and the random-phase approximation in the equation-of-motion framework. The results were compared with the DI-EOMCC results (*J. Phys. B-At. Mol. Opt.* **2015**, *48*, 115009).

Interatomic coulombic decay using equation of motion coupled cluster: Interatomic Coulombic decay (ICD) is an efficient and ultrafast radiation less decay mechanism which can be initiated by removal of an electron from the inner-valence shell of the atom or molecule. Generally, the ICD mechanism occurs in weakly bound clusters. CAP/EOM-CC method was used for the study. It consisted the combination of complex absorbing potential (CAP) with the equation-of-motion coupled-cluster (EOM-CC) method. This technique was applied to determine the lifetime of an auto ionized, inner-valence excited state of the $(HF)_N$; N=2,3. THE CAP/EOMCC was also used to study the lifetime of 2s inner valence excited state of Ne atom in Ne- X; X = Ne, Mg, Ar, system at various inter nuclear distances. The lifetime of ICD in Ne-X; X = Ne, Mg, Ar, systems. CAP/ EOMCC was also used to study the auger decay of core hole and double core hole states (*J. Chem. Phys.* **2015**, *143*, 24305).

Resonance of CO_2 : The potential energy curve for the resonance states of CO^-_2 was studied upon bending as well as symmetric and asymmetric stretching of the molecule. Specifically, the C–O bond length was stretched from 1.1 Å to 1.5 Å and the bending angles were changed between 180° and 132°. Upon bending, the low energy resonance state was split into two components i.e., $^2A_1$, $^2B_1$ due to the Renner Teller effect, which behave differently as the molecule is bent (*J. Chem. Phys.* **2014**, *141*, 164113).

Potential energy surface using extended coupled cluster: Extended coupled cluster method was used for the potential energy surface (PES) study using coupled and a decoupled approximation. HF, N_2 and C_2 were studied as test systems. N_2 and C_2 being doubly and triply bonded, were considered to be interesting systems for PES study. For efficient and accurate calculation of potential energy surfaces of HF, N_2 and C_2 molecules ECC method was used. ECC equations were solved in a coupled as well as decoupled manner (*Chem. Phys. Lett.* **2014**, *612*, 209).

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Extensive atomistic simulations and statistical analyses are combined to probe biologically relevant macromolecular phenomena. It included understanding the pathways that led to self-assembly of amyloidogenic proteins responsible for proteopathic diseases (Alzheimer's, Parkinson's and Prion diseases, and type-II diabetes). The important modes of association, free energy barriers and the conformational propensities were calculated and benchmarked against relevant experimental data to yield mechanistic insights. Interfacial simulations with nanomaterials were used to understand how the disease prone pathways may be blocked and the information potentially used in the design of suitable therapeutics. In addition, protein behavior at extremes of temperatures ('cold' and 'heat' denaturation) were studied with the aim of understanding how their thermal stabilities can be controlled. The work showed the relevance for the food and cryo-preservation industries.

Sustainable Chemical Industry

Mathematical and computational modeling

Development and application of new methods for excited state processes in bio-chromophores

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The major activities included development and application of electronic structure methods that can be used to understand excited state processes in molecules, where strong correlations are crucial. The hybrid QM/MM methods were developed based on the electronic structure methods. The group is being involved in studying the various excited state and ionization mediated processes in melanin and related molecules.

Low scaling hybrid QM/MM method: A perturbative approximation was developed for hybrid equation of motion coupled cluster/ effective fragment potential method that can accurately estimate solvatochromic shifts for ionization and excitation energies. The main aim of this work was to develop computationally cheap methods that are capable of calculating excited state energies and properties (*J. Chem. Phys.* **2014**, *140*, 94101).

Components of the interaction energy that affects IR spectra: The various components of the interaction energy in case of weakly bound complexes and the major component that is correlated with the shift in the vibrational spectra were reported. It was noticed that the red shift was due to electrostatic interactions for fluorinated phenyl-acetylene the acetylenic CH stretch (*Phys. Chem. Chem. Phys.* **2014**, *16*, 25247, **2015**, *17*, 434).

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Modeling gating charge and voltage changes in response to charge separation in membrane proteins : Measurements of voltage changes in response to charge separation within membrane proteins can offer fundamental information on mechanisms of charge transport and displacement processes. An attempt was made to solve this problem by using a coarse-grained model of membrane proteins, which included an explicit description of the membrane, the electrolytes, and the electrodes. The model evaluated the gating charges and the electrode potentials upon charge transfer within the protein. Interestingly, it was found that charge-separation processes with different spatial directions (but the same distance perpendicular to the membrane) can give similar observed voltage changes (*P. Natl. Acad. Sci.* USA **2014**, *111*, 11353).

Structural order of water molecules around hydrophobic solutes: Lengthscale dependence and solute-solvent coupling: If life can be considered a massive self-assembly process, water mediated interactions provide the driving force. Although hydrophobicity is a well-defined macroscopic quantity, the understanding at the molecular level is quite poor. Using extensive molecular dynamics simulations it was demonstrated that in complex biomolecule water, structure and dynamics would be dynamically coupled to the local chemical and topological heterogeneity of the solute both static and dynamic.

Sustainable Chemical Industry

Chemical engineering science

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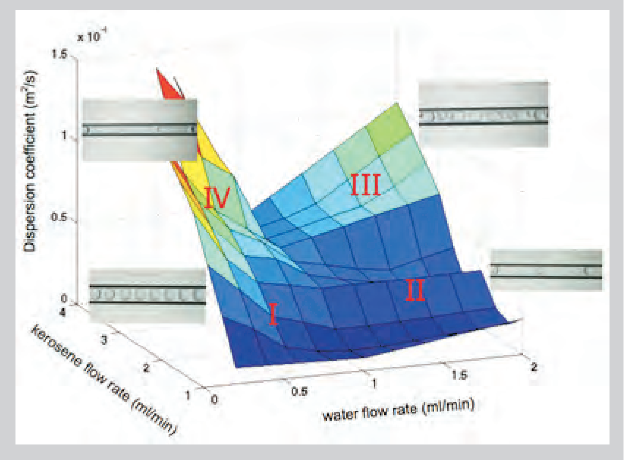
Effect of interfacial mass transfer on the dispersion in segmented flow in straight capillaries: The effect of interfacial mass transfer on the extent of dispersion in liquid–liquid segmented flow in straight capillaries was studied. Dispersion coefficient was seen to go through a minimum with increasing flow rates in the absence of interfacial mass transfer. The physicochemical properties of both the phases and slug lengths were seen to vary along the capillary length in the presence of mass transfer. The extent of dispersion was always higher in the presence of interfacial mass transfer. Simulations of a 1st order interfacial reaction considering varying slug lengths showed a significant change in optimum operating parameters than the conventional approach. The approach is now being extended for segmented flows with reactions (*AIChE J.* **2015**, DOI: 10.1002/aic.14945; *Can. J. Chem. Eng.* **2014**, *92*, 2166).



Understanding interfacial precipitation in small capillaries: Particle laden flows in small channels often leads to clogging making them inoperable for long time continuous operation. In order to control the flow of solids in micro-capillaries, it is necessary to understand the mechanism of solid generation and also the relative rates of different associated phenomena. A detailed analysis of these factors for a wide range of flow regimes (viz. slug, droplet, stratified, annular etc.) helped to quantify the conditions that can help avoid clogging of small channels. A few interesting features of interfacial precipitation were also observed for liquid–liquid and gas–liquid–liquid systems.

Computational chemistry based approach for prediction of kinetics of highly exothermic reactions: Nitration of aromatic as well heterocyclic substrates is very important for variety of applications. An approach was developed based on Hammett theory for the estimation of reaction kinetics using quantum chemical calculation (usage of p-EDA descriptor) to facilitate a reliable design of reactors to produce the important nitro-derivatives. The computed values of substitution constants of various functional groups on aromatic substrates were found close match with experimental values for halogenated as well as non-halogenated derivatives of benzene and also for the heterocyclic compounds. The established approach helped to quantify the effect of sulfuric acid strength and temperature on rate constant in a very accurate way (error below 5%).

Sustainable Chemical Industry

Chemical engineering science

Two-phase flow boiling in small channel

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The identification of boiling regimes was carried out with time series analysis, energy balance and reported literature. The presented experimental results are useful to gain the insight into complex boiling flows in tubes and will provide a sound basis for further work in this area.

Two phase flow boiling in small channels: A brief review: Boiling flows are encountered in a wide range of industrial applications such as boilers, core and steam generators in nuclear reactors, petroleum transportation, electronic cooling and various types of chemical reactors. Many of these applications involve boiling flows in conventional channels (channel size ≥ 3mm). Flow boiling regimes, dry out, flow instabilities, heat flux and wall temperature profiles are some of the key design issues in such flows. An attempt was made to provide a perspective and to present available information on boiling in small channels in terms of channel size, flow regimes, heat transfer correlations, pressure drop, critical heat flux and film thickness. The strengths and weaknesses of published approaches and computational models of boiling in small channels were also identified (*Sadhana* **2013**, *38*, 1083).

Two phase flow boiling in 19 mm tube: Experiments and CFD modeling: Heat transfer coefficient, flow boiling regimes, flow instabilities, pressure drop and condition like dry out are some of the key issues in every boiling flow study. It observed that limited experimental data base available on 19mm ID channel diameter i.e. a typical tube diameter of steam generator. The experimental set-up was designed for studying boiling flows in 19 mm ID tube in such a way that different flow regimes occurring in a steam generator tube (from pre-heating of sub-cooled water to dry-out) could be investigated by varying inlet conditions. A special feature of these experiments was that time-dependent temperatures were measured at four locations along the channel. The steady-state temperature was estimated and identification of flow boiling regimes was done with transient characteristics using time series analysis. Experimental data and corresponding results were well in agreement with the reported correlations and observations.

Two phase flow boiling pressure drop in small channels: The focus was on pressure drop in two phase flow boiling in tubes of 19 mm diameter. The reported results cover a reasonable range of heat and mass flux conditions such as 9 – 27 kW/m^2 and 2.9 – 5.9 kg/m^2 s respectively. The various existing correlations were assessed against experimental data for the pressure drop in a single, vertical channel during flow boiling of water at near-atmospheric pressure. A special feature of these experiments was that time-dependent pressures were measured at four locations along the channel. The steady-state pressure-drop was estimated and identification of flow boiling regimes was done with transient characteristics using time series analysis. Experimental data and corresponding results are compared with the reported correlations. The results are useful to understand the key aspects of flow boiling in small channels (*Procedia IUTAM* **2015**, *15*, 313).

Void fraction measurement using electrical capacitance tomography and high speed photography: The measurement of two-phase flow parameters such as flow regime and void fraction is considerably important and play an important role in characterization of the hydrodynamic behavior of such gas-liquid two phase systems. According to industrial applications; it is essential to develop measurement technique for void fraction measurement which can work in hot and opaque systems. An attempt was made to establish Electrical Capacitance Tomography (ECT) facility for measuring void fraction and flow regimes as well as develop suitable data processing methodologies. The focus was to measure void fraction using ECT technique and compares it with conventional and high speed photography technique. It will give guidelines of using ECT technique for hot and opaque systems like boiling flows (*Chem. Eng. Res. Design* **2015**, *94*, 1).

Resource Centers

Catalyst Pilot Plant

The Catalyst Pilot Plant (CPP) is well equipped with the required facilities for the scale-up studies at different scale of operations. It houses the fixed bed reactors for the performance evaluation of the catalysts in various hydrocarbon conversion reactions of academic and industrial importance. CPP is well equipped with an array of physico-chemical characterization facilities.

The process for the preparation of the proprietary catalyst for CSIR-NCL's process of selective hydrogenolysis of glycerol to 1,2-propanediol was scaled up and the product was formulated with sufficient crushing strength. 15 Kg of an optimum zeolite-based adsorbent for the generation of oxygen was prepared and supplied. The proprietary catalyst developed by BPCL R&D Centre, Noida was scaled up to 2.5 kg per batch level and 8 kg catalyst was supplied (in powder form) to BPCL. In order to create and sustain the specialized knowldge competencies, we also focussed on the following research areas :

- Oxyanion-induced hydrothermal crystallization of Sn-BEA molecular sieves.
- Fly ash/NiFe2O4 composite for the removal of Congo red from aq. solutions.
- Zeolite-based micro/mesoporous composites for specialty chemicals.
- Catalyst screening, kinetics and catalytic process optimization for various heterogeneous biomass conversion reactions.

Central NMR Facility

This Resource Center provides support to all the scientific activities of the laboratory. The scientists associated with this Center also carry out research activities on application of solid state and solution state NMR spectroscopy in diverse areas of chemical, biological and materials sciences. The Center maintains and operates five NMR spectrometers operating at 200, 300, 400, 500 and 700 MHz and a ECX 400 spectrometer. AV300 is a wide bore spectrometer dedicated to solid state NMR while the standard bore AV500 and 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. Although, the primary users of this facility are from the research community within the laboratory, the facility is open to researchers in other educational institutions and industries. Apart from the technical support, the Center also plays an integral part in the basic and applied research activities of the Laboratory.

During the year, the NMR Facility analyzed about 58,000 samples in solution state and 1000 samples in solid state including 500 samples from industries, other R&D and academic institutes generating the ECF of Rs. 52.8 lakhs.

AV-700 NMR spectrometer

Center for Materials Characterization

Centre for Materials Characterization is a central facility for routine and advanced characterization of materials, catering the requirements of the entire research community at CSIR-NCL. The centre is equipped with various instruments, such as single crystal and powder X-ray diffractometers, Scanning electron microscopes, Transmission electron microscopes, X-ray photoelectron spectroscope, Mass spectrometers, SQUID magnetometer, Raman Spectrometer, etc. which are used for R&D projects of the Laboratory. During the year, more than twenty thousand samples were analysed out of which five percent of the samples were from outside CSIR-NCL generating considerable amount of ECF for the laboratory.

Digital Information and Knowledge Resource Center

Digital Information and Knowledge Resource Center (DIKRC) comprises Network Administration Unit and the Knowledge Resource Center.

Network Administration Unit takes care of planning, procurement, installation, operation as well as maintenance of necessary hardware, software assets. The unit has deployed a new high core router and a switch to increase the throughput of the network traffic. The entire Wi-Fi technology of the guest house was revamped by deploying strong and highly secured wireless devices that enhanced the wireless signal strength by six times. The unit has established LAN connectivity in the newly constructed buildings such as HR-IV hostel, Indus Magic, MBL, Converges, etc. by providing more than 900, 1Gbps network ports. The unit has also established 'TIRE-II' type 'DATA CENTER' premises of about 800 Sq. Ft. in the newly constructed 'Converges' building. The center looks after the web based 'Access Control and Time Management' system and 'IP based Camera Surveillance system'. The unit has upgraded the LAN connectivity of more than 600 network points from 100 mbps to 1 Gbps. A software based network device was installed in order to deploy VoIP and SIP technology to control the multimedia communication. The unit takes care of MS Exchange 2010 server based E-mailing system for more than 1800 E-mail users and anti-spamming solution is also maintained.

Knowledge Resource Centre manages the both archival print resources and contemporary digital resources. It has subscribed to various print & E resources to fulfill the objective of providing critical information support. KRC has a collection of 1.43 lakh documents including books and bound volumes of journals. During the year 34 books were purchased and access to major publisher's online journals was available through CSIR-NISCAIR consortium project. Theses were submitted by research students and the links were provided on intranet to the awarded theses. Access to various online journals was made available; moreover Nature journals, Science, Taylor & Francis, American Institute of Physics & American Physical Society journals were also subscribed. Web of Science, Thomson Patent database & Questel Orbit databases were made accessible. During the year 35 students, 8 corporate members and 50 casual visitors availed the services of library. A training program was organized for effective utilization of Thomson Innovation, a Patent database, & SciFinder.

National Repository of Molecules

A small initiative was started to establish a platform having small molecule repository and a screening set up to run a pre-clinical discovery program under a 12FYP program in CSIR-NCL. A library consisting of ~11,000 samples from both natural and synthetic origin was developed. All these compounds were collected from different neighboring Institutes, Colleges and University Departments for biological activity.

Biological screening: The protocols for pre-clinical discoveries of small molecule inhibitors against tuberculosis were already developed (Khan et al. 2008, Singh et al. 2011, Sarkar et al. 2012). Currently it was possible to screen >100 plates for screening in one set. The activity consisted of primary screenings, dose response effect, specificity against gram + ve and gram-ve bacteria and cytotoxicity against different cell lines. The anti-proliferative assay protocols were used to check the cytotoxicity of potential anti-tubercular inhibitors. A parallel study on pancreatic cancer established the use of nanoparticles as potential therapeutic agent (*RSC Adv.* **2014,** *4,* 7666; *J. Nat. Prod.* **2014,** 76; *Med. Chem.,* **2015,** *7,* 979; *Int. J. Antimicrob. Ag.* **2015;** *J. Mater. Chem. B.* **2015,** *2,* 3190).

Transfer of novel diagnostic technique to industry: A Tech Transfer agreement with a start-up company for the development, manufacturing and marketing the kit (PCT/IN2013/000115) was signed by CSIR-NCL.

National Collection of Industrial Microorganisms

NCIM is dedicated to the isolation, identification, collection, preservation, and distribution of authentic microbial strains to industries and academia for biotechnological applications. It generated an ECF of ₹219 lakh through supply of 8000 microbial strains. Around 400 microbial strains were lyophilized for their long-term preservation. Nearly 45 new microbial strains were received for deposition. DNA extraction, PCR amplification, and sequencing protocols for bacteria, fungi, yeast and algae have been optimized and implemented. About 200 in-house strains were authenticated by molecular methods like sequencing. Standardized certificate of analysis for the microbial cultures has been obtained and latest catalog of microbial strains has been made available in the form of hard copy and online version at http://www.ncl-india.org/files/NCIM/Catalogue.aspx.

S & T Support Services

Business Development

Business Development Division (BDD) facilitates through the discussions regarding technologies, research proposals, business negotiations, research valuation, IP ownership and contracts management of all research projects performed in CSIR-NCL, right from the start to its conclusion. MIS is also responsible for the budgeting of the laboratory. IT group of BDD has important role for the development, operation and management of various IT applications.

Publication and Science Communication

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

A conference management tool was deployed to manage the conferences including the International Conference on Structural and Inorganic Chemistry, 17th CRSI National Symposium in Chemistry, Frontiers in Electronic Structure Theory and The 14th Theoretical Chemistry Symposium during the year.

International Conference on Structural and Inorganic Chemistry

December 04-05, 2014, CSIR-NCL, Pune

General Scope

ICSIC, Pune 2014 will bring together academicians from around the globe to present and discuss the latest and most exciting aspects of structural and inorganic chemistry. This conference, jointly hosted by NCL-Pune, IISER-Pune, and SP Pune University-Pune, will build a vital forum for exchanging new ideas among the world's leading Inorganic Chemists – in a constructive and interdisciplinary atmosphere. The conference will provide a common platform to strengthen the international network of inorganic and organometallic chemists.

It is with great pleasure we invite the inorganic and organometallic chemistry community to actively participate in this important event. The scientific program consists of presentations by eight foreign speakers, eight Indian speakers and two poster sessions.

Important Dates

Registration Close	|	Oct 15, 2014
Abstract Submission	|	Oct 31, 2014
Abstract Acceptance	|	Nov 10, 2014

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Announcement

Programme schedule uploaded

Registration Open

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17th CRSI National Symposium in Chemistry

February 06-08, 2015, CSIR-NCL, Pune

9th CRSI-RSC Symposium

February 05, 2015.

NEW ...onse for CRSI 2015. We are closing the registration for managing infrastructure and logistics

General Scope

CRSI National Symposium in Chemistry (CRSI-NSC) is a series of highly successful and one of the best attended symposia in chemistry that started in 1999 at IISc, Bangalore. The symposium has grown in size over the years, and has attracted over 900 participants in recent years, thus transforming itself into the most important annual Chemistry Symposium in India. CSIR-NCL is happy to host CRSI-NSC once again, after CRSI-NSC-04 on 2002, and CRSI-NSC-11 on 2009. It is with great pleasure we extend invitation to the chemistry fraternity to participate in this important event. The scientific programme will consist of plenary lectures, various medal lectures, invited lectures and poster presentations.

Important Dates

Last date for Registration	|	[illegible]
Last date of submission	|	[illegible]
abstract acceptance date	|	[illegible]
9th CRSI-RSC Joint Symposium	|	[illegible]

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Announcement

Updated accommodation list with con...

Maps and directions for accommodati...

Scientific Program

Accommodation Available

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Engineering Services

Engineering Services Unit takes care and provide back up of all engineering aspects like Civil, Mechanical and Electrical. The unit helps Scientists in Glass Blowing services which is a unique facility at CSIR–NCL. It takes care of very basic needs like Water, Electricity, Generator backup, Compressed Air, Vacuum, Air Conditioning and other scientific needs. The unit provided support to install and function the equipments like NMRS, XRDS, GCS properly in the Lab. ESU also support to facilitate the Communication and Networking setup.

ESU takes care of required back up related to Electrical, Air–Conditioning, and Civil Engineering Services to organize national and international seminars.

No.	Work Category	Work Percentage
1	Lab and Colony Renovations	40
2	Creation of Electric sub-station set up	10
3	New generator back up supply	20
4	Creation of concrete roads	10
5	Creation of hostel accommodation for students	20

Instrumentation and Communication

Instrumentation:
Prototype development was done for real time data acquisition and control for green house using LabVIEW. Application was developed in the first phase for temperature monitoring of different plants in Green House. Controls were made effective with reference to the temperature range programmed by the user. Web publishing of real time data was done so that Project Leader can monitor real time temperature on his desktop.

Communication System: WiFi telephony implementation
Successful implementation of WiFi telephony using Alcatel Omni PCX Enterprise communication system was done. It was implemented in the Communication area domain using SIP softphone implementation on mobile that enabled WiFi connectivity. It required a communication system to be interfaced with whole network to execute. Analog, digital, IP, SIP and WiFi telephony were made functional. New generation technology mobiles are SIP compliant and WiFi enabled and hence linking with OXE had no problem. Globally Corporate world prefers using SIP telephony on mobile with WiFi implementation.

Human Resource Management

Project Training: More than 473 intern students pursuing the courses like M.Sc., M.Pharm., B.E., M.E., B.Tech., M.Tech. at various colleges, universities and Indian institutes including IITs, IISERs, and NITs as well as foreign institutes completed their Summer/Winter Projects at CSIR–NCL.

Guest workers: Thirty two guest–workers worked at CSIR–NCL including fellows of various Indian Sciences and Engineering Academies. One student from abroad was also trained.

Institutional visits: The Unit coordinated thirteen institutional visits mainly of students pursuing professional courses in chemical sciences, medical sciences, agricultural sciences, engineering sciences, besides basic and applied sciences from postgraduate colleges located across the India.

CSIR-UGC NET Examination: The tests were conducted at Pune centre on June 22, 2014 and December 21, 2014 for 20755 and 19969 registered candidates respectively.

वित्त एवं लेखा

1.	निधि की उपयोगिता	
	सीएसआईआर अनुदान राशि	
	परियोजनाएँ	(₹ लाख में)
	नेटवर्क (सी/एफ सहित)	3196.516
	गैर–नेटवर्क	12010.037
	NMITLI परियोजनाएँ	290.259
	ईएमआर एवं वैज्ञानिक पूल	948.299
	प्रयोगशाला आरक्षित निधि	835.392
	बाहरी वित्तपोषित परियोजनाएँ	2062.156
	विविध जमा राशि	58.807
	बाहरी निकायों की ओर से भुगतान	367.905
	प्रायोजित सम्मेलनों/संगोष्ठियों हेतु अमानत	68.886
	कुल	19838.257
2.	प्रयोगशाला आरक्षित निधि का अर्जन	(₹ लाख में)
	वर्ष के दौरान अतिरिक्त निधि (सीएसआईआर के अलावा) के निवेश पर अर्जित ब्याज के माध्यम से प्रयोगशाला आरक्षित निधि का अर्जन	78.047
	अन्य लेखाशीर्षों से	522.473
	कुल	600.520
3.	31.3.2015 को अतिरिक्त निधि का निवेश (₹ लाख में)	2495.700
4.	आपत्ति–पुस्तिका मदों का निपटारा	523
	वर्ष के दौरान किए गए समायोजन	(₹ लाख में)
	निजी	3893.350
	यात्रा भत्ता /छुट्टी यात्रा रियायत	52.620
	स्थानीय	126.590
	कुल	3206.448
5.	निम्न लिखित प्रकार के वाउचर तैयार किए गए	
	भुगतान	18823
	प्राप्त राशि	4449
	टी.ई.	184
	कुल	23456

Finance and Accounts

1.	**Funds Utilization**	
	CSIR Grant	
	Projects	(₹in lakh)
	Network	3196.516
	Non – network	12010.037
	NMITLI Projects	290.259
	EMR & Scientist Pool	948.299
	Laboratory Reserve	835.392
	Externally Funded Projects	2062.156
	Misc. Deposits	58.807
	Payment on behalf of outside bodies	367.905
	Deposits for Sponsored conf. / seminars	68.886
	Total	**19838.257**
2.	**Generation of Lab Reserve**	(₹in lakh)
	Through earning of interest on investment of surplus funds (other than CSIR) during the year	78.047
	From other heads	522.473
	Total	**600.520**
3.	**Investment of surplus funds as on 31.3.2015 (₹in lakh)**	2495.700
4.	**Clearance of OB items**	523
	Adj. made during the year	(₹ in lakh)
	Private	3893.350
	TA/LTC	52.620
	Local	126.590
	Total	**3206.448**
	No. of items	
5.	**Following types of vouchers were generated**	
	Payment	18823
	Receipt	4449
	TE	184
	Total	**23456**

भंडार एवं क्रय (Stores & Purchase)

भंडार एवं क्रय में निम्नलिखित गतिविधियों हेतु पहल की गईः—

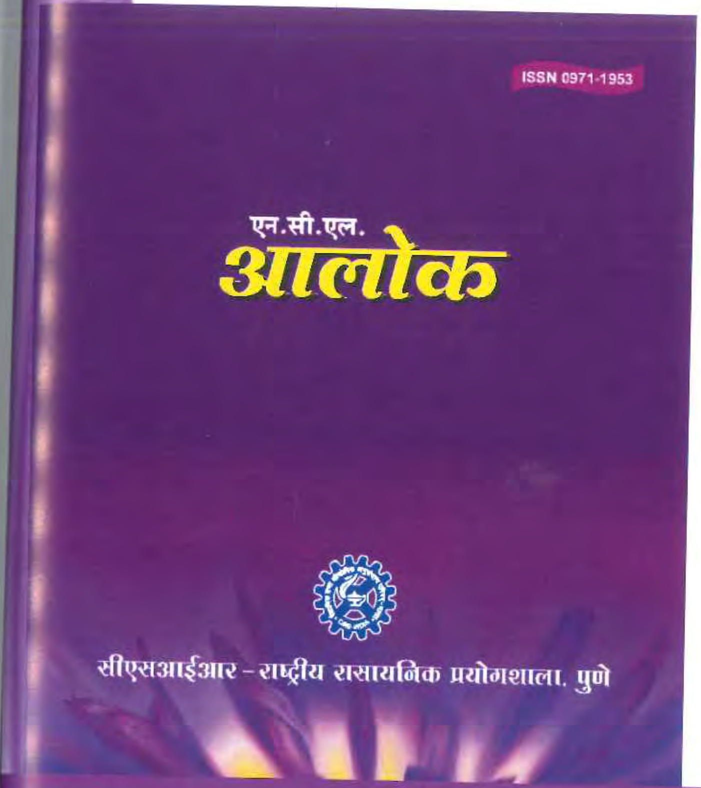
- ❖ ऑनलाइन मांगपत्र के द्वारा एक दिन के भीतर आर्डर पूरा करके, दो दिन के भीतर आपूर्ति की जाना जारी है ।
- ❖ साल्वेंट गोडाउन का नवीनीकरण किया गया तथा संबंधित मुद्दों को हल किया गया।
- ❖ स्टेशनरी स्टॉक की जांच की गई तथा स्थानीय खरीद को कम करने के लिए इसमें नई वस्तुएं जोड़ी गई।
- ❖ FVC बिल प्रमाणन को सुव्यवस्थित किया गया।
- ❖ नॉन मूविंग एवं स्लो मूविंग आइटम्स की समीक्षा की गई।
- ❖ ईआरपी कार्यान्वयन जारी है।
- ❖ उच्च मूल्य वाली विभिन्न प्रकार की वस्तुओं की उपलब्धता हेतु वर्ष 2014.15 के दौरान 12 प्रेस निविदाएं जारी की गई।

Initiatives adopted in Stores and Purchaseequipments like NMRS, XRDS, GCS properly in the Lab. ESU also support to facilitate the Communication and Networking setup.

- ❖ Online indents are continued to place the order within a day & supplies within two days.
- ❖ Solvent godown has been renovated and issues regularized.
- ❖ Stationery stocks reviewed & new items added to minimize the local purchase.
- ❖ FVC bills certification has been streamlined.
- ❖ Review of non-moving and slow moving items has taken place.
- ❖ ERP implementation is in progress.
- ❖ 12 Press tenders were issued during 2014-15 for procurement of various high value items.

भंडार एवं क्रयः उपलब्धियां (Stores and Purchase: Accomplishments):

मद	संख्या		मूल्य (₹ करोड़ में)	
	2013 -14	2014 -15	2013 -14	2014 -15
कुल प्राप्त एवं निष्पादित मांगपत्र	1207	1523	44.50	29.81
कुल दिए गए ऑर्डर (आयातित)	190	193	16.16	15.16
कुल दिए गए ऑर्डर (स्वदेशी : ऑनलाइन आरसी ऑर्डर सहित)	950	1216	20.71	22.54
कुल प्राप्त सामग्री (आयातित)	240	1007	36.00	11.31
कुल प्राप्त सामग्री (स्वदेशी)	870	2376	57.88	18.57
स्थानीय खरीद (ऑनलाइन आरसी ऑर्डर सहित)	7841	8852	17.15	5.29
भंडार से जारी की गई कुल सामग्री	16771	24160	9.31	-
वित्तीय वर्ष 2014.15 के दौरान समायोजित बकाया शेष	-	-	-	17.07
वित्तीय वर्ष 2014.15 के दौरान सीमा शुल्क से छूट प्राप्त राशि का उपयोग	-	-	-	07.07
वित्तीय वर्ष 2014.15 के दौरान उत्पाद शुल्क से छूट प्राप्त राशि का उपयोग	-	-	-	8.54



Annexures

Patents Granted: Foreign

Title	Inventor(s)	Country/ Region and Grant No.
Pip 3 Antagonist	Ramana Venkata Chepuri; Alexei Degterev	US: 8628961
Lactic Acid-Isosorbide Copolyesters And Process For Preparation Thereof	Bhaskar Bhairavnath Idage; Susheela Bhaskar Idage; Sivaram Swaminathan	US: 8633294 B2
Transesterification Catalyst Process For Preparation Thereof And A Process For Transesterification Using The Catalyst	Darbha Srinivas; Rajendra Srivastava; Paul Ratnasamy	KR: 10-1366063
Nadi Tarangini:Ayurvedic Pulse–Based Diagnostic System Incorporating Machine Learning	Amol Arvind Kulkarni; Ramesh Anna Joshi; Rohini Ramesh Joshi; Nayana Tushar Nivangune; Manisha Abhiman Jagtap; Bhat Ashok;Joshi Aniruddha; Kulkarni Anand; Kulkarni Bhaskar; Jayaraman Valadi; Chandran Sharat	CN: 101815466 B
Surface Modified Porous Polyethylene As Reservoir Scaffolds For Pancreatic Cells	Ulhas Kanhaiyalal Kharul; Harshada Ramesh Lohokare; B L V Prasad	US: 8663618
	B L V Prasad	EP: 2545105 B1
		AU: 2011225694
	B L V Prasad; Virginia D Britto	JP: 5603442
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	US: 8674131 B2
		CN: ZL201080045396.1
Continuous Flow Process For The Preparation Of Sulphoxide Compounds	Amol Arvind Kulkarni; Ramesh Anna Joshi; Rohini Ramesh Joshi; Nayana Tushar Nivangune; Manisha Abhiman Jagtap	IL: 217402
A Novel Ph Sensitive Copolymer Composition And A Process Thereof	Suvarnapathaki Rupali Kedar; Kulkarni Mohan Gopal Krishna	EP: 1940911 B1
Optically Variable Product Security Feature	Guruswamy Kumaraswamy	CN: 102282218 B
Room Temperature Electrochemical Process For Synthesizing Titanium Dioxide Nanoneedles	Rajeshkumar Shankar Hyam; Reshma Kanta Bhosale; Satishchandra Balkrishna Ogale	AU: 2010204075
		CN: 102272049 B
		JP: 5547211
		EP: 2376386 B1
Abpbi Based Porous Membranes	Ulhas Kanhaiyalal Kharul; Harshada Ramesh Lohokare	US: 8715783
		AU: 2011219494
Improved Process For Production Of Tert-Butyl Amine	Vijay Vasant Bokade; Praphulla Narahar Joshi; Prashant Suresh Niphadkar	US: 8722935 B2
		CN: 201180035077.7
Microcapsules Containing Biocide And Preparation Thereof By Solvent Evaporation Technique	Parshuram Gajanan Shukla; Sivaram Swaminathan	US: 8722071
Inhibitory Activity Of Bytteneria Species	Dhiman Sarkar; Swati Pramod Joshi; Upasana Singh; Ketki Dilip Shurpali; Roshan Rajan Kulkarni	CN: 201180014904.4

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

Title	Inventor(s)	Country/ Region and Grant No.
A Novel Dicarbonic Initiator And Its Application For The Synthesis Of Alpha Gamma Difunctional Polydienes Polystyrenes And Sbs Or Sis Triblock Copolymers In Non–Polar Solvent Without Additives	Gnanou Vyes; Matmour Rachid; More Arvind Sudhakar;Wadgaonkar Prakash Purushottam	KR: 10–1408152
New Process For The Preparation Of The Antiepileptic Drug Lacosamide	Murugan Muthukrishnan; Mohammad Mujahid; Rashant Pramod Majumdar	US: 8748660 B2
Fe(Iii) Complex Of Biuret–Amide Based Macrocyclic Ligand As Peroxidase Enzyme Mimic	Sayam Sengupta; Chakadola Panda; Munmun Ghosh	US: 8754206 B2
Nanogold Loaded Sharp Edged Carbon Bullets As Gene Carrier	Prasad LV Bhagavatula; Periyasamy Shanmugham Vijayakumar; Othalathara Ushar Raj Abhilash; Bashir Mohammad Khan	US: 8759054 B2
Enzymes From Beauveria Sp. And Process For Preparation Thereof	Seeta Laxman Ryali; Shiv Shankar; Snehal Vijay More; Harish Bansilal Khandelwal; Chandra Babu Kannan Narasimhan; Saravanan Palanivel; Padmanabhan Balaram	US: 8765447 B2
Accelerated Gelation Of Regenerated Fibroin	Nagarkar Shailesh Prakash; Lele Ashish Kishore	US: 8779097 CN: ZL201080033991.3
Transesterification Catalyst Process For Preparation Thereof And A Process For Transesterification Using The Catalyst	Darbha Srinivas; Rajendra Srivastava; Paul Ratnasamy	CA: 2625437
Method For The Preparation Of Biofuels From Glycerol	Dharbha Srinivas; Lakshmi Saikia; Paul Ratnasamy	CA: 2718474
A Composition For Ph Dependent Release Of Therapeutic Agent	Ramesh Muthusamy; Mohan Gopalkrishna Kulkarni	JP: 5592902
Process For Producing Fatty Acids	Darbha Srinivas; Satyarthi Jitendra Kumar; Thirumalaiswamy Raja; Deshpande Shilpa Shirish	US: 8802876
Process For The Preparation Of Hydroxyacetone Via Glycerol Dehydration	Chandrashekhar Vasant Rode; Amol Mahalingappa Hengne; Ajay Ashok Ghalwadkar; Rasika Bharat Mane; Pravinkumar Hansraj Mohite; Hari Shankar Potdar	US: 8809593
Gastroretentive Extended Release Composition Of Therapeutic Agent	Ramesh Muthusamy; Mohan Gopalkrishna Kulkarni	US: 8808669
Process For The Preparation Of L–Lactide Of High Chemical Yield Optical Purity	Bhaskar Bhairavnath Idage; Sivaram Swaminathan	EP: 2539332 B1
Graft Copolymer Composition With Ph Dependent Behaviour	Ramesh Muthusamy; Mohan Gopalkrishna Kulkarni	EP: 2545089 B1
Ph Sensitive Graft Copolymer	Muthusamy Ramesh; Mohan Gopalkrishna Kulkarni	US: 8822605 B2

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

Title	Inventor(s)	Country/ Region and Grant No.
Cealo3 Perovskites Containing Transition Metal	R Nandini Devi; Satyanarayana Veera Venkata Chilukuri	JP: 5610408
Electrochemical Process For Synthesis Of Graphene	Dhanraj Bhagwanrao Shinde; Vijayamohanan Kunjikrishnan Pillai	US: 8834701
Substituted 14-Dioxa-8-Azaspiro [45] 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 Bommena Vittal; Gawali Bhimrao Bodhanrao; Reddy Vaddu Venkata Narayana	US: 8841296
Optically Variable Product Security Feature	Guruswamy Kumaraswamy	AU: 2009329038
14-Triazole Derivatives And Their Antimycobacterial Activity2	Dhiman Sarkar; Sunita Ranjan Deshpande; Shailaja Pramod Maybhate; Sayalee Ramchandra Chavan; Anjali Prabhakar Likhite.; Sampa Sarkar; Arshad Khan; Preeti Madhukar Chaudhary	US: 8865910B2
Nitrite Reductase(Nirbd) As Novel Anti-Tubercular Drug Target	Dhiman Sarkar	US: 8877452
Process For The Preparation Of L-Lactide Of High Chemical Yield Optical Purity	Bhaskar Bhairavnath Idage; Sivaram Swaminathan	US: 8895760 B2 CN: ZL201180020676.1
Process For Producing Hydrocarbon Fuel	Darbha Srinivas; Rajendra Srivastava; Paul Ratnasamy	CA: 2625767
Sulfonic Acid Functionalized Swcnts A Key To Increase The Conductivity Of Nafion Membranes For Pemfcs Applications	Vijayamohanan K Pillai; R Kannan; Bhalchandra A Kakade	EP: 2253038 B1
Dna Loaded Supported Gold Nanoparticles Process For The Preparation And Use Thereof	Prasad L V Bhagavatula; Periyasamy Shanmugham Vijaykumar; Othalathara Usharraj Abhilash; Bashir Mohammad Khan	EP: 2462227 B1
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	CN: ZL201080045396.1
Perylene bisimide polyester Blend Films For Photovoltaic Applications	Asha Syama Kumari; Nisha Simon Kumari	EP: 2675843 (B1)

Patents Granted: Indian

Title	Inventor(s)	Patent No.
A Process For The Preparation Of Cellulose Based Porous Membrane Useful For The Seperation Of Biomolecules	Adikane Harshavardhan Vishavanath; Thakar Dnyyaneshwar Maruti; Kharul Ulhas Kanhaiyalal	258360
An Improved Process For The Preparation Of Functionalized Polystyrene	Sarika Babasaheb Deokar; Ramesh Shivajirao Ghadage; Arika Kotha; Chelanattu Khizhakke Madath Raman Rajan; Surendra Ponrathnam	258440
Process For Synthesis Of Alpha–Substituted Acroleins	Deshpande Raj Madhukar; Diwakar Makarand Madhukar; Chaudhari Raghunath Vitthal	258695
Polyvalent Imprinted Polymers And Preparation Thereof	Kulkarni M G; Khandare J J;	259667
An Improved Process For The Preparation Of Β-Amino Alcohols	Shivarkar Anandkumar Balasaheb; Gupte Sunil Purushottam; Chaudhari Raghunath Vitthal; Joshi Ramesh Anna; Bhide Sunil Ram	260818
Process For The Preparation Of Sustained Release Agents For Oral Care Products	Kumaraswamy Guruswamy	262826
Water Soluble Macromonomers Containing Terminal Unsaturation And A Process For The Prepration Thereof	Kulkarni Mohan Gopalakrishna; Patil Prerana Maruti	264183

Ph.D. Theses

Academy of Scientific and Innovative Research (AcSIR)

Author	Title	Guide(s)
Agarkar S.	Dye sensitized solar cell: Optimizing materials, methods and optoelectronic effects	Ogale, S. B.
Bhavsar R. S.	Polymeric ionic liquids (PILs): Synthetic approaches and gas permeation studies with an emphasis on CO_2 separation	Kharul, U. K.
Das R.	Particle size and morphology dependent magnetic properties of rare-earth manganites with potential multiferroic property	Poddar, P.
Dey C.	Polyoxometalate as building units to design functional metal organic hybrid materials	Banerjee, R
Goriya Y. M.	Metal catalyzed sequential carbon-carbon and/or carbon-nitrogen bond formation	Ramana, C. V.
Kundu T.	Structural characteristics of amino acid derived metal organic frameworks for water adsorption and proton transport	Banerjee, R.
Pachfule P. S.	Functionalization and interpenetration in metal organic frameworks for reversible H_2 storage	Banerjee, R.
Palaniselvam T.	Development of cost-effective nitrogen-doped carbonaceous materials for oxygen reduction reaction in polymer electrolyte membrane fuel cells	Kurungot, S.
Panda T. K.	Functionality and dimentionality effect on variation of CO_2 uptake and proton conduction in metal organic frameworks	Banerjee, R.
Pandey P. R.	Elucidation of mechanism and energetics of wetting of model surfaces and characterization of structural and dynamical properties of biologically inspired systems by molecular simulations	Roy, S.
Sadhu S.	Study of the fundamentals of nucleation and growth mechanism behind the formation of titania nanostructures for photovoltaic application	Poddar, P.
Sharma P. R.	Functionalized celluloses and their nanoparticles: Synthesis, properties and applications	Varma, A. J.
Shinde V. S.	Gold catalysis: Development of relay catalytic branching cascades and chemosensors for detection of gold ions	Patil, N. T.
Vijayadas K. N.	Structural investigations on sequence-specific Änt-Pro	Sanjayan, G. J.

Ph.D. Theses

Savitribai Phule Pune University...cont'd

Author	Title	Guide(s)
Acham V. R.	Metal fluoride supported palladium: Synthesis, characterization and industrially important catalytic applications	Umbarkar, S. B.
Banerjee A.	Charged peptide nucleic acid analogues: Ethano-locked PNA and beta-gamma-bisubstituted PNA	Kumar, V.A.
Banerjee A.	Novel synthesis of transition metal oxide nanostructures and related composites for energy, environment and sensing applications	Jog, Jyoti
Bansode S. B.	Study of glycation and drug induced protein crosslinking	Kulkarni, M. J.
Chaithanya Kiran I. N.	Asymmetric synthesis of bioactive molecules via hydrolytic kinetic resolution of alkoxy epoxides, dihydroxylation of alkenes and synthetic moethodologies involving oxidative cyclization of styrenese and esterification of aldehydes	Sudalai, A.
Chandra P.	Molybdenum peroxo species in various structural environment for oxidation reactions	Umbarkar, S. B.
Chanmal C. V.	High dielectric constant PVDF based nanocomposites for applications in low thermal emissivity and field effect devices	Jog, Jyoti
Chavan P. N.	Synthetic studies towards tamiflu and biotin	Chavan, S. P.
Chavan P. S.	Biochemical and microbial profiling of yeasts to identify their role in wine making	Deshpande, M. V.
Chepuri V. S. K.	Isatogens: Reactions and synthetic utility	Ramana, C. V.
Chikate Y. R.	Development of efficient strategies for control of Lepidopteran insect pest	Giri, A. P.
Daramwar P. P.	Biotransformation of santalene derivatives from Indian sandalwood: Santalum album	Thulasiram, H. V.
Das S.	Studies toward the total synthesis of didemniserinolipid B, Notoryne and Kumausallene	Ramana, C. V.
Debgupta J.	CdSe and its hybrid materials for energy applications	Vijayamohanan, K.
Deepa A. K.	Depolymerization of Lignin over heterogeneous catalyst having acidic functionality	Dhepe, Paresh L.
Devalankar D.	Asymmetric synthesis of bioactive molecules and new synthetic methodologies to gamma-butyrolactones, epoxy esters and chromanes	Sudalai, A.
Dutta A. K.	Geometrical derivatives of energy surfaces and spectroscopic properties of open shell molecules and molecular excited scates: A coupled cluster investigation	Pal, S. & Vaval, N.
Ghosh A.	Study of molecular properties and resonance within the coupled cluster framework	Vaval, N.
Gokhale R. R.	Novel synthesis of functional carbon forms and their energy applications	Jog, Jyoti
Golegaonkar S. B.	Elucidating molecular mechanism of antiglycation compounds by proteomic approaches	Kulkarni, M. J.

Ph.D. Theses

Savitribai Phule Pune University...cont'd

Author	Title	Guide(s)
Gujar P. D.	Studies on acidic phytase from Aspergillus niger mutants	Khire, J.
Haldar S.	Chemical finger-printing, metabolic profiling, and biotransformation of Neem (Azadirachta indica) limonoids	Thulasiram, H. V.
Jadhav D.	Visible light photoredox catalysis in sp3 C-H activation of t-amines for C-C bond formation reaction	Pandey, G.
Jaokar T.	Structural studies of selected mitochondrial complex-I subunits	Suresh, C. G.
Joshi R. R.	Simulation and optimization of chemical process plants	Kulkarni, B. D.
Joshi R. S.	Tailoring potent plant protease inhibitor against Helicoverpa Armigera proteases	Giri, A. P.
Kale G.R.	Dry autothermal reforming of fuels	Kulkarni, B. D.
Kale S. M.	Development and application of DNA markers for genetic improvement of linseed	Gupta, V. S.
Kamble D. A.	Enantioselective synthesis of bioactive molecules via metal-catalysed kinetic resolution of benzylic alcohols and azido epoxides, alpha-aminoxylation of aldehydes and methodology involving diazidation of alkenes	Sudalai, A.
Kanna N.	Green catalytic processes for selective oxyfunctionalization of hydrocarbons and biomass derived feedstocks	Satyanarayana, C. V. V.
Kommagalla Y.	[Metal]-catalyzed carbon-carbon and carbon-heteroatom bond formaton: Synthesis of biologically active heterocyclic compounds	Ramana, C. V.
Kona C. N.	Studies towards the synthesis of cephalosporolides E/F & H and gold catalyzed [1,3] O-C rearragement	Ramana, C. V.
Kulkarni S. V.	Bioremediation of petroleum hydrocarbons polluted sites for the conservation of soil microbial diversity	Deshpande, M. V. & Ranade, D. R.
Kumari Nisha	Solution-processable random copolyesters containing perylenebisimide and oligo (P-Phenylenevinylene) by reactive blending	Asha, S. K.
Lale G. J	Gibberellin production: Strain improvement and process optimization in stirred tank reactor	Gadre, R. V.
Mahajan M. B.	Synthesis and studies on the magnetic properties of nanosized oxides of Co, Ni, Cu and Zn	Joy, P. A.
Mahajan Neha	Efficacy of diverse Capsicum annuum protease inhibitors against the adaptive plasticity of Helicoverpa armigera proteases	Giri, A. P.
Manna A.	C-C bond formation and electron-proton transfer reations in unusual media	Anil, Kumar
Mathai E. K.	Investigation of molecular and segmental motions in polymers using solid-state NMR and development of new experiments using symmetry based pulse sequence	Rajamohanan, P. R.

Ph.D. Theses

Savitribai Phule Pune University...cont'd

Author	Title	Guide(s)
Mishra D.	Structural, conformational and reactivity studies on DNA base pairs and phospholipids using density functional theory (DFT)	Pal, S.
Nardele C. G.	Photoresponsive liquid crystalline azobenzene polyesters: Design, synthesis and self organization study	Asha, S. K.
Pandhare S. B.	Dioxomolybdenum complexes-synthesis and catalytic application in oxidation reactions	Umbarkar, S. B.
Patel P.	Studies on structure-function relationship of enymes involved in lignin biosynthesis	Agrawal, D. C. & Suresh, C. G.
Pathan M. Y.	Enantioselective synthesis of phoracantholide I, mexiletine, enciprazine, esmolol, atenolol, xibenolol via alpha-aminoxylation of aldehyde and application of recyclable catalysis in organic transformation	Mulla, S. A. R.
Rohamare S. B.	Structural and functional studies on kinetically stable serine protease from Nocardiopsis Sp. NCIM 5124	Gaikwad, S. M.
Samanta A.	Surface functionalized noble metal nanoparticles and their encapsulation in porous silica: A synthesis, characterization and catalytic study	Nandini, Devi R.
Senthil Kumar B.	Asymmetric synthesis of pyrazolidines, pyrrolidines, indolines and tetrahydroquinolines via organocatalyzed sequential reactions	Sudalai, A.
Shaikh M.	Sythesis,characterization and catalytic activity of micro-mesoporous inorganic solids for biolubricant preparation	Srinivas, D.
Shankar P.	Development of molecular approaches for the control of Odoiporus longicollis (Oliver), a major pest of bananas and plantains in Asia	Lalitha, S. K.
Sharma P.	Immobilization of metal complexes (Pd,Mn) over mesoporous materials: Synthesis characterization and application for oxidation, hydrogenation & C-C coupling reactions	Singh, A. P.
Sharma R.	Study of glycosyltransferases and other stress-related proteins encoded in chickpea genome and analysis of their structures and functions using molecular modelling and docking	Suresh, C. G.
Shurpali K. D.	Biochemical studies on redox regulation in different dormancy models of mycobacteria	Sarkar, D.
Srivastava P. L.	Characterization of the genes involved in santalene biosynthetic pathway in Indian sandalwood Santalum Album Linn	Thulasiram, H. V.
Suresh K. K.	Repositioning of drugs for novel uses and understanding the molecular mechanism of drug toxicity by chemical proteomic approach	Kulkarni, M. G.

Network Projects

Title	Project Leader(s)
A multi-scale Simulation and Modeling Approach to Designing Smart Functional Materials for use in Energy, Electrochemistry and Bio-mimetics (MSM)	Dr. Kumar Vanka
Advanced Drug Delivery System (ADD)	Dr. Sen Gupta Sayam
Affordable Cancer Therapeutics (ACT)	Dr. Chavan S. P.
Biocatalysts for Industrial Applications & Greener Organic Synthesis (BIAGOS)	Dr. Thulasiram H. V.
Bioprospection of plant resources and other natural products (BioprosPR)	Dr. Kadoo N. Y.
Catalysts for Specialty Chemicals (CSC)	Dr. Dhepe Paresh
Catalysts for Sustainable Energy (Ecat)	Dr. Srinivas D.
Centre for BIOtherapeutic Molecule Discovery (BioDiscovery)	Dr. Sanjayan G. J. and Dr. Giri A. P.
Centre for Surface and Interface Science Research (CSISR)	Dr. Gopinath C. S. and Dr. Vinod C. P.
Clean Coal Technology (TapCoal)	Dr. Srinivas D.
Creating Intellectual Property and capabilities for the development of improved security features and subtrates for the Indian currency note (FUTURE)	Dr. Premnath V.
CSIR-NCL OSDD Outreach Center	Dr. Karthikeyan M. and Dr. Ramana C. V.
CSIR-NCL-IGIB Joint Research Initiative: Interfacing Chemistry and Biology	Dr. Thulasiram H. V.
Development of Functional food and their formulations for potential health benefits of common man (FUNHEALTH)	Dr. Giri A. P.
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. and Dr. Kamble Sanjay P.
Emerging and re-emerging challenges in infectious disease: System based drug design for infectious diseases (SPLenDID)	Dr. Argade N. P.
Encapsulated Microorganisms for Environmental Protection (EMEP)	Dr. Gadre R. V.
Energy Efficient Technologies (E2++)	Dr. Kharul U. K.
Genome Dynamics in cellular organization, differentiation and enantiostasis (GenCODE)	Dr. Fernandes Moneesha

Network Projects...cont'd

Title	Project Leader(s)
Genomics of medicinal plants and agronomically important traits (PlaGen)	Dr. Giri A. P.
Host Interactome analysis: Understanding the role of Host molecules in Parasitic Infection (HOPE)	Dr. Ram Rup Sarkar
Hydrogen Energy: Overcoming materials challenges in PEMFC towards generation, separation, storage and conversion of hydrogen (HYDEN)	Dr. Kharul U. K.
Inherently Safer Practices for Industrial Risk Reduction (INSPIRE)	Dr. Karthikeyan M.
Innovate, develop and up-scale modular, agile, intensified and contineous (Indus MAGIC) processes and plants	Dr. Ranade Vivek Vinayak
Innovative solutions for Solar Energy storage	Dr. Gopinath C. S.; Dr. Shelke Manjusha and Dr. Avadhani Chilukuri Ver
Integrated NextGen approaches in health, disease and environmental toxicity (INDEPTH)	Dr. Kulkarni Mahesh J.
Man as a Superorganism: Understanding the Human Microbiome (HUM)	Dr. Suresh C. G.
Membrane and Adsorbent Technology Platform for Effective Separation of Gases and Liquid (MATES)	Dr. Desale Girish R.
Metabolic profiling of human body fluids by MS and NMR (CMET)	Dr. Venkateswarlu Panchagnula
Molecules to Materials to Devices (M2D)	Dr. Prasad B. L. V. and Dr. Das Amitava
Nanomaterials: Applications and impact on Safety, Health and Environment (NanoSHE)	Dr. Ahmad Absar
National Repository of Moelcules (NORMS)	Dr. Sarkar Dhiman
Natural products as Affordable Healthcare Agents (NaPAHA)	Dr. Thulasiram H. V.
Neurodegenerative Diseases: Causes and Corrections (miND)	Dr. Kulkarni Mahesh J.
New Approaches towards Understanding of Disease Dynamics and to Accelerate Drug Discovery (UNDO)	Dr. Sarkar Dhiman
Non-Infringing Chemistry and Engineering for Pharmaceuticals –(NICE-P)	Dr. D. Srinivasa Reddy

Network Projects...cont'd

Title	Project Leader(s)
Nuclear Magnetic Resonance Centre for Advanced Research (NMRCAR)	Dr. Rajamohanan P. R.
Organic reactions in generating innovative and natural scaffolds (ORIGIN)	Dr. Ramana C. V.
Plant Diversity: Studying adaptation biology and understanding/exploiting medicinally important plants for useful bioactives (SIMPLE)	Dr. Kadoo N. Y.
Plant-Microbe and Soil Interactions (PMSI)	Dr. Kadoo N. Y.
Recovery of water from domestic waste water using membrane based systems	Dr. Kamble Sanjay P.
Research Initiative for Low Emissions (RILE)	Dr. (Mrs.) Umbarkar S. B.
Screening molecules in lead exploration (SMiLE)	Dr. Kulkarni Mahesh J.
Technologies and Products for Solar Energy Utilization through Networks (TAPSUN)	Dr. Krishnamoorthy K.
Towards Understanding Skin Cell Homeostasis (TOUCH)	Dr. Fernandes Moneesha
Up gradation of facilities / National Repository of molecules and National Collection of Industrial Micro Organisms Resource Cantre (NCIMRC)	Dr. Dharne Mahesh S.
Zero Emission Research Innitiative for Solid Wastes from Leather (ZERIS)	Dr. E. Deenadayalan

CSIR-NCL Customers

Indian Customers

- Aarti Industries Ltd.
- Aceto Chem Pvt. Ltd.
- Aether Industries Ltd.
- Ajeet Seeds Ltd.
- Amar Equipments Pvt. Ltd.
- Anupam Rasayan India Ltd.
- ATC ENSYS Private Ltd.
- Aura Innovations Pvt. Ltd.
- Bayer CropScience Ltd
- Biopore Surgicals Pvt. Ltd.
- Cadbury India Ltd.
- Centaur Pharmaceuticals Pvt. Ltd.
- Crompton Greaves Ltd.
- CSIR–Tech Private Ltd.
- Cummins India Ltd.
- DSM India Private Ltd.
- Emcure Pharmaceuticals Ltd.
- Entrepreneurship Development Centre (EDC)
- Gadre Marine Exports Pvt. Ltd.
- GMM Pfaundler Ltd.
- Godavari Sugar Mills Ltd.
- Invictus Oncology P. Ltd.
- Jay Chemicals
- Johnson & Johnson Ltd.
- Kan Biosys Pvt. Ltd.
- KPIT Technologies Limited
- Mott MacDonald Pvt. Ltd.
- Prashant Industries
- Racold Thermo Ltd.
- Rallis India Ltd.
- Ranbaxy Laboratories Ltd.
- Reliance Industries Ltd.
- S C Johnson Products Pvt. Ltd.
- Sandoz Private Limited
- SeQuent Scientific Ltd.
- Shantani Proteome Analytics Pvt. Ltd.
- Shogun Organics Ltd.
- Tata Chemicals Ltd.
- Tridiagonal Solutions P. Ltd.
- Unichem Laboratories Limited
- Vinati Organics Limited (Mumbai)

Foreign Customers

- Arkema France SA
- Benefuel Incorporation
- General Cable Corporation
- GlaxoSmithKline LLC
- Shell Technology Centre
- Solvay SA
- Solvay Speciality Polymers, Italy
- Unitel Technologies Inc.

Publicly Funded Customers

- Bharat Petroleum Corporation
- GAIL (India) Limited

Dateline CSIR-NCL

08/05/2014	National Technology Day Lecture on 'Changing India in Global S&T Landscape' by Dr. T. Ramasami, Former Secretary, Department of Science & Technology, Govt. of India, New Delhi
02/06/2014	Prof. J. W. McBain Memorial Lecture by Prof. Anthony K. Cheetham, Fellow of Trinity College, University of Cambridge, UK on Recent developments in Metal Organic Frameworks
04/07/2014	Research Scholars Meet –Address by Honourable Dr. A. P. J. Abdul Kalam, Former President of India
26/09/2014	CSIR Foundation Day Lecture on 'Travails of a chemist at crossroads: A life in CSIR and beyond' by Prof. K. N. Ganesh, Director, IISER, Pune
15/10/2014–17/10/2014	Workshop on Organic Photovoltaices for Solar Energy conversion
29/10/2014–31/10/2014	3rd Indo-French Bilateral Symposium on Catalysis for Sustainable & Environmental Chemistry
30/10/2014–31/10/2014	International Meet on 'Recent Advances in Polymer Science'
04/12/2014–05/12/2014	International Conference on Structural and Inorganic Chemistry
15/12/2014	The L. K. Doraiswamy Honor Lecture in Chemical Engineering by Prof. Joan F. Brennecke, University of Notre Dame
18/12/2014	The 14th Theoretical Chemistry Symposium
03/01/2015	NCL Foundation Day lecture by Prof. Sudhir Kumar Sopory, VC, JNU, New Delhi, on 'An Insight into Plant Life : Perception, feelings and survival strategies'
10/01/2015	NCL Alumni – Global Meet 2015 and Dr. K. Anji Reddy Memorial Lecture by Dr. A. V. Rama Rao on the occasion of NCL Global Alumni Meet
06/02/2015–08/02/2015	17th CRSI National Symposium in Chemistry
27/02/2015	The National Science Day Lecture on "Recent strides in Indian Space mission" by Dr. K. Radhakrishnan
28/02/2015	Inauguration of "Hall of Residence–IV" by Dr. M. O. Garg, DG–CSIR

Awards / Recognitions

Anil Kumar	• A member of Executive Council of CODATA (ICSU Committee on Data for Science and Technology) • CRSI Silver Medal
Asha S. K.	• CRSI Bronze Medal
B. L. V. Prasad	• Fellow of the Indian Academy of Sciences
C. V. Rode	• A Fellow of the Indian National Academy of Engineering
D. Srinivas	• A member of the Editorial Board of the Indian Journal of Chemistry, Sec A
M. V. Deshpande	• Lifetime Achievement Award 2014-15 from the Indian Chitin and Chitosan Society
Neelanjana Sengupta	• Raman Research Fellowship
Pradeep Kumar	• Fellow of Indian National Science Academy • A National Representative for the Chemistry and the Environment Division Committee an IUPAC body
Rahul Banerjee	• NASI-SCOPUS Young Scientist Award for 2014
Satishchandra Ogale	• A Member of Editorial Advisory Board of a Journal ACS–Applied Materials & Interfaces
Sourav Pal	• RPG Life Sciences Padma Vibhushan Prof. M. M. Sharma Medal • Chemcon Distinguished Speaker Award • Professor Sadhan Basu Memorial Lecture
Syed Dastager	• Raman Research Fellowship
Ulhas Kharul	• VASVIK research award 2013
Vivek Ranade	• VASVIK research award 2014

Outreach Programme

This is the science outreach activity of CSIR–NCL and faculty from Indian Institute of Science, Education and research, Pune. The objective is to boost the excitement of science and technology among school children. Following talks were organized during the year.

Topic	Speaker
Using Physics Chemistry and Mathematics to Understand Biology	Dr. Chetan Gadgil, CSIR-NCL
Virtual Chemistry: Building labs inside computers	Dr. Suman Chakrabarthy, CSIR-NCL
An Information Super-Highway in Plants: A tale of tour and detour	Dr. Anjan Banerjee, IISER-Pune
Space Exploration Driven by "Curiosity"	Dr. Goutam Chattopadhyay, NASA Jet Propulsion Laboratory, Caltech, USA
The Circle of Life: An Introduction to the wonderful world of Animal Development	Dr. Girish Ratnaparkhi, IISER Pune
To stick or not to stick that is the question: How and why do cells stick?	Dr. Nagaraj Balasubramanium, IISER-Pune
Fighting Diseases with Math	Dr. Ramrup Sarkar, CSIR-NCL
Looking at life beyond the limit of the eye at the "atomic" unit of life	Chaitanya Athale, SER, Pune
What makes gold so special and precious? My experiences as an engineer and a scientist	Dr. Sanat Kumar, Columbia University, New York
Game Theory and Behaviour	Prof Neelesh Dahanukar, IISER-Pune
Chemistry of Food	Dr. Magesh Nandagopal, CSIR-NCL
Origin and Evolution of the Earth	Dr. Rahul Chopra, Foundation for Liberal and Management Education, Pune

सीएसआईआर–एनसीएल की राजभाषा कार्यान्वयन संबंधी रिपोर्ट

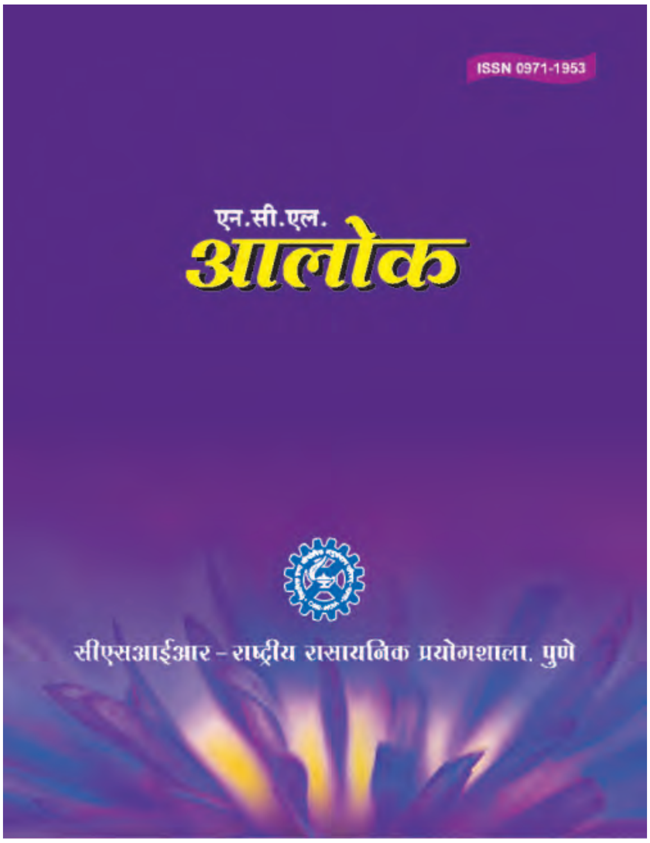
भारत सरकार की राजभाषा नीति तथा राजभाषा संबंधी नियमों का अनुसरण करने की दृष्टि से सीएसआईआर– राष्ट्रीय रासायनिक प्रयोगशाला (एन.सी.एल.) में प्रत्येक स्तर पर गहन प्रयास किए जाते हैं। सीएसआईआर–एन.सी.एल. एक वैज्ञानिक प्रयोगशाला है, जहां अधिकांश कार्य वैज्ञानिक तथा तकनीकी स्वरूप का होता है तथा शेष प्रशासनिक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

प्रत्येक तिमाही में प्रयोगशाला की राजभाषा कार्यान्वयन समिति की 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 तथा नगर के हिन्दी शिक्षण योजना की सहायक निदेशक बाहरी प्रेक्षक के रूप में उपस्थित रहते हैं ।

प्रयोगशाला 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।

वैज्ञानिक कार्यों में राजभाषा के प्रयोग को बढ़ावा देने हेतु तथा राजभाषा हिन्दी के प्रचार –प्रसार की दृष्टि से यहाँ समय–समय पर वैज्ञानिक संगोष्ठी का आयोजन हिन्दी भाषा में किया जाता है ।इसी क्रम में प्रयोगशाला में दिनांक 19 जून, 2014 को 'जैविकीय महत्व के प्राकृतिक एवं अप्राकृतिक उत्पादों का संश्लेषण' नामक विषय पर एकदिवसीय राष्ट्रीय विज्ञान संगोष्ठी का आयोजन किया गया ।

प्रयोगशाला में 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 ।



सीएसआईआर–एनसीएल की राजभाषा कार्यान्वयन संबंधी रिपोर्ट

प्रयोगशाला में प्रतिवर्ष हिन्दी पखवाड़ा समारोह का भव्य आयोजन किया जाता है । इस वर्ष 15–29 सितंबर, 2014 के दौरान हिन्दी पखवाड़ा आयोजित किया गया । इस अवसर पर स्टाफ के लिए विभिन्न हिन्दी प्रतियोगिताओं तथा कार्यक्रमों का आयोजन किया जाता हैं । हिन्दी पखवाड़ा के आरंभ में हिन्दी दिवस के अवसर पर प्रतिवर्ष प्रयोगशाला की वार्षिक गृहपत्रिका "एनसीएल आलोक" का विमोचन किया जाता हैं। प्रयोगशाला के हिन्दी कक्ष द्वारा प्रतिदिन हिन्दी सुविचार तथा अँग्रेजी 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 पत्र इत्यादि द्विभाषी रूप में तैयार किए गए हैं। प्रयोगशाला की वैबसाइट 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 ।

सीएसआईआर–एनसीएल की राजभाषा कार्यान्वयन संबंधी रिपोर्ट

प्रयोगशाला में आयोजित होने वाले समारोहों, व्याख्यानों एवं संगोष्ठियों की रिपोर्ट हिन्दी एवं अँग्रेजी दोनों भाषाओं में सीएसआईआर–समाचार में प्रकाशनार्थ राष्ट्रीय विज्ञान संचार एवं सूचना स्त्रोत 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 ।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 तथा वैज्ञानिक विभिन्न विद्यालयों तथा महाविद्यालयों के विद्यार्थियों के लिए विज्ञान संबंधी व्याख्यान हिन्दी में देते है।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 3 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 पत्रें 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।

सीएसआईआर–एनसीएल में हिन्दी पखवाडा समारोह का आयोजन

सीएसआईआर–एनसीएल में दिनांक 15 से 29 सितंबर, 2014 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 छात्रें ने बड़ी संख्या में उत्साहपूर्वक प्रतिभाग लिया।

हिन्दी पखवाड़ा समारोह के दौरान निम्नांकित गतिविधियां आयोजित की गई–

1. दिनांक 15 सितंबर, 2014 – हिन्दी पखवाड़ा शुभारंभ एवं 'एनसीएल–आलोक' का लोकार्पण
2. दिनांक 16 सितंबर, 2014 – शब्द ज्ञान प्रतियोगिता
3. दिनांक 17 सितंबर, 2014 – सामान्य ज्ञान प्रतियोगिता
4. दिनांक 18 सितंबर, 2014 – हिन्दी काव्यपाठ प्रतियोगिता
5. दिनांक 19 सितंबर, 2014 – हिन्दी शुद्धलेखन प्रतियोगिता (केवल चतुर्थ श्रेणी कर्मचारियों के लिए)
6. दिनांक 23 सितंबर, 2014 – हिन्दी कार्यशाला
7. दिनांक 29 सितंबर, 2014 – पखवाड़ा समापन एवं पुरस्कार वितरण समारोह

दिनांक 15 सितंबर, 2014 को प्रयोगशाला में हिन्दी पखवाड़ा शुभारंभ तथा वार्षिक राजभाषा पत्रिका **'एन.सी.एल.–आलोक'** का लोकार्पण कार्यक्रम आयोजित किया गया। इस अवसर पर मुख्य अतिथि के रूप में आकाशवाणी, पुणे के उपमहानिदेशक श्री आशीष भटनागर तथा अध्यक्ष के रूप में प्रयोगशाला के निदेशक डॉ. सौरव पाल उपस्थित थे। मुख्य अतिथि श्री आशीष भटनागर ने अपने संबोधन में कहा कि 'वास्तव में भारतीय भाषाओं के समारोह का आयोजन पूरे भारतीय जनमानस के साथ जुड़ा हुआ है। यह अवसर हमें अपनी स्वाधीनता और राष्ट्रीय अस्मिता की याद दिलाता है।' 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। निदेशक डॉ. सौरव पाल ने अपने संबोधन में कहा कि 'इस अवसर पर हम सभी केवल हिन्दी ही नहीं बल्कि सभी भारतीय भाषाओं के माध्यम से देश की अखण्डता बनाए रखने की प्रतिज्ञा भी करते हैं। ये भाषाएँ ही हमारी भारतीयता की पहचान हैं। अतः हमें हिन्दी के साथ–साथ अन्य भारतीय भाषाओं का भी सम्मान करते हुए राजभाषा के विकास की दिशा में सतत रूप से प्रयास करते रहना होगा।

दिनांक 29 सितंबर, 2014 को आयोजित हिन्दी पखवाड़ा समापन एवं पुरस्कार वितरण समारोह के दौरान कार्यक्रम के अध्यक्ष के रूप में उपस्थित निदेशक डॉ. सौरव पाल ने कहा कि 'हिन्दी पखवाडा मनाना भारत सरकार की राजभाषा नीति को सफल बनाने की दिशा में किए जा रहे उपायों में से एक है। इस प्रकार के आयोजन द्वारा हम अपने रोज के कामकाज में राजभाषा के प्रयोग का संकल्प लेते हैं। इस अवसर पर हम प्रयोगशाला की ओर से वार्षिक राजभाषा पत्रिका एनसीएल आलोक को प्रकाशित करते हैं और विभिन्न प्रतियोगिताएँ आयोजित करके कर्मचारियों को हिन्दी में काम करने के लिए प्रेरित करते हैं। मुझे विश्वास है कि हमारी प्रयोगशाला के सभी वैज्ञानिक और अधिकारी, कर्मचारी अपना अधिकाधिक कार्य हिन्दी में करके राष्ट्रसेवा में अपना अमूल्य योगदान देंगे।

सीएसआईआर–एनसीएल में हिन्दी पखवाडा समारोह का आयोजन

इस अवसर पर मुख्य अतिथि के रूप में उपस्थित डॉ. सुधीर कुमार (प्राध्याापक– इग्नू) 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। जिस प्रकार हम अपने राष्ट्रध्वज और राष्ट्रगीत का सम्मान करते हैं, उसी तरह हम सबको अपनी राजभाषा – राष्ट्रभाषा हिन्दी् का भी सम्मान करना चाहिए और अपनी भाषा का अधिक से अधिक प्रयोग करके उसके विकास में अपना योगदान देना चाहिए।

समारोह के आरंभ में श्री उमेश गुप्ता, वरिष्ठ हिन्दी अधिकारी ने हिन्दी पखवाड़े की प्रासंगिकता पर प्रकाश डाला। समारोह की कार्यवाही का संचालन हिन्दी अधिकारी श्रीमती स्वाति चढ्ढा ने किया । अंत में श्रीमती प्रेमा बालकृष्णन, प्रशासन नियंत्रक ने सभी के प्रति धन्यवाद ज्ञापित किया ।

सीएसआईआर–एनसीएल में राष्ट्रीय विज्ञान संगोष्ठी का आयोजन

भारत सरकार की राजभाषा नीति का अनुसरण करते हुए दिनांक 19 जून, 2014 को कार्बनिक रसायन प्रभाग की ओर से 'जैविकीय महत्व के प्राकृतिक एवं अप्राकृतिक उत्पादों का संश्लेषण' नामक विषय पर एकदिवसीय राष्ट्रीय विज्ञान संगोष्ठी का आयोजन हिन्दी माध्यम से किया गया।

इस संगोष्ठी में डॉ. विश्वकर्मा सिंह, आईआईटी, मुंबई, डॉ. विनोद कुमार तिवारी, बी.एच.यू., वाराणसी, डॉ. सुधीर कुमार, इग्नू, पुणे, डॉ. वैशाली शिंदे, पुणे वि.वि., पुणे, अतिथि व्याख्याता के रूप में उपस्थित थे। उद्घाटन सत्र में वरिष्ठ हिन्दी, अधिकारी श्री उमेश गुप्ता, ने सभी अतिथि व्याख्याताओं, उपस्थित प्रतिभागियों एवं वैज्ञानिक वर्ग का स्वागत करते हुए कहा कि राजभाषा के माध्यम से इस प्रकार की संगोष्ठियों का आयोजन राजभाषा तथा वैज्ञानिक अनुसंधान दोनों क्षेत्रें के लिए आवश्यक है। इस अवसर पर उन्होंने प्रयोगशाला में किए जा रहे राजभाषा उन्नयन संबंधी प्रयासों तथा गतिविधियों की भी जानकारी दी। संगोष्ठी के संयोजक तथा कार्बनिक रसायन प्रभाग के प्रमुख डॉ. प्रदीप कुमार त्रिपाठी ने सभी उपस्थित जनों का स्वागत करते हुए संगोष्ठी की प्रस्तावना देते हुए कहा कि 'आज अंतर्राष्ट्रीय स्तर पर हिन्दी के बढ़ते कदम देखकर सभी को प्रसन्नता होना स्वाभाविक है, किन्तु हमारे ही देश में बहुत से क्षेत्रों में हमारी इस भाषा को वह सम्मान प्राप्त नहीं है, जिसकी वह अधिकारिणी है। अतः हमारा उत्तरदायित्व हैं कि अन्य सभी क्षेत्रों के साथ–साथ विशेष रूप से वैज्ञानिक साहित्य की सम्पदा अपनी राजभाषा में बढ़ाएं। अच्छे और आदर्श अनुवाद उपलब्ध हों, मौलिक वैज्ञानिक साहित्य को प्रचुर मात्र में लिखा जाये और इस महत्वपूर्ण कार्य के लिए वैज्ञानिक संगोष्ठियां हिन्दी माध्यम से की जाएं एवं हिन्दी भाषा में वैज्ञानिक पारिभाषिक शब्दावली का निर्माण भी हो।

सीएसआईआर–एनसीएल में राष्ट्रीय विज्ञान संगोष्ठी का आयोजन

उद्घाटन सत्र के अध्यक्ष के रूप में एनसीएल के निदेशक डॉ. सौरव पाल उपस्थित थे। उन्होंने इस अवसर पर कहा कि हम सब जानते हैं कि हिन्दी राजभाषा, सम्पर्क भाषा, जनभाषा के सोपानों को पार कर विश्वभाषा बनने की ओर अग्रसर है किन्तु तकनीक और विज्ञान से संबंधित क्षेत्रें में हिन्दी का प्रयोग अत्यंत कम होता है। आज राष्ट्रभाषा के रूप में विकसित होने के लिए हिन्दी भाषा में पर्याप्त विज्ञान सम्बन्धी साहित्य अपेक्षित है। साथ ही अधिकांश वैज्ञानिक शोधकार्य अंग्रेजी भाषा में ही होने के कारण जन साधारण तक उसकी जानकारी नहीं पहुंच पाती है। अतः राजभाषा हिन्दी के माध्यम से इस संगोष्ठी का आयोजन करके हम वैज्ञानिक कार्यों को हिन्दी भाषा में करने का संदेश भी दे रहे हैं।

उद्घाटन सत्र के पश्चात संगोष्ठी तीन सत्रें में आयोजित की गई। प्रथम सत्र में डॉ.. विश्वकर्मा सिंह, आईआईटी, मुंबई, डॉ. विनोद कुमार तिवारी, बी.एच.यू., वाराणसी, डॉ. वैशाली शिंदे, पुणे वि.वि., पुणे ने अपने शोधपत्र प्रस्तुत किए। इस सत्र की अध्यक्षता एनसीएल के कार्बनिक रसायन प्रभाग के प्रमुख वैज्ञानिक डॉ. एस. पी. चव्हाण ने की।

द्वितीय सत्र में डॉ. सुधीर कुमार, इग्नू, पुणे, डॉ. एच. बी. बोराटे, एनसीएल तथा डॉ. श्रीनिवास रेड्डी, एनसीएल ने प्रस्तुतियां दीं। द्वितीय सत्र की अध्ययक्षता डॉ. ए. पी. सिंह, प्रमुख–उत्प्रेररण प्रभाग, एनसीएल द्वारा की गई।

तृतीय सत्र में दिव्या त्रिपाठी, शोधछात्र, एनसीएल, डॉ. आशीष भट्टाचार्य, वरिष्ठ वैज्ञानिक, एनसीएल ने अपनी प्रस्तुतियां दीं। तृतीय सत्र की अध्यक्षता डॉ. ए. जे. वर्मा, प्रमुख–बहुलक अभियांत्रिकी प्रभाग, एनसीएल ने की।

सीएसआईआर–एनसीएल में राष्ट्रीय विज्ञान संगोष्ठी का आयोजन

सभी सत्र अध्यक्षों द्वारा प्रत्येक प्रस्तुति के पश्चातत उसकी विवेचनापूर्ण समीक्षा करते हुए उस विषय पर अपने मौलिक विचार भी प्रस्तुत किए गए तथा उपस्थित शोधछात्रें तथा वैज्ञानिकों को भी चर्चा में सम्मिलित किया गया।

संगोष्ठी के समापन सत्र में निदेशक डॉ. सौरव पाल ने आयोजकों को संगोष्ठी के सफल आयोजन हेतु बधाई दी तथा प्रसन्नता व्यक्त करते हुए कहा कि इस प्रकार के आयोजनों द्वारा ही हम हिन्दी भाषा के माध्यम से विभिन्न प्रकार के अनुसंधान कार्यों को जनमानस तक पहुंचा सकते हैं। उन्होंने कहा कि एनसीएल में प्रतिवर्ष राजभाषा हिन्दी के माध्यम से ऐसी वैज्ञानिक संगोष्ठियों का आयोजन किया जाना चाहिए। अंत में डॉ. आर. ए. जोशी, प्रमुख वैज्ञानिक, कार्बनिक रसायन प्रभाग, एनसीएल द्वारा धन्यवाद ज्ञापन प्रस्तुत किया गया। संगोष्ठी का संचालन हिन्दी अधिकारी श्रीमती स्वााति चढ्ढा द्वारा किया गया।

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